Modelling, Data Analytics and AI in Engineering Conference

Book of Abstracts

Porto 2 -5 July 2024

https://madeai-eng.org/

Contents

Modelling, Data Analytics and AI in Engineering

In today's rapidly evolving science and technology landscape, modelling, data analytics, and artificial intelligence (AI) play pivotal roles in reshaping problem-solving strategies across diverse industrial sectors. From aerospace and automotive to chemical, construction, energy, healthcare, materials, and transportation, these transformative technologies address complex challenges and drive innovation.

The intersections of modelling, data analytics, and AI are deeply rooted in their mathematical and computational frameworks. However, a regrettable trend persists: these disciplines are often studied in isolated silos within engineering and science programs, lacking extensive interdisciplinary collaboration. To unlock their full potential as breakthrough solutions at the engineering forefront, integration using a holistic systems approach becomes imperative.

Join us at the MadeAI conference, where accomplished researchers and industry leaders from the global communities of computer science, engineering, and mathematics converge to exchange ideas. Explore the fusion of modelling, data analytics, and AI in engineering and unearth new opportunities. This conference aims to foster research and innovation in the realms of modelling, data analytics, and AI within engineering. The conference themes span a wide spectrum:

- Foundational Principles and Methodologies: Delve into the core principles underpinning modelling, data analytics, and AI.
- Chemical Engineering Applications: Explore how these technologies enhance materials and processes engineering.
- Civil Engineering Utilization: From building design to energy management, environmental protection, geotechnical analysis, and structural engineering, discover the impact of modelling, data analytics, and AI.
- Electrical Engineering Integration: Dive into electronic, computer, power, and optical engineering domains, where these tools drive innovation.
- Mechanical Engineering Incorporation: Acoustics, aerospace, automotive, manufacturing, marine, thermal, and sports engineering all benefit from the integration of modelling, data analytics, and AI.
- Interdisciplinary Exploration: Uncover synergies and collaborative opportunities across disciplines, including but not limited to biomedical engineering, petroleum engineering, robotics, and automation.
- Other relevant topics

The MadeAI conference serves as a catalyst for advancing research and shaping the future of engineering through the convergence of these powerful technologies.

Chairs

Prof. Chenfeng Li FLSW
Swansea University, United Kingdom

Prof. F.M. Andrade Pires
University of Porto (FEUP), Portugal

Scientific Committee

Prof. Franz Baader, Technische Universität Dresden, Germany
Prof. René de Borst, University of Sheffield, United Kingdom
Prof. Francisco Chinesta, ENSAM ParisTech, France
Prof. Cong Gao, Nanyang Technological University, Singapore
Prof. Roger G. Ghanem, University of Southern California, USA
Prof. Mark A. Girolam, Cambridge University, United Kingdom
Prof. Surya R. Kalidindi, Georgia Institute of Technology, USA
Prof. George Em Karniadakis, Brown University, USA
Prof. Wing K. Liu, Northwestern University, USA
Prof. Witold Pedrycz, University of Alberta, Canada
Prof. Stefanie Reese, RWTH Aachen University, Germany
Prof. Horst D. Simon, ADIA Lab, Abu Dhabi
Prof. Katia Sycara, Carnegie Mellon University, USA
Prof. Alexandre Tkatchenko, University of Luxembourg, Luxembourg
Prof. Philip Torr, Oxford University, United Kingdom
Prof. Peter Wriggers, Leibniz University Hannover, Germany
Prof. Tong Zhang, Hong Kong University of Science and Technology, China

A probabilistic conditional generative learning methodology to predict liquid fuel physicochemical properties

Rodolfo S. M. Freitas [1, a], Xi Jiang [1]

[1] School of Engineering and Materials Science, Queen Mary University of London, Mile End Road, London E1 4NS, UK

E-mail: rodolfo.dasilvamachadodefreitas@qmul.ac.uk, xi.jiang@qmul.ac.uk

Liquid synthetic fuels like Oxymethylene Dimethyl Ethers (OMEx) will play a key role shortly in the transport sector, especially in difficult-to-decarbonize transport sectors such as shipping, road freight, and aviation transport. For the rapid integration of synthetic fuels into current infrastructures for storage, transport, and direct injection in combustion engines, the physicochemical properties associated with fuel composition must be known. This represents a significant challenge since synthetic fuels are often composed of complex mixtures and the physicochemical properties depend on fuel composition variability linked with production source and process. In light of the design of alternative fuels, machine-learning (ML) models can be a powerful tool to yield accurate predictions of fundamental fuel properties from the chemical compositions of the fuels. In the present work, a probabilistic conditional generative learning methodology is used to develop quantitative structure-property relationship models. Such a framework integrates variational auto-encoders (VAE) and generative adversarial networks (GANs) that enable the end-to-end training of predictive models. Here, the fuel structure is represented by molecular descriptors and deep-learning molecular fingerprints. This approach allows a mathematical characterization of a chemical structure used to select the most relevant features that describe the chemical structure of the fuel, allowing the construction of interpretable models. The present methodology is employed to build predictive models for the cetane number and sooting tendencies of primary components of alternative fuels. The results show that the approach can predict accurately the fuel properties from the chemical structure. Also, the methodology is extended to inverse fuel design by exploring the chemical space to learn fuel blends matching the desired properties, leveraging the design of alternative fuels toward fully sustainable combustion.

[a] Presenting Author

Reconstruction Porous Media Microstructure using Descriptor Subjected VAE

XIANGYUN GE [1, a] , LIYUAN WANG [2] , CHENFENG LI [3]

[1] Swansea University, E-mail: 2021547@swansea.ac.uk

[2] Swansea University, E-mail: 2336281@swansea.ac.uk

[3] Swansea University, E-mail: c.f.li@swansea.ac.uk

Porous media are pores contained materials which allow fluids to pass through them. This kind of material can be found in various natural and engineered systems, such as soils, rocks, biological tissues, and synthetic materials like foams and membranes. The study of porous media involves understanding the PSPP(Processing-Structure-Properties-Performance) relationship within these materials, especially regarding how fluids move and react within the pores. Microstructure structure can be acquired from lab test including X-ray or SEM(scanning electron microscope) which is time-consuming and labor-intensive or digital reconstructing which is highly efficient. Profiting from the development of AI recently, machine learning based and deep learning based method have been employed in porous media microstructure reconstruction and superior to traditional method with better versatility and higher efficiency. Core part of digital reconstruction is to find a method to generate images and compare the descriptors of generated images with original images.

VAE(Variational autoencoder) has been demonstrated to possess the capacity to generate reconstructions of porous media. However, the reconstruction of porous media using this method simply focus from computer vision points of view and ignored descriptors during training process. We propose an extension of standard VAE method, combing a ResNet to consider descriptors in training process. The accuracy of the generated microstructures is validated through a statistical comparison between synthetic and real datasets using several descriptors.

Keywords: Microstructure reconstruction, Porous Media, Variational Autoencoder

[a] Presenting Author

Fresh Concrete Flow Simulation: CFD and CFD-DEM modelling

Shuai Shu[1, a], Chenfeng Li[2]
[1] Swansea University, E-mail: 2021388@swansea.ac.uk
[2] Swansea University, E-mail: c.f.li@swansea.ac.uk

Concrete is a mixture of five components: cement, coarse aggregate, fine aggregate, water and chemical admixtures. Self-compacting concrete (SCC) was developed to obtain better workability in its fresh state without weakening the hardened concrete strength by adding only a small amount of admixture.

Concrete is a mixture of varieties of components. While for modelling purpose, depending on the scale of observation, there are different ways to look into it. For example, the most two common perspectives are regarding the whole thing as pure fluid or a mixture of coarse aggregate and mortar. Obviously, the former requires a Computational Fluid Dynamics (CFD) solver while the latter requires a numerical technique for Computational Fluid Dynamics-Discrete Element Method (CFD-DEM) modelling. In all numerical methods for CFD, the Finite Volume Method (FVM) is the most popular because of its maturity, accuracy and computational cost. Therefore, the FVM-based commercial software ANSYS Fluent is used in the study and a C++ in-house code is used for CFD-DEM simulation.

There are various standard tests to validate the workability of SCC, including slump flow test, V-funnel test, L-box test, etc., in the lab. Among those, the slump flow test is the most commonly used test on site. In this study, a slump flow test was modelled and simulated by both CFD and CFD-DEM approaches, and the results are compared.

[a] Presenting Author

Physics informed neural networks for modeling dynamic linear elasticity

Vijay Kag [1, a], Venkatesh Gopinath [1]
[1]Bosch Research and Technology Center, Bangalore, India
fixed-term.Vijay.Kag@in.bosch.com

Recently, there has been a surge of data-based approaches coupled with physics-based models to solve many engineering problems. One such innovative method is the Physics-Informed Neural Network (PINN) which was introduced by Raissi et al. [1]. At present, the PINN method has been utilized successfully in multiple domains, where it is used for forward and inverse modeling.

We are motivated by the study of Haghighat et al. [2] where they have used PINN to obtain the material properties of a unit square subjected to a static vertical load. They used the Finite Element Method (FEM) to solve the problem and used that data to train the PINN model. They also mention the use of PINN in performing sensitivity analysis, where they train the PINN with a range of linearly elastic material parameters λ and μ and then use that information to obtain sensitivity of the solution for unknown material parameters.

In this work, we study a cantilever beam subjected with an oscillating load on the free end of the beam. The oscillating load means that the problem is of transient nature. We have considered linear elastic material. We show the results for the forward problem, where one finds the solution and the inverse problem, where one finds the material parameters given the solution to the problem. For calculating the data loss, we only use sparse data from the boundary nodes of the domain using FEM simulations. We also show the results from the sensitivity study which paves the way for cost effective material parameter identification in practical scenarios. Based on our work, we believe such methods could have applications in the domain of vibration analysis, where one analyzes the mechanical response of a structure subjected to vibrations.

Reference:

[1] Raissi, P. Perdikaris, and G. E. Karniadakis, “Physics-informed neural networks: A deep learning framework for solving forward and inverse problems involving nonlinear partial differential equations”, J. Comput. Phys. 378, 686–707 (2019).

[2] Haghighat, E., Raissi, M., Moure, A., Gomez, H., Juanes, R., 2021b. “A physics-informed deep learning framework for inversion and surrogate modeling in solid mechanics”, Comput. Methods Appl. Mech. Engg. 379, 113741.

[a] Presenting Author

An AI-mediated Axisymmetric Drop Shape Analysis for Surface Tension Measurement

Dmitri Lyalikov[1], Soorna Choheili[2], Marie Gerber[1], Charlotte Broyard[1], Ehsan Atefi [1,a], and Farrukh Fattoyev [2],

[1a] Manhattan College, USA, E-mail: ehsan.atefi@manhattan.edu

[1] Manhattan College, USA

[2] University of Waterloo, Canada

Axisymmetric drop shape analysis and pendant drop tensiometry are attractive approaches in the petroleum and biomedical industries for determining the interfacial tension, characterization of reservoir substances, and estimating the surface roughness. Emerging machine learning approaches show the promise of greater accuracy and far less computational demand for interfacial tension analysis compared to iterative numerical methods based on the Young-Laplace equation for colloids. To the best of our knowledge, deep learning models have only been evaluated on artificially generated drop profiles. To provide a framework for the industrial realization of machine learning methods on noisy, imperfect experimental images, we present a flexible, highly precise platform for the prediction of biphasic liquid interfacial tension. This platform utilizes a big library of pendant drop images for training XGBoost, the state-of-the-art gradient boosting machine learning architecture, for generating a predictive model. We provide a front-end image processing framework, capable of extracting characteristic features from real pendant drop images. This provides an interface to a physics-informed XGBoost model exhibiting greater than 99.2 percent accuracy in predicting surface tension. Our platform has been tested on several experimental drops with surface tension ranging from 20 $mJ/m^!$ to 72 $mJ/m^!$. One main advantage of this platform is the capability of being retrained for ultralow interfacial tension values.

[a] Presenting Author

Investigating the Impact of Rebar Spacing and Concrete Workability on the Generation of Defects within Bored Piles Using CFD

Thomas Mitchell [1,a]
[1] Swansea University, E-mail: 904633@swansea.ac.uk

The aim of this study is to investigate how rebar spacing and concrete workability affect flow mechanisms and the generation of defects within bored piles. Defects such as mattressing, inclusions, voids and poor adhesion between the concrete and rebar are regularly observed in industry, and whilst there are plenty of theories regarding their creation, there is a need for numerical modelling to help provide more insight and evidence into the root causes. A pure CFD (Computational Fluid Dynamics) approach has been taken – using the open-source software OpenFOAM - to model the gravity-driven tremie concreting process and capture flow interactions between air, support fluid, concrete, and the rebar structure. Defect Severity Grids have been produced: identifying observed key flow features, how their likelihood varies based on rebar spacing and concrete workability, and finally linking the flow features to the generation of physical defects. A 3D, high-fidelity model is used to explicitly model the rebar within the pile, capturing detailed flow mechanisms and features such as mattressing, concrete differential, cover-zone gradient and concrete recesses behind rebar. It can be concluded that concrete workability and rebar spacing are dependent variables, which can compound to create undesirable flow features. A clear trend is observed that both decreasing concrete workability and reducing clear spacing between rebar increase these undesirable flow features that could lead to an increased likelihood of defects such as mattressing, inclusions, voids and insufficient bonding between concrete and rebar.

[a] Presenting Author

Supervised Regression Models as Alternatives to Numerical Prediction Equations for Mechanical Material Properties of Bitumen

Dr Elaine Simone Goosen [1, a]
[1] Civil Engineering, Stellenbosch University, E-mail: esgoosen@sun.ac.za

Bitumen is viscoelastic – mechanical responses are functions of temperature (T) and loading rate (ρo). Simplifications during the modelling are required to avoid vast testing. The time-temperature superposition principle states that, within the linear viscoelastic range, either a change in T or ρo can affect identical changes in stiffness or relaxation. The principle allows the super-positioning of isotherms at various temperatures over limited frequencies to form a behavioural curve at a single temperature over a broader frequency domain. Figure 1 indicates how temperature isotherms of complex shear stiffness, G*, are shifted to form a single stiffness curve, i.e. a master curve. The magnitude with which each isotherm is moved is the shift factor, α. Figure 2 indicates the resultant master curves for G* and relaxation, represented here by the phase angle (8), along with the shift function. The shift function allows shift factors to be calculated for any temperature, enabling the translation of the master curves to the relevant temperature where either G* or 8 must be known. These calculations require three optimised numerical equations: one each for G*(ρo), 8(ρo), and α(T). If the bitumen is considered at various oxidation levels (or ages), the required number of models increases with factor three for each additional age. Ordinary numerical equations for shift functions (Modified Kaelble) and master curves (Generalised Logistic, GL, and Christensen-Anderson-Marasteanu, CAM) are also often restricted to the G* and 8 ranges for which they are appropriate.

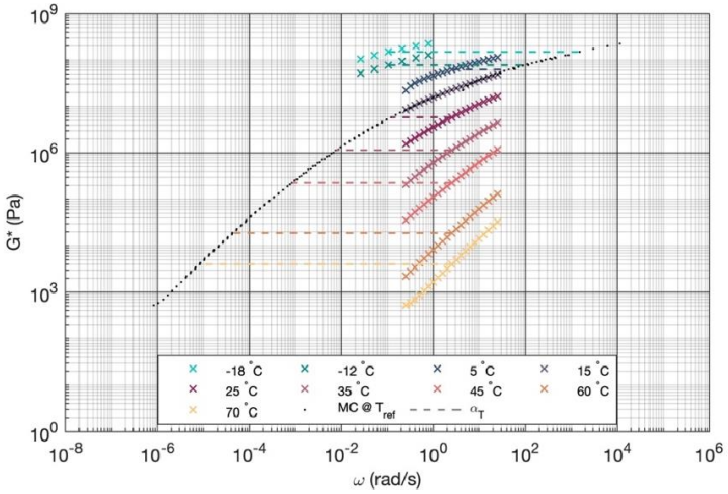


Figure 1: Isotherm shift to form a master curve at T_{ref}

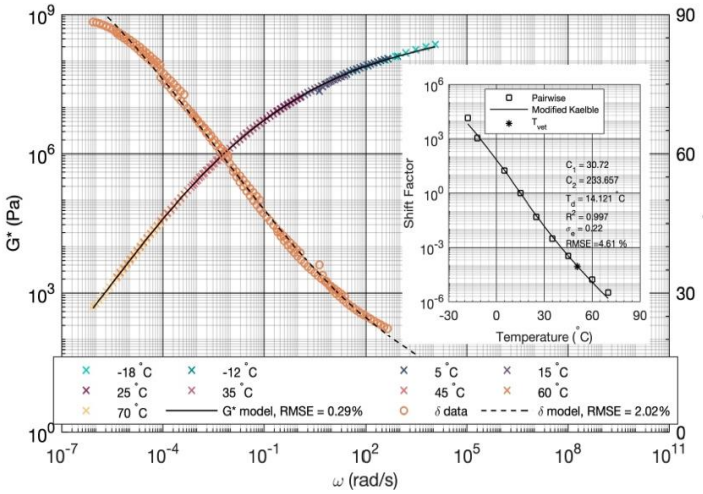


Figure 2: G and master curves at T_{ref} with shift function*

This work investigates applying simple multivariate (ρo, T, and oxidation level) and multilabel (G* and 8) prediction models as alternatives to multiple optimised numerical prediction models.

[a] Presenting Author

Test isotherms are pre-processed by calculating and applying shift factor matrices to create a data frame containing master curves at each test temperature (Figure 3), creating an interpolation field for both G* and 8. The logarithm of μ and G* is taken, and the age feature is replaced with dummy categorical columns. The resulting dependent variable matrix dimensions depend on the number of test observations and oxidation levels. The data in Figure 3 results in an 8437 x 7 data frame, of which 20% are assigned to the test set. MultiOutputRegressor from the sklearn multioutput library is used in conjunction with KNeighbors (KNN), RandomForest (RF), Bagging (BR), AdaBoost (ADB), and SVR (SVM) regressors. Hyperparameters are honed, and models are optimised with GridSearchCV using fivefold cross-validation. Figure 4 indicates the resulting RF predictions for a data frame containing entries for five ages.

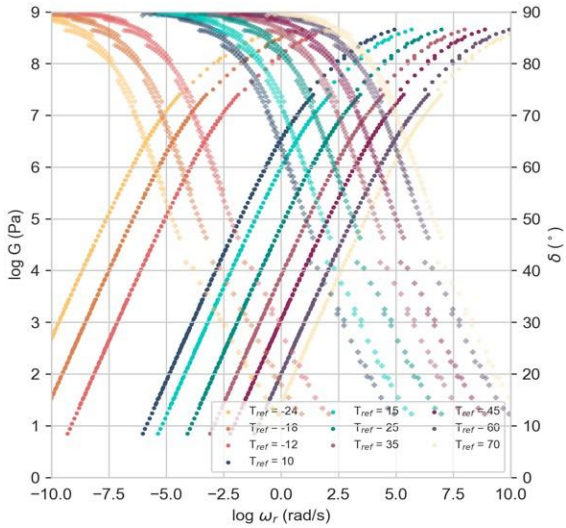


Figure 3: Input data example per oxidation level

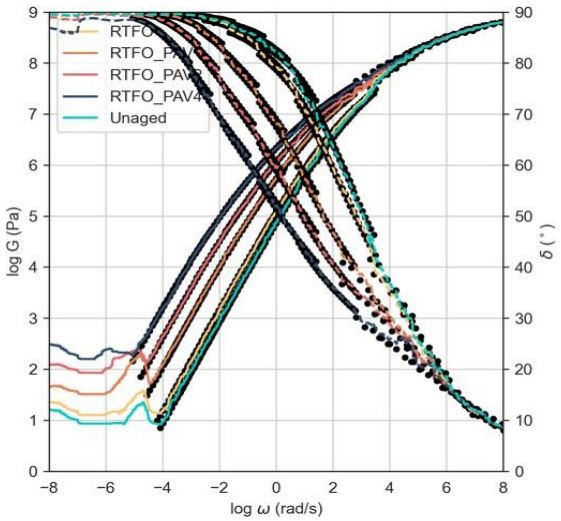


Figure 4: Trained RF model for T = 25℃

Table 1 compares the NRMSE of the supervised models to numerical equations. All G* predictions are acceptable (NRMSE < 2%). One advantage of the supervised models is seen in the accuracy of 8 models – specifically, those similar to discrete mathematical models (i.e. KNN, RF, BR and ADB). Secondly, while three numerical equations must be fitted for each bitumen oxidation level, one supervised model can be fitted to all ages to predict multiple labels – avoiding additional errors due to shift models. Lastly, while the fit range for the numerical equations, must be limited, the supervised models show accuracy over the entire data domain.

Table 1: NRMSE comparison of numerical equations and supervised regression models

Property	Numerical Equations				SkLearn Models					
	Age	**Modified Kaelble**	**GL**	**CAM**	**Data**	**KNN**	**RF**	**BR**	**ADB**	**SVM**
log G* (Pa)	Original	6,18	2,18	0,292	Train	0	1,09	1,13	0,25	1,89
	RTFO	6,44	1,67	0,341	Test	1,38	2,13	2,19	1,72	1,88
	RTFO & PAV1	5,4	0,85	0,466	All	0,62	1,36	1,41	0,8	1,88
	RTFO & PAV2	6,86	0,83	0,533						
	RTFO & PAV4	4,67	0,88	0,718						
	Average	**5,91**	**1,28**	**0,47**		**0,62**	**1,36**	**1,41**	**0,80**	**1,88**
	Rank	N/A	4	1		2	5	6	3	7

δ (°)	Original	6,18	1,55	2,67	Train	0	1,15	1,17	0,78	3,89
	RTFO	6,44	1,58	2,64	Test	3,59	2,96	2,97	3,13	3,91
	RTFO & PAV1	5,4	1,68	3,99	All	1,6	1,68	1,69	1,56	3,9
	RTFO & PAV2	6,86	2,71	4,84						
	RTFO & PAV4	4,67	2,36	6,41						
	Average	5,91	1,98	4,11		1,60	1,68	1,69	1,56	3,90
	Rank	N/A	5	7		2	3	4	1	6

Visual Material Characteristics Learning for Circular Healthcare

Federico Zocco[a] and Shahin Rahimifard

Centre for Sustainable Manufacturing and Recycling Technologies (SMART), Wolfson School of Mechanical, Electrical and Manufacturing Engineering, Loughborough University, England, UK. E-mail: federico.zocco.fz@gmail.com, s.rahimifard@lboro.ac.uk

The linear take-make-dispose paradigm at the foundations of our traditional economy is proving to be unsustainable due to waste pollution and material supply uncertainties. Hence, increasing the circularity of material flows is necessary. In this paper, we make a step towards circular healthcare by developing several vision systems targeting three main circular economy tasks: resources mapping and quantification, waste sorting, and disassembly. The performance of our systems demonstrates that representation-learning vision can improve the recovery chain, where autonomous systems are key enablers due to the contamination risks. We also published two fully-annotated datasets for image segmentation and for key-point tracking in disassembly operations of inhalers and glucose meters. The datasets and source code are publicly available.

[a] Presenting Author

Discrete Ritz method

Zhao Jing*, Lei Duan, Siqi Wang
School of Aeronautics, Northwestern Polytechnical University, Xi'an 710072, Shaanxi, China,
E-mail: jingzhao@nwpu.edu.cn

Abstract:

In the past century, the Ritz method could not be applied to complex geometric problems due to the complexity of constructing a global trial function to approximate structural behaviours and the difficulty of numerical integration in complex geometric domains. This fact has led to a large number of literatures examining the problems of two-dimensional (2D) and three-dimensional (3D) structures having regular geometries. Reddy[1] indicated that the Ritz method is a true "meshless" method because it uses a global trial function for solving the problem, thus eschewing the necessity for meshes or nodes in the solution process. However, engineering problems are significantly more complex with irregular geometries, preventing the Ritz method from being applied, despite the fact that it is "meshless", efficient, and accurate.

To resolve this problem, this study presents a novel numerical method, discrete Ritz method (DRM), for the static, stability and vibration analysis of 2D and 3D structures with arbitrary geometries[2-4].

The problem is formulated in a standard geometric domain (rectangle for 2D and cuboid for 3D problems), and arbitrarily shaped structures can be simulated by assigning cutouts within the standard geometric domain. Geometries of structures are characterized by using level set functions. By combining the extended interval integral, Gauss quadrature, variable stiffness characterization, the strain energy of the structure is modelled in the standard geometric domain, discretized using Gauss points, and is characterized by variable stiffness, which characterizes the material distribution and structure geometry simultaneously. In this manner, DRM transforms the problem into a discrete energy system which allows the geometric boundary of the structure to vary in the standard geometric domain. The orthogonal polynomials are used as the global admissible function to approximate structural behaviours. The deformation of arbitrarily shaped structures can be numerically simulated by setting the stiffness and thickness of Gauss points within the cutouts to zero. New formulations in DRM have resulted in completely standard energy functionals and computation procedures for arbitrarily shaped 2D/3D structures.

Keyword: Discrete Ritz method, Complex geometries, Cutouts, Variable stiffness, Orthogonal polynomials

[1] Reddy JN, Srinivasa AR. Misattributions and misnomers in mechanics: Why they matter in the search for insight and precision of thought. Vietnam J Mech, 2020, 42(3): 283-291.

[2] Jing Z, Duan L. Discrete Ritz method for buckling analysis of arbitrarily shaped plates with arbitrary cutouts. Thin-Walled Structures, 2023, 193: 111294.

[3] Jing Z, Duan L. Free vibration analysis of three-dimensional solids with arbitrary geometries using discrete Ritz method. Journal of Sound and Vibration, 2024, 571: 118132.

[4] Jing Z. Variable stiffness discrete Ritz method for free vibration analysis of plates in arbitrary geometries. Journal of Sound and Vibration, 2023, 553: 117662.

Strength of Arrays with Randomly Displaced Micropillars

Z DOMANSKI [1, a], AZ GRZYBOWSKI [2], N SCZYGIOL [3]

[1] Czestochowa University of Technology, E-mail: zbigniew.domanski@pcz.pl

[2] Czestochowa University of Technology, E-mail: andrzej.grzybowski@pcz.pl

[3] Czestochowa University of Technology, E-mail: norbert.sczygiol@pcz.pl

We consider an ensemble of arrays of vertical pillars located on flat substrates and subjected to a sudden load applied axially. Due to local overloadings, some pillars crush, and loads carried by these pillars flow to intact ones accordingly with a load-transfer rule directly resulting from the elastic properties of employed materials. Because the load transfer itself originates from stresses that emerge inside of substrate in the presence of applied loads the strength of a given array also depends on all pillar-to-pillar distances.

In this work, we analyse how mutual pillar positions influence an overall system's strength. With this aim, we generate an ensemble of arrays with pillar positions randomly varying in the vicinities of nodes of a square lattice. Employing a fibre-bundle-model framework we simulate a sudden loading process. It turns out that an average array’s strength computed from our ensemble is smaller than that of an array with perfectly positioned pillars.

[a] Presenting Author

On the Blackjack-Type Problems with Random Limit and its Applications in Overlading Protection

AZ GRZYBOWSKI [1, a], Z DOMANSKI [2], N SCZYGIOL [3]

[1] Czestochowa University of Technology, E-mail: andrzej.grzybowski@pcz.pl

[2] Czestochowa University of Technology, E-mail: zbigniew.domanski @pcz.pl

[3] Czestochowa University of Technology, E-mail: norbert.sczygiol@pcz.pl

This presentation is devoted to the optimal stopping problems which share some features with the blackjack type games, thus they are called blackjack-type optimal stopping problems. The scheme of these decisions–making setups is the following: a decision-maker sequentially observes the values of a sequence of nonnegative random variables. After each observation, she/he has to decide whether to stop or to continue. If the decision-maker decides to stop, then she/he obtains a payoff which is the greater, the greater is the sum of already observed values. However, if this sum exceeds a given positive number – a limit stated in the problem - then the decision-maker loses all or part of his payoff. Here, some theoretical results concerning the solutions to such problems are presented. Next, an extension of this class of problems to the ones with a random limit is introduced, discussed, and then illustrated with the application to the problem of arrays-of-pillars overloading protection.

[a] Presenting Author

Global Search Methos as Tools for Classifier-Learning Problems with Unequal Error Costs

AZ GRZYBOWSKI [1, a], Z DOMANSKI [2], N SCZYGIOL [3]

[1] Czestochowa University of Technology, E-mail: andrzej.grzybowski@pcz.pl

[2] Czestochowa University of Technology, E-mail: zbigniew.domanski @pcz.pl

[3] Czestochowa University of Technology, E-mail: norbert.sczygiol@pcz.pl

Classification is the process of predicting the class of given data points. Here we consider problems that belong to the category of supervised learning. In supervised learning problems, an algorithm makes predictions using the given dataset and is learned/corrected by the "supervisor". The learning process stops when the algorithm achieves a level of performance that is acceptable to the decision-maker.

The presentation aims to analyse and compare the performance of some classes of global search methods that were adopted in our studies for such supervised learning in problems with unequal error costs. Apart from pointing at the Genetic Algorithm as the best tool for considered classifier-learning tasks, our simulation experiments revealed also that the proportions between the weights of specific classification errors have a significant impact on the proportions between related probabilities of those errors' occurrence. Moreover, it is observed, that apart from the error weights, the weights assigned to correct classifications are also significant. Thus, this observation concerning machine learning is in line with the operant-conditioning principle formulated by Skinner to explain the human learning nature.

[a] Presenting Author

Computation of the Magnetic Polarizability Tensor (MPT) Characterisation of Realistic Metallic Targets

James Elgy [1, a], Paul D. Ledger[2]

[1] Keele University, Keele, Staffordshire, UK, ST5 5BG E-mail: j.elgy@keele.ac.uk

[2] Keele University, Keele, Staffordshire, UK, ST5 5BG, E-mail: p.d.ledger@keele.ac.uk

The use of metal detection is now a mature and well understood topic, with example applications in security screening, detection of unexploded ordnance, and food safety. However, current metal detection implementations rely on the simple thresholding of measured field perturbations, which then alerts an operator, and lack the ability to non-invasively characterise and identify an object. The Magnetic Polarizability Tensor (MPT) provides an inexpensive characterisation of a conducting metallic object and has explicit formula for the computation of its coefficients for arbitrary shaped objects, which in combination with machine learning (ML) classification can be used to identify the object. This is underpinned by a rigorous mathematical theory for the characterisation they provide [1] and several laboratory measurements [2]. In this talk we use realistic examples to discuss the use of the open-source MPT-Calculator software
[3] for the efficient computation of the MPT over a wide frequency range with the aim of constructing large dictionaries for ML classification. This includes the use of a hp-finite elements approach in combination with an adaptive proper orthogonal decomposition (POD) reduced order modelling for fast computation, a-posteriori error estimates to provide certificates of accuracy, and the handling of highly magnetic objects via the use of prismatic boundary layer approaches and hp-finite element refinements.

[1] P. D. Ledger, W. R. B. Lionheart, *The spectral properties of the magnetic polarizability tensor for metallic object characterisation*, Math. Methods Appl. Sci. 43 (1) (2020) 78–113.

[2] J. Elgy, P. D. Ledger, J. L. Davidson, T. Özdeğer and A. J. Peyton, *Computations and measurements of the magnetic polarizability tensor characterisation of highly conducting and magnetic objects*, Eng. Comput. 40 (7\8) (2023) 1778–1806.

[3] MPT-Calculator, *MPT-calculator/MPT-calculator: July 2023 Release of the MPT-calculator project*, GitHub. Available at: https://github.com/MPT-Calculator/MPT-Calculator (Accessed: 05 February 2024).

[a] Presenting Author

Neural Network-based methodology to predict the deformation of 3D printed stiffeners on pre-stretched soft membranes

Paolo Marcandelli, Daniel Calegaro, Stefano Mariani

[1]Polytechnic University of Milan, E-mail: paolo.marcandelli@polimi.it; daniel.calegaro@polimi.it; stefano.mariani@polimi.it

Abstract: In this work, a deep learning strategy is exploited to learn and predict the deformation of stiffeners, 3D printed onto a pre-stretched soft membrane. The working process reads as follows: the fabric support is stretched until a pre-defined level; a specific geometry of stiffener is printed on top of it; the membrane is finally released, and the influence on the induced deformation of the sample is observed. Fused deposition modeling was carried out by means of a Voron 2.4 3D printer, specifically calibrated for PLA printing on a Lycra fabric. To study how the different stiffener patterns can affect the buckled configuration, several samples featuring different dimensions and geometries were printed. A finite element (FE) model was then set to numerically reproduce the results obtained in the experimental campaign. In addition to the data obtained from the laboratory tests, FE simulations conducted with a calibrated numerical model were used to construct a wider training dataset. In the neural network, a pretrained YOLO (You Only Look Once) model was used to extract the relevant pattern features, in terms of the in-plane dimensions before the release. Then, a regression network is added to predict the out-of-plane deflection. Results are shown to testify the capability of the proposed approach, and its efficiency for a future shape optimization of the 3D printed geometry to attain specific targets of coupled system response.

Keywords: Deep learning, Neural Networks, Yolo, 3D printing

* Paolo Marcandelli

An enhanced BP neural network for analyzing SHM data and predicting structural performance of in-service fabricated bridges

Shenao Zhang Qiwen Jin Yan Su Shuanhai He

Shenao Zhang[1], School of Civil Engineering, Henan University of Technology, Zhengzhou, China. Email:2370520726@qq.com

Qiwen Jin[2], School of Civil Engineering, Henan University of Technology, Zhengzhou, China. School of Highway, National Engineering Laboratory for Bridge Structural Safety, Chang'an University, Xi'an, China. Email:jqw.sinx123@163.com

Yan Su[3,] Department of Foreign Languages, Xi'an Jiaotong University City College, Shaanxi, China. Emial:suyan822@163.com

Shuanhai He[4], School of Highway, National Engineering Laboratory for Bridge Structural Safety, Chang'an University, Xi'an, China.

Corresponding author email: jqw.sinx123@163.com

Presenting Author: Shenao Zhang

Structural Health Monitoring (SHM) has recently been widely applied to new built and, in particular, in-service bridges, providing a more complete and accurate assessment of structural performance. However, there is also an urgent need to effectively analyze large amounts of structural monitoring data, followed by predicting bridge performance and providing scientific support for maintenance and management decisions. This paper is devoted to the analysis and prediction of massive in-service bridge monitoring data by using BP neural network method, specifically including: (1) Taking the displacement and strain sample monitoring data of an existing prefabricated simple supported girder bridge as an example, BP neural network method is applied to analyze and predict the sample monitoring data, and error analysis is also carried out to evaluate the accuracy of BP neural network method; (2) Considering the improved BP neural network method, applying it again to analyze and predict the sample monitoring data, and further performing error analysis to evaluate the accuracy of the improved BP neural network method; (3) The change in structural performance of in-service prefabricated bridges is further reversed in accordance with the analysis results of the monitoring data in order to better guide the maintenance and management of prefabricated bridge structures. Results show that BP neural network method can effectively analyze and predict bridge structure monitoring data, and error is small. The analysis and prediction errors of bridge structure monitoring data can be further reduced by the improved BP neural network method. In particular, the transverse distribution performance of the superstructure of the prefabricated bridge can be further revealed. This study can be used for the intelligent analysis and processing of bridge monitoring data, and can also be used as a reference for further analysis and evaluation of the service performance of bridge structures.

Keywords: in-service bridge monitoring data, BP neural network, error analysis, prefabricated simple supported girder bridge, structural transverse distribution performance

Modelling and Simulation of Patients Access to Healthcare System

I.C. Obagbuwa[1*], N. Mphuthi [2], E.S. Maseko[3], K. Matabane[4] and P.E. Baisitse[5]

[1*] Department of Computer Science and Information Technology, Sol Plaatje University, South Africa, Ibidun.obagbuwa@spu.ac.za

[2] Department of Computer Science and Information Technology, Sol Plaatje University, South Africa, 202000784@spu.ac.za

[3] Department of Computer Science and Information Technology, Sol Plaatje University, South Africa, 202000696@spu.ac.za

[4] Department of Computer Science and Information Technology, Sol Plaatje University, South Africa, 201900206@spu.ac.za

[5] Department of Computer Science and Information Technology, Sol Plaatje University, South Africa, 201902507@spu.ac.za

Patient access to healthcare is the cornerstone of all patient interactions with the health industry. Modeling and simulation in healthcare understand the interdependency between infrastructure and human-oriented variables in complex systems. The study simulated a clinic using the data assumption, personal experience, and inspection of the behaviour and activities of the facility. The project aimed to simulate a model to better understand the system's behaviour and increase the patient's access to healthcare. Factors looked at to accomplish this goal were the consultation rooms, the number of staff, and the working hours. The conceptual model was compared with the computerised model to validate and verify the model's accuracy. The analysis of inputs and outputs, alongside the experimentation, shows that the time from input data is almost evenly distributed, and the output indicates negative skewness in the results, which shows that the patients receive little care/insufficient care. There exists less to no refusal of patients. Given that only the stochastic arrival part of the clinic was simulated, for future work, we shall simulate the whole clinic for better results and performance.

Keywords: Modelling, simulations, Arena simulation software, Patients, HealthCare

Modelling Human Behaviour Using Discrete Event Simulation for South Africa Restaurants

I.C. OBAGBUWA[1*], F.L. MOTSHABI[2], C. STANDER[3] and T. NYENYA[4]

[1*] Department of Computer Science and Information Technology, Sol Plaatje University, South Africa, Ibidun.obagbuwa@spu.ac.za

[2] Department of Computer Science and Information Technology, Sol Plaatje University, South Africa, 201900815@spu.ac.za

[3] Department of Computer Science and Information Technology, Sol Plaatje University, South Africa, 201902396@spu.ac.za

[4] Department of Computer Science and Information Technology, Sol Plaatje University, South Africa, 202000980@spu.ac.za

Customer satisfaction plays an essential role in maintaining relationships with restaurants. The type of service one receives can influence how one thinks/ behave. Discrete Event Simulation can be used to model such systems to see the interaction in a restaurant from when the customer arrives and places an order until they receive their meal. Taking into consideration that a restaurant is a queuing system, this might have a significant impact on behavioural decision-making. The aim is to develop a simulation model to simulate customer behaviour, measure the restaurant's performance, understand the situation better, and simulate new improvements. The system's basic structure is modelled using discrete event simulation, including all the parties involved, all the discrete events in time, and how they relate to each other. It is then verified to look for potential bottlenecks and failures within the system. The model can also allow users to predict how long an order could take and how system changes affect the simulation's effectiveness.

Keywords: Discrete Event Simulation, restaurant, customer behaviour

Improving Corrosion Data Modelling through an Evolutionary Algorithm Approach

Anibal Marrero[1], Juan J. Santana[2,a], David Greiner[3]

[1] Escuela de Ingenierías Industriales y Civiles, Universidad de Las Palmas de Gran Canaria (ULPGC), E-mail: anibal.marrero102@alu.ulpgc.

[2] Departamento de Ingeniería de Procesos, Universidad de Las Palmas de Gran Canaria (ULPGC), E-mail: juan.santana@ulpgc.es

[2] Instituto Universitario de Sistemas Inteligentes y Aplicaciones Numéricas en Ingeniería (SIANI), Universidad de Las Palmas de Gran Canaria (ULPGC), E-mail: david.greiner@ulpgc.es

Corrosion is a worldwide spread problem which it is estimated to have a direct cost of over 3% of the world Gross Domestic Product annually. The experts on corrosion point out that up to 25% of costs caused by corrosion annually can be saved if currently available corrosion control techniques are applied. Organic coatings are a widely studied and applied technique for extending the life span of metals exposed to various environmental conditions. The performance and behaviour of the organic coatings against corrosion can be tested with techniques such as Electrochemical Impedance Spectroscopy (EIS). Thus, information on the electrochemical behaviour of the metal–coating system, as well as the presence of pores and defects, can be extracted from EIS data analysis.

EIS experimental data modelling can be achieved using several commercial software packages that utilize non-linear regression algorithms with accurate fits. However, they are highly dependent of initial values for parameters and hence present serious problem of convergence to the optimum. Evolutionary algorithms (EAs) do not show these problems and have been proven to be a robust solution in the optimization field. In previous works [1], electrochemical systems, consisting of a coated metal probe in contact with a test solution, were modeled by means of two time–constants equivalent electrical circuits, obtaining very accurate fits. In this work, more complex systems characterized by three time constants are modeled by using state of the art differential evolution approaches. Results are promising, and it is expected in the near future that EAs based optimization methods prevail in the field of electrochemical systems modelling, such as coatings or batteries.

This Word has been partially funded by MCIN/AEI/10.13039/501100011033/FEDER, UE under Grant PID2021-127445NB-I00.

[1] F. González et al., *Engineering Computations*, 39-9 (2019) 2960-2982.

Keywords: Evolutionary Algorithm, EIS, corrosion, coatings

Defending Against Deepfakes: Perturbation-based Adversarial Detection with AI

Saminder Dhesi[1], Laura Fontes[1,*], Isibor Kennedy Ihianle[1], David Ada Adama[1], Pedro Machado[1,*]

[1] *Department of Computer Science*,
Nottingham Trent University
Nottingham, UK
{N0774151,N1119003}@my.ntu.ac.uk
{ isibor.ihianle,david.adama,pedro.machado}@ntu.ac.uk

Abstract: Deep learning constitutes a pivotal component within the realm of machine learning, offering remarkable capabilities in tasks ranging from image recognition to natural language processing. However, this very strength also renders deep learning models susceptible to adversarial examples, a phenomenon pervasive across a diverse array of applications. These adversarial examples are characterized by subtle perturbations artfully injected into clean images or videos, thereby causing deep learning algorithms to misclassify or produce erroneous outputs. This susceptibility extends beyond the confines of digital domains, as adversarial examples can also be strategically designed to target human cognition, leading to the creation of deceptive media, such as deepfakes. Deepfakes, in particular, have emerged as a potent tool to manipulate public opinion and tarnish the reputations of public figures, underscoring the urgent need to address the security and ethical implications associated with adversarial examples. This article delves into the multifaceted world of adversarial examples, elucidating the underlying principles behind their capacity to deceive deep learning algorithms. We explore the various manifestations of this phenomenon, from their insidious role in compromising model reliability to their impact in shaping the contemporary landscape of disinformation and misinformation. To illustrate progress in combating adversarial examples, we showcase the development of a tailored Convolutional Neural Network (CNN) designed explicitly to detect deepfakes, a pivotal step towards enhancing model robustness in the face of adversarial threats. Impressively, this custom CNN has achieved a precision rate of 76.2% on the DFDC dataset.

Keywords: Deepfakes, Adversarial Attacks, CNN, GAN

* Presenting author

This article proposes a state-of-the-art DeepFake detector network that utilises machine learning techniques to mitigate adversarial attacks on autonomous systems that are vulnerable to deepfakes. To evaluate the efficacy of the proposed approach, a transferable white-box attack via perturbations was developed to pose a practical threat to the deepfake detection system. The attack was applied to a variety of Deepfake Detection Challenge (DFDC) and COVID datasets, to demonstrate the effectiveness of the proposed algorithms on Deep Learning (DL) techniques such as Convolutional Neural Network (CNN) and Generative Adversarial Network (GAN). The proposed approach showed promising results for detecting deepfakes, achieving a precision value of 76.2% on the DFDC dataset. However, this result can be improved by increasing the volume of media in the datasets. The detection models were able to distinguish between real and fake media and can be applied in real-life scenarios such as the COVID dataset. To evaluate the system's robustness against adversarial attacks,

white-box attacks via perturbation were applied to distort the images. The Real vs. Fake dataset's classification probability was reduced from 10.9 to $2.26e^{-18}$ with the addition of perturbation, and the COVID dataset's probability was reduced from 11.1 to $1.46e^{-16}$. The proposed method offers an effective approach to detecting deepfakes by incorporating adversarial examples through white-box attacks that use perturbations to decrease classification probability.

The proposed work on mitigating adversarial attacks and detecting deepfakes has significant ethical impacts. Deepfakes, which are manipulated media that appear real, can be exploited to deceive, manipulate public opinion, spread misinformation, and facilitate cybercrime. The proposed DeepFake detector network aims to address these ethical concerns by safeguarding truth and trust in digital media, mitigating social and political manipulation, and protecting privacy and consent. This work has implications for individuals, organizations, and society as a whole.The proposed work on mitigating adversarial attacks and detecting deepfakes has significant ethical impacts. Deepfakes, which are manipulated media that appear real, can be exploited to deceive, manipulate public opinion, spread misinformation, and facil- itate cybercrime. The proposed DeepFake detector network aims to address these ethical concerns by safeguarding truth and trust in digital media, mitigating social and political manipulation, and protecting privacy and consent. This work has implications for individuals, organizations, and society as a whole. From a business perspective, the impact of Artificial Intelligence (AI) in relation to deepfake detection and AI-based technologies is notable. By incorporating AI-powered deepfake detection systems, businesses can enhance trust and reliability in their digital media content. This helps demonstrate their commitment to authentic communication, transparent marketing practices, and reliable representation of products or services. Additionally, implementing robust deepfake detection mechanisms safeguards brand reputation by proactively identifying and addressing potential threats that manipulate brand images or spread false information. Furthermore, integrating deepfake detection systems into cybersecurity strategies strengthens defences against malicious activities such as impersonation, unauthorised access, and fraud, ensuring the integrity and authenticity of digital interactions. From a business perspective, the impact of AI in relation to deep- fake detection and AI-based technologies is notable. By incorporating AI-powered deepfake detection systems, businesses can enhance trust and reliability in their digital media content. This helps demonstrate their commitment to authentic communication, transparent marketing practices, and reliable representation of products or services. Additionally, implementing robust deepfake detection mechanisms safeguards brand reputation by proactively identifying and addressing potential threats that manipulate brand images or spread false information. Furthermore, integrating deepfake detection systems into cybersecurity strategies strengthens defences against malicious activities such as impersonation, unauthorized access, and fraud, ensuring the integrity and authenticity of digital interactions.

Investigating the Impact of Weight Initialisation Strategies on Performance of Liquid State Machines

Pavithra Koralalage[1], Ireoluwa Fakeye[1], Jason Smith[2], Isibor Kennedy Ihianle[1],Salisu Wada Yahaya[1] and Andreas Oikonomou[1], Pedro Machado[1,*]

[1]Department of Computer Science, Nottingham Trent University
Nottingham, NG11 8NS, UK
Emails: {N1043138,N1112313}@my.ntu.ac.uk,
{ isibor.ihianle, salisu.yahaya, andreas.oikonomou,pedro.machado}@ntu.ac.uk
[2]B Department of Mathematics, Nottingham Trent University
Nottingham, NG11 8NS, UK
Email: jason.smith@ntu.ac.uk

Abstract: Spiking Neural Networks (SNNs) emerged as a promising solution in the field of Artificial Neural Networks (ANNs), attracting the attention of researchers due to their ability to mimic the human brain and process complex information with remarkable speed and accuracy. This research aimed to optimise the training process of Liquid State Machines (LSMs), a recurrent architecture of SNNs, by identifying the most effective weight range to be assigned in SNN to achieve the least difference between desired and actual output. The experimental results showed that by using spike metrics and a range of weights, the desired output and the actual output of spiking neurons could be effectively optimised, leading to improved performance of SNNs. The results were tested and confirmed using three different weight initialisation approaches, with the best results obtained using the Barabasi-Albert random graph method.

Keywords: Spiking Neural Networks (SNN), Liquid State Machine (LSM), Victor Purpura Distance, Van Rossum Distance, Excitatory Synapses, Inhibitory Synapses, NEST, Weight initialisation, random weights, Barabasi-Albert graph, Erdos Renyi graph

* Presenting author

Based on the results of the research, it can be concluded that the difference between the input spike train and output spike train, as measured by both Victor Purpura (VP) and Van Rossum (VR) distances, increases as the weights of the synapses increase. The Victor Purpura distance has a clearer distinction when the neuron population is large, and for such populations, the relationship between weights and the VP orVR distances follows an exponential pattern.

In the LSM experiments, the VP distance remained constant, while the VRdifference was affected by the weight range. This highlights the importance of using multiple spike metrics when observing network behaviour. The relationship between weights and spike metric differences was consistent across all network topologies tested in the research. The identified weight range for LSM topology is the optimal range for assigning excitatory synapses in order to minimise the spike metric difference. As further research, the weight range for inhibitory synapses can be determined in order to result in a similar spike train to the input spike train. The current implementation does not take into account lateral inhibition, so this will be a future area of research to observe the impact of this property on training optimisation. Additionally, the propagation delays of pre-synaptic neurons have not been considered in the

current research, so this will also be a future area of investigation to improve the accuracy of the solution.

From a societal perspective, the findings of this research have implications for the broader field of Artificial Intelligence (AI). Understanding the relationship between synaptic weights and spike metric differences contributes to the development of more efficient and accurate neural network models. These advancements can positively impact various AI applications, such as image recognition, natural language processing, and autonomous systems, leading to improved performance and reliability. Moreover, the optimisation of training processes based on these findings can reduce computational resources and energy consumption, making AI systems more sustainable. In terms of novel exploitation and business models, the research outcomes offer opportunities for developing specialised AI solutions. Companies can leverage the insights gained from this research to create advanced neural network architectures with optimised synaptic weights. Such innovations can be applied in areas like anomaly detection, pattern recognition, and predictive analytics, enabling businesses to make more informed decisions and enhance operational efficiency. Additionally, organisations specialising in AI hardware and software can incorporate these findings into their products and services, providing customers with more efficient and accurate AI tools.

Quantifying Power Consumption and Trade-offs of Heterogeneous Devices for AI Inference

Ivica Matic[1], Francisco de Lemos[1], Isibor Kennedy Ihianle[1], David Ada Adama[1], Pedro Machado[1,*]

[1] Department of Computer Science School of Science and Technology, Nottingham Trent University, Nottingham, UK, Emails: ivica.matic2018@my.ntu.ac.uk, {francisco.lemos,isibor.ihianle,david.adama,pedro.machado}@ntu.ac.uk

Abstract: Modern-day life is driven by electronic devices connected to the internet. The emerging research field of the Internet-of-Things (IoT) has become popular, just as there has been a steady increase in the number of connected devices. Although these devices are utilised to perform Computer Vision (CV) tasks, it is essential to understand their power consumption against performance. We report the power consumption profile and analysis of the NVIDIA Jetson Nano board while performing object classification. The authors present an extensive analysis regarding power consumption per frame and the output in frames per second using YOLOv5 models. The results show that the YOLOv5n outperforms other YOLOV5 variants in terms of throughput (i.e. 12.34 fps) and low power consumption (i.e. 0.154 mWh/frame).

Keywords: Internet of things, edge computing, NVIDIA Jetson Nano, Power consumption, Deep learning inference

* Presenting author

The subject covered in this paper has several impacts on ethical intelligent decision-making. By analysing the power consumption and data throughput of the NVIDIA Jetson Nano (NJN) when running different variants of the YOLOv5 model, the authors provide valuable insights into the energy efficiency and performance trade-offs in Artificial Intelligence (AI) in- ference at the edge. This information is essential for making informed decisions regarding the deployment of AI systems in resource-constrained environments. Ethical decision-making in this context involves considering the environmental impact and sustainability of AI systems, ensuring they operate efficiently without unnecessarily depleting resources.

Moreover, the study demonstrates that combining both Central Processor Units (CPU) and Graphics Processor Units (GPU) resources on the NJN outperforms using the CPU alone for YOLOv5 inference. This finding highlights the importance of heterogeneity in AI systems for achieving optimal performance. Ethical intelligent decision-making involves considering the most efficient allocation of computational resources to minimising energy consumption and maximising performance while adhering to any constraints or limitations.

From a business perspective, the project opens up future exploitable application areas. The authors show that the NJN offers lower power consumption and higher data throughput compared to combining the CPU performance with cloud services like Azure. This finding suggests that the NJN can be a cost-effective solution for AI inference at the edge, where real-time processing and low latency are crucial. Businesses can leverage the NJN to develop AI applications that require on-device processing, such as autonomous vehicles, surveillance systems, industrial automation, and robotics.

Furthermore, the authors highlight the ease of use and AI acceleration capabilities of the NJN and similar NVIDIA boards, thanks to full Compute Unified Device Architecture (CUDA) support. This accessibility and compatibility with popular frameworks and libraries like TensorFlow, Darknet, and PyTorch make it easier for businesses to adopt and integrate AI technologies into their existing workflows. It creates a thriving community with abundant knowledge, tips, and advice, facilitating the development and deployment of AI applications.

Neural network potential-based molecular dynamics study on the pollutant formation mechanism of ammonia-hydrogen co-firing

Zhihao Xing [1, a], Xi Jiang [1*]
[1] Queen Mary University of London
E-mail: zhihao.xing@qmul.ac.uk
E-mail: xi.jiang@qmul.ac.uk

Compared to fossil fuels, the combustion of ammonia and hydrogen does not produce carbon emissions. Both ammonia and hydrogen are renewable energy sources capable of meeting long-term energy demands. However, due to limitations in their combustion characteristics, using ammonia or hydrogen individually as fuels presents various drawbacks. For example, hydrogen is highly explosive, while ammonia ignition is challenging. A feasible solution is the co-firing of ammonia and hydrogen, which can mitigate the disadvantages associated with the individual use of these fuels. In the combustion of ammonia and hydrogen, a key challenge lies in the emission of nitrogen oxides (NO_X, including NO and NO_2) and nitrous oxide (N_2O), which significantly impacts human health and gives rise to significant environmental issues. Further refinement and understanding of the mechanisms underlying NO_X and N_2O formation are urgently needed. In this study, we trained two neural network potentials (NNPs) based on the density functional theory (DFT) calculated training dataset for the ammonia and ammonia-hydrogen combustion systems for the first time. The NNPs have the accuracy of DFT and the efficiency of empirical force fields. For the thousand-atom systems, the computational speed of the NNP is 1.272 ns/day.

These NNPs were employed to predict the mechanisms underlying the generation of NO_X and N_2O during ammonia-hydrogen combustion, as well as the influence of hydrogen addition on ammonia decomposition. The results indicate that both the addition of hydrogen and the reduction of equivalence ratio (increasing oxygen content) contribute to the promotion of ammonia consumption and the generation of NO and NO_2. This is attributed to the enhancement of the oxidative environment within the system resulting from both strategies, facilitating the oxidation of NH_X (NH_2 and NH) to form NO and further oxidising NO to produce NO_2. An interesting observation is that the addition of hydrogen inhibits the generation of N_2O, while the addition of oxygen promotes N_2O production. We attribute this to the fact that the decomposition of hydrogen stimulates the production of H radicals, leading to the inhibition of the crucial intermediate product HNNO formation reaction (NH + NO → HNNO), which is essential for N_2O generation. Furthermore, our simulations provide insights into detailed chemical reactions at the atomic scale, which is hard to achieve by experimental studies and chemical kinetics simulations. The obtained complete chemical reaction pathways contribute to a better understanding of the entire ammonia-hydrogen combustion process, facilitating the mitigation of pollutant generation at its source.

[a] Presenting Author

Keywords: Ammonia, hydrogen, NO_X, N_2O, neural network potential, reactive molecular dynamics.

A Fuzzy Controller for Energy Management in a Hydrogen-powered Solid Oxide Fuel Cell Vehicle

Ibrahim KASAR [1,a], Abbas FOTOUHI [1], Ali NABAVI [1]
[1] Cranfield University, E-mail: ibrahim.kasar@cranfield.ac.uk

Development and popularization of various electrified vehicles is a rising trend worldwide to reduce energy consumption and environmental pollution [1]. One of the solutions proposed for the next generation of vehicles is fuel cell technology[2]. Unlike the proton-exchange membrane (PEM) fuel cell, Solid oxide fuel cells (SOFC) have not received enough attention as a power source in the transportation sector. However, with the development of the technology, its advantages over other types of fuel cells, such as fuel flexibility and high energy efficiency, have made SOFC an interesting option [3], [4]. This study aims to design and simulate a new fuzzy controller for energy management in a hydrogen-powered SOFC vehicle. A 1 kW SOFC stack is modelled and tested. The SOFC model is then scaled up to be used in a full-vehicle powertrain system, which is a series hybrid electric vehicle model. In such a configuration, we need an energy management system (EMS) to control the flow of electrical energy from the SOFC to the battery and also from the battery to the vehicle propulsion system. There are some constraints as well such as maintaining the battery State-of-Charge (SOC) around a set point (i.e. 60%). For that purpose, a fuzzy controller is developed to manage the interactions between all powertrain components. The presented EMS model has two inputs: the total power demand of the vehicle and the battery SOC, whereas it has one output: the SOFC discharge current, which charges the battery. Figure 1 displays a simulation case study in which the full-vehicle model is simulated according to the Worldwide Harmonized Light Vehicle Test Procedure (WLTP). The results include the WLTP speed profile, the battery SOC, the SOFC current, and the total power demand. As it is expected, the power demand increases during accelerations. The yellow curve in the graph shows the battery SOC, which is successfully maintained around the set point using the proposed fuzzy EMS. As shown in the figure, the EMS increases the SOFC current when the power demand increases. The next step is to check if the SOFC is able to respond to that demand quickly and effectively or not.

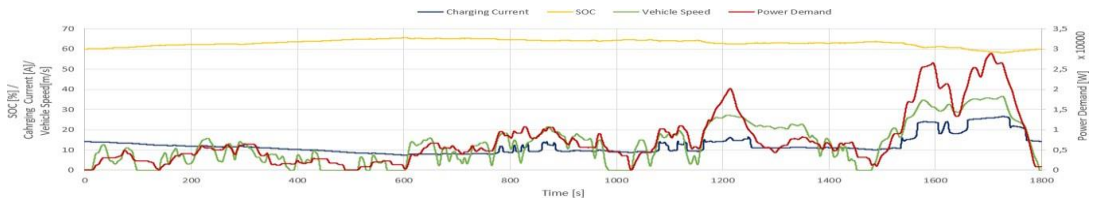


Figure 1 WLTP Simulation: battery SOC, SOFC charge current, and total power demand.

In order to make sure that the SOFC can follow the fuzzy EMS commands in the real world, experimental tests are conducted on a 1 kW SOFC stack and one test result is illustrated in

[a] Presenting Author

Figure 2. According to the result, the SOFC is capable of providing the required current in such a dynamic condition quite well. Indeed, the pulse tests are intentionally designed to measure how quickly and effectively the SOFC stack responds to rapid and short-term load changes in real-world applications. Figure 2 demonstrates a comparison between the actual current values coming out from the SOFC against the target current values. An average error of 0.1 A was achieved in that case.

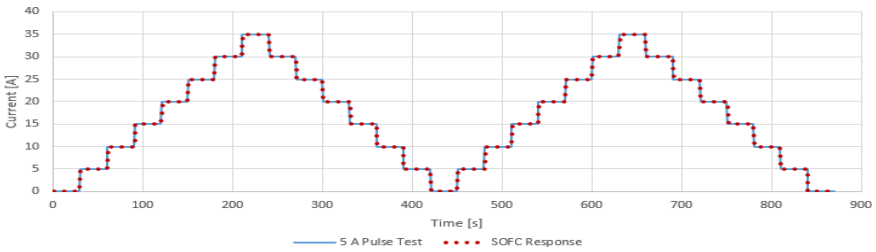


Figure 2 Comparison of the SOFC's output current and the target values

The results of this study demonstrate the potential use of SOFC technology in the automotive sector due to its high energy efficiency, compatibility with various fuels, and environmentally friendly qualities. This study contributes to bridging the gap between the theoretical simulation studies on SOFC vehicles and the practical applications of that technology. Implementation and testing of a full-scale hydrogen-powered SOFC vehicle will be a significant advancement in green propulsion technologies, and the EMS plays an important role in the realisation of that goal. In addition to the proposed fuzzy controller, other AI-based methods could be used to achieve the same goal.

References

[1] J. Y. Yong, V. K. Ramachandaramurthy, K. M. Tan, and N. Mithulananthan, "A review on the state-of-the-art technologies of electric vehicle, its impacts and prospects," *Renewable and Sustainable Energy Reviews*, vol. 49. Elsevier Ltd, pp. 365–385, May 16, 2015. doi: 10.1016/j.rser.2015.04.130.

[2] B. Tanç, H. T. Arat, E. Baltacıoğlu, and K. Aydın, "Overview of the next quarter century vision of hydrogen fuel cell electric vehicles," *Int J Hydrogen Energy*, vol. 44, no. 20, pp. 10120–10128, Apr. 2019, doi: 10.1016/j.ijhydene.2018.10.112.

[3] V. Malik, S. Srivastava, M. K. Bhatnagar, and M. Vishnoi, "Comparative study and analysis between Solid Oxide Fuel Cells (SOFC) and Proton Exchange Membrane (PEM) fuel cell - A review," in *Materials Today: Proceedings*, Elsevier Ltd, 2021, pp. 2270–2275. doi: 10.1016/j.matpr.2021.04.203.

[4] M. Singh, D. Zappa, and E. Comini, "Solid oxide fuel cell: Decade of progress, future perspectives and challenges," *International Journal of Hydrogen Energy*, vol. 46, no. 54. Elsevier Ltd, pp. 27643–27674, Aug. 05, 2021. doi: 10.1016/j.ijhydene.2021.06.020.

Generative adversarial framework for calibrating stochastic geometry models to ASSB cathode microstructures

O. Furat[1], A. Bielefeld[2], J. Janek[2], V. Schmidt[1]

[1]Ulm University, Institute of Stochastics, 89069 Ulm, Germany[1]

[2]Justus-Liebig University Giessen, Center for Materials Research, 35392 Giessen, Germany

This talk introduces a computational method for training digital twins to generate virtual 3D microstructures of all-solid-state-battery (ASSB) cathodes through stochastic geometry models, calibrated by microscopy image data. These digital twins can be used for systematic variation of model parameters to create various structural scenarios, exploited as geometry input for numerical simulations of electrochemical properties [1,2,3]. For calibrating models that can generate virtual 3D microstructures by stochastic simulation, generative adversarial networks (GANs) have gained increased popularity [4]. While GANs offer a data-driven approach for modeling complex microstructures, the systematic variation of model parameters for generating diverse 3D morphologies can be difficult. In contrast to this, relatively simple models of stochastic geometry (based on Gaussian random fields) allow parameter-driven structure variation, but can fall short in mimicking complex ASSB microstructures. Combining GANs with advanced stochastic geometry models (like excursion sets of more general random fields) overcomes these limitations. These parametric hybrid models are flexible enough to represent ASSB cathode microstructures, enabling the systematic exploration of different structures. Moreover, by combining stochastic and numerical simulations, the impact of morphological descriptors on electrochemical performance can be investigated and quantitative structure-property relationships can be established. Thus, the presented method, will allow for the generation of a wide spectrum of virtual 3D microstructures, that can be used for identifying microstructures of ASSB cathodes with optimized electrochemical properties.

References

[1] B. Prifling et al. (2021). Front. in Mater. 8 (2021), 786502.

[2] O. Furat et al. (2021). npj Comput. Mater. 7, 105.

[3] E. Schlautmann et al. (2023). Adv. Energy Mater. 13, 2302309.

[4] S. Kench and S.J. Cooper (2021). Nat. Mach. Intell. 3, 299-305.

GeoBiked: A Dataset with Geometric Features and Automated Labeling Techniques to Enable Deep Generative Models in Engineering Design

Phillip Mueller [1, 2 a], Sebastian Mueller [1 a], Bai Li [1], Lars Mikelsons [2]
[1] BMW Group, E-mail: [phillip.mueller; sebastian.mm.mueller; bai.li]@bmw.de
[2] University of Augsburg, E-mail: [phillip.mueller; lars.mikelsons]@uni-a.de

As AI-driven approaches begin to emerge in the field of engineering design, a critical challenge lies in overcoming the scarcity of geometrically detailed datasets and developing efficient methods for curating domain-specific data. This gap significantly impedes the advancement of Deep Generative Models (DGMs) for structural design tasks. While it is possible to synthesize aesthetically pleasing images, the absence of geometrically and structurally rich datasets for image generation models leads to difficulties in producing designs that meet the geometric constraints essential in engineering design applications. Addressing this bottleneck is crucial to democratize the utilization of DGMs for practical applications in engineering design. Our work introduces a comprehensive solution centered around the *BIKED* dataset proposed by Regenwetter et al. [1].

Our updated and enriched version of the dataset contains 4355 samples of diverse bicycle images, each geometrically normalized to ensure consistency across the dataset. Beyond the mere visual representation, the dataset is annotated with 10 different structural, technical, and semantic features. We further extended the dataset by adding 12 reference points for each sample, describing their geometric characteristics. Therefore, each bicycle can be differentiated into its structural and semantic components. The extensive annotation facilitates a multitude of generative tasks, such as Geometry-to-Image or Feature-to-Image generation. By standardizing the image resolutions at both 256x256 and 2048x2048 pixels, the dataset ensures versatility and applicability across varying generative contexts.

An additional contribution of our work is the automatic assignment of natural language descriptions to the images. Comparing different methodologies to solve this task, we first bootstrap the vision-language capabilities of *GPT-4V* [2], passing all images through the model and instructing it to generate text descriptions of the bicycles. We investigate open-source vision-language models such as *Imp-v1* [3] and *moondream1* [4], to circumvent GPT's paywall and token-limit, finding that *GPT-4V* significantly outperforms them in this task.

We further investigate the applicability of *GPT-4V* for automatic feature detection in images, based on the models' abilities for solving complex reasoning tasks [5], [6]. Since performance in such tasks significantly varies depending on the complexity and novelty of the task [7], we propose a simple mechanism to verify domain-specific understanding. We instruct *GPT-4V* to detect existing features in our *GeoBike*-dataset and compare the results to the ground-truth, observing reliable feature detection. This approach is extended to the identification of additional features in the images, namely the handlebar types of the bicycles. We thereby

[a] Presenting Author

illustrate the capability of the technique for autonomous feature recognition and categorization.

Collectively, these contributions are aimed at lowering the barrier to applying generative methods in engineering design. The dataset serves as a foundation for developing and testing engineering-oriented generative models. The proposed methodologies for automatic labeling through powerful pretrained models aim to extend the application of DGMs to more domains, previously hindered by the necessary effort of manual dataset curation.

Bike Style	BMX	Mountainbike	Touring
Fork Type	Stiff	Sprung	Stiff
Frame Thickness	XL	XL	XS
Rim Style Front	Spoked	Spoked	Spoked
Rim Style Rear	Spoked	Spoked	Spoked
Bottle on Seattube	No	No	Yes
Bottle on Downtube	No	No	Yes
Wheel Diameter Front	486 mm	699 mm	680 mm
Wheel Diameter Rear	486 mm	699 mm	680 mm
Chainring Teeth	28	42	50
Natural Language Descriptions	*A fixed-gear bicycle with a single speed drivetrain and minimalistic design, featuring an upright handlebar and dual caliper breaks.* *Unleash your inner daredevil with the top-tier BMX bike, engineered for extreme stunts and unstoppable action in any terrain.*	*A mountain bike featuring a robust frame with hardtail design, a suspension fork in the front, knobby tires for traction on rough terrain and multiple gears.* *Conquer the trails with our rugged mountain bike, built to take on the toughest terrains with ease and precision – your ultimate companion for outdoor adeventures.*	*A touring bicycle with drop handlebars, a multi-gear derailleur system, rear pannier rack and water bottle holders, designed for long-distance travel and commuting.* *Embark on epic journeys with our deluxe touring bicycle, your road-worthy vessel equipped with essential gear and comfort for the long haul – adventure awaits!*
Image			

Figure 1: Examples from our GeoBiked dataset with exemplary text-prompts.

References

[1] Regenwetter, L., Curry, B., Ahmed, F., 2021. “BIKED: A Dataset for Computational Bicycle Design with Machine Learning Benchmarks”. *Preprint: arXiv:2103.05844*

[2] OpenAI. 2023. “GPT-4V(ision) System Card. *OpenAI: https://cdn.openai.com/papers/GPTV_System_Card.pdf*

[3] Shao, Z., Ouyang, X., Yu, Z., Yu, J., 2024. “Imp-v1: An Empirical Study of Multimodal Small Language Models”, *Huggingface: https://huggingface.co/MILVLG/imp-v1-3b*

[4] vikhyatk. 2024. “moondream1 [Model]“, *HuggingFace: https://huggingface.co/vikhyatk/moondream1*

[5] Wei, J., Wang, X., Schuurmans, D., et al., 2023. “Chain-of-Thought- Prompting Elicits Reasoning in Large Language Models”. *Preprint: arXiv:2201.11903*

[6] Singh, M., Cambronero, J., Gulwani, S., et al., 2023. “Assessing GPT4-V on Structured Reasoning Tasks”, *Preprint: arXiv:2312.11524*

[7] Liu, H., Ning, R., Teng, Z., et al., 2023. “Evaluating the Logical Reasoning Ability of ChatGPT and GPT-4”, *Preprint: arXiv:2304.03439*

Fast analysis of transport phenomena in melt during Cz-Si single crystal growth by using Hybrid-PINNs

Tsuyoshi Miyamoto [1, a], Yuto Takehara [1], Yasunori Okano [1,*], Sadik Dost [2]
[1] Department of Material Engineering Science, Osaka University,
E-mail: okano.yasunori.es@osaka-u.ac.jp
[2] Department of Mechanical Engineering, University of Victoria

Silicon (Si) bulk single crystals are mostly grown by the Czochralski (Cz) technique. To grow high quality Si crystals with this method, it is essential to have a real-time control of the transport phenomena occurring in its melt. Classical numerical simulations for this purpose do not only require long computational times but also cannot utilize an analysis in real-time. Physics Informed Neural Networks (PINNs) [1] on the other hand are proven to be a very powerful tool for this objective. PINNs are machine learning tools that learn the governing equations of the system involved and provide fast predictions. Naturally, the predictions satisfy the physical laws. Takehara *et al.* [2] developed a method by using PINNs to provide fast predictions for the transport phenomena occurring in the Si melt of the Cz process. The Cz-Si melt was subjected to an applied vertical magnetic field to suppress natural convection.

In this study, we developed a machine learning model, called Hybrid-PINNs, in the absence of an applied magnetic field. The objective was to overcome the above-mentioned simulation time issues. The architecture of Hybrid-PINNs developed in this study is shown in Fig. 1. The input parameters were the imposed temperature boundary conditions ($T_\mathrm{l}, T_\mathrm{r}, T_\mathrm{h}$), the speed of the seed crystal rotation ω_s, and the melt height h. The numerical results, governing equations, and boundary conditions were learned.

Figure 2 presents the flow velocity (left) and temperature distributions (right) in the Si melt, obtained from the numerical simulation and Hybrid-PINNs. Numerical simulations required about 45 minutes of computation time, whereas Hybrid-PINNs could make predictions in only about 0.1 seconds, even for different boundary conditions.

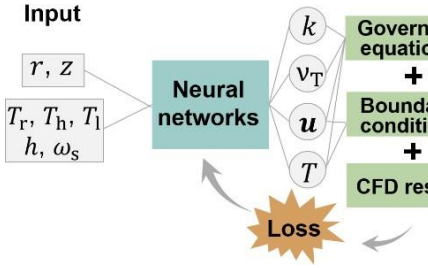


Fig. 1 The architecture of Hybrid-PINNs for predicting temperature and flow velocity at different parameters.

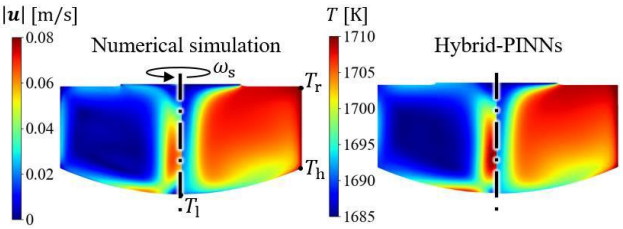


Fig. 2 Numerical simulation result and Hybrid-PINNs prediction at $(T_\mathrm{l}, T_\mathrm{r}, T_\mathrm{h}, \omega_\mathrm{s}, h) = (1690\ \mathrm{K}, 1710\ \mathrm{K}, 1710\ \mathrm{K}, 2\ \mathrm{rpm}, 0.25\ \mathrm{m})$.

References

[1] Raissi, M. *et al.*, *J. Comput. Phys*, **378**, 686 (2019).
[2] Takehara, Y. *et al.*, *J. Chem. Eng. Japan*, **56,** 2236656 (2023).

Two-tailed confidence-interval-based fuzzy testing method for Six Sigma Quality Index

Kuen-Suan Chen [1, a], Chun-Min Yu [1,*]

[1] National Chin-Yi University of Technology, E-mail: kuensuan.chen@gmail.com (K. S. Chen); E-mail: yu2013000@gmail.com

The Industry 4.0 concept promotes the networked environment and management of smart manufacturing and inspires innovation in global industry. Production data is transmitted and shared between products and manufacturing equipment through the Internet of Things. Manufacturers can leverage shared production data and big data analytics models to achieve better process quality and efficiency. Reducing defective products can not only reduce the scrap rate and rework rate, but also reduce social losses such as product maintenance costs and environmental pollution, create more profits for manufacturers, and improve product quality and industrial competitiveness. This paper proposes a novel evaluation method for process quality.

Under the assumption of normal process, let the random variable X be a normal distribution with process mean μ and process standard deviation σ, that is, $X \sim N\left(\mu,\sigma^2\right)$. The Six Sigma method promoted by Motorola in 1986 can effectively reduce the process variation as well as the product defective rate. The Six Sigma method promoted by Motorola allows the process average to deviate from the process target by 1.5 standard deviations (1.5 σ). Meanwhile, there will be 3.4 defects per million opportunities (DPMO). When the process average deviates from the target value by 1.5 standard deviations and the process standard deviation is 1/6 of the tolerance, the process quality is said to reach the level of 6σ. Chen et al. revised the process capability index based on this definition and proposed a Six Sigma Quality Index (SSQI) as follows:

$$Q_{pk} = \frac{d - |\mu - T|}{\sigma} + 1.5$$

where $T = (USL + LSL)/2$, a target value, and $d = (USL - LSL)/2$, which means half the length of the specification interval. USL and LSL are the upper and lower specifications, respectively. When the process average deviates from the target value by 1.5 standard deviations, and the process standard deviation is 1/k of the tolerance, then $|\mu - T| = 1.5|k$, $d = k\sigma$, and

[a] Presenting Author

$$Q_{pk} \geq Q_{pk}(k) = \frac{1-(1.5|k)}{1|k} + 1.5 = k$$

Obviously, when process quality level is *k-sigma*, then the value of Q_{pk} is at least equal to k. Under the assumption of normality, a mathematical relationship of inequality between index Q_{pk} and the process yield can be expressed as follows:

$$yield \geq 2\Phi\left(Q_{pk} - 1.5\right) - 1$$

where $\Phi(\bullet)$ is the cumulative function of standard normal distributions. Obviously, index Q_{pk} can reflect the process yield and quality level. Therefore, the Six Sigma Quality Index is not only a bridge between businesses and customers but also a tool for internal engineers to evaluate, analyze and propose improvement suggestions on processes. However, the index contains unknown parameters, so that it must be estimated from the sampled data. In order to improve the accuracy of estimation and overcome the uncertainty of measurement data, this paper first based on the results of statistical inference derives the confidence interval of index Q_{pk} and then proposes a two-tailed confidence-interval-based fuzzy testing method as an evaluation method for process quality. This two-tailed fuzzy testing method is based on the confidence interval, so that it can reduce the risk of misjudgment caused by sampling errors, and it is more reasonable than the statistical testing method.

Research on AI Vision for Emotion Recognition in Archery Athletes

Wei-Ting Lin [1], Chia-Chin Chiang [2], Yi-Chian Chen [3, a], Hsiu-Chuan Hsu [4,5], Jian-Hao Chen [5]

[1] Department of Physical Education Office, National Kaohsiung University of Science and Technology, Kaohsiung, Taiwan, E-mail: titan08148@nkust.edu.tw

[2] Department of Mechanical Engineering, National Kaohsiung University of Science and Technology, Kaohsiung, Taiwan, E-mail: ccchiang@nkust.edu.tw

[3] Department of Occupational Safety and Hygiene, Fooyin University, Kaohsiung, Taiwan, E-mail: candiceycchen@gmail.com

[4] Department of Computer Science, National Chengchi University, Taipei, Taiwan, E-mail: hcjhsu@nccu.edu.tw

[5] Graduate Institute of Applied Physics, National Chengchi University, Taipei, Taiwan, E-mail: howie0108@gmail.com, hcjhsu@nccu.edu.tw

This article focuses on the application of artificial intelligence algorithms to the intensive training of archery athletes, aiming to record the emotional states of students with comparable athletic experience during their learning and training processes. How to win competitions ultimately relies heavily on the training content that is devised. Sporting events are often momentary and highly tense, demanding athletes to possess strong mental resilience. It's evident that the athlete's psychological state significantly affects their performance during both training and competitions. In the process of devising training routines, obtaining insights into athletes' emotional responses and variations under various circumstances can serve as valuable references for training. By tailoring training methods or competition strategies based on athletes' emotional states, we can formulate more personalized and effective approaches. Given the flourishing development of artificial intelligence across various domains, this study employs convolutional neural networks for athlete emotion recognition. We utilize datasets provided by AffectNet and the Real-world Affective Faces Database (RAF-DB) for facial emotion recognition as samples for neural network learning. In addition to the emotion databases, we establish a custom tennis match emotion database in this research to analyze athletes' emotional reactions during tennis matches.

This study categorizes the AffectNet dataset into seven emotions: Neutral, Happy, Sad, Surprise, Fear, Disgust, and Anger. These seven human emotions serve as the target emotions for training the model. The model's learning on the AffectNet dataset, the research aims to assess its ability to discern the emotions of ethnic chinese athletes. The study utilizes a custom athlete emotion database as the validation dataset to evaluate whether the model can accurately interpret the emotions of ethnic chinese athletes (Figure 1). In addition to the AffectNet dataset, the research employs the RAF-DB dataset as the training dataset for emotion recognition. A comparison is made between the models trained on AffectNet and RAF-DB to analyze the differences between the two. The study also conducts training on a convolutional neural network using the self-created athlete emotion database. The goal is for the model to learn the

[a] Presenting Author

emotional responses of Chinese athletes during training sessions. Given the significance of neutral, happy, sad, and fearful emotions in athletes' on-court reactions, these four human emotions are defined as the training targets for the model to learn.

The study utilized the EfficientNet model to train on a self-created emotion database of Chinese athletes, achieving an accuracy of 64%. The research also compared the accuracy of the SE_Resnet network on the AffectNet dataset and the RAF-DB dataset. The RAF-DB dataset exhibited relatively higher validation accuracy in the same categories compared to the AffectNet dataset. However, this was expected as RAF-DB has significantly fewer data and less complexity compared to AffectNet, leading to higher expected performance in validation accuracy.The study further compared using AffectNet as a pre-trained model for facial emotion data and applying it to training on the RAF-DB dataset. The obtained validation accuracy increased by 15% compared to training directly on the RAF-DB dataset. This result indicates that AffectNet offers a more diverse dataset for facial emotion data.

Upon analysis, the study found that using the AffectNet pre-trained model resulted in more accurate and uniform emotion classification on the RAF-DB dataset. The confusion matrix revealed that the classification accuracy is directly proportional to the number of photos in each category, shown as Figure2. In the AffectNet dataset, the "Disgust" category had the fewest photos, resulting in lower accuracy in the confusion matrix. Conversely, the "Happy" category had the highest number of photos, leading to the highest accuracy in the confusion matrix. However, due to the overall low photo count and uneven distribution of categories, the model tended to overclassify other categories as "Happy" or "Neutral."

Keywords: Archery Athletes, Emotional, AffectNet, Databases

Neutral Happy Sad

Figure 1. Facial features from the athlete database.

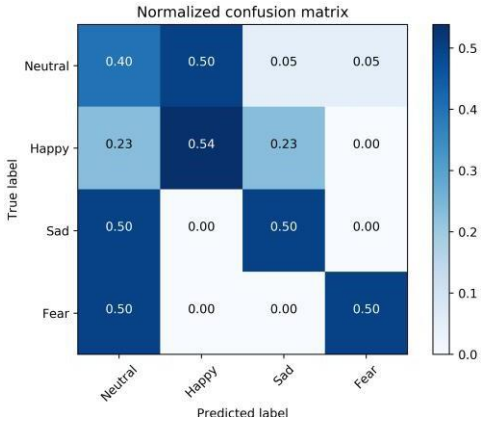


Figure 2. The confusion matrix displays the model's prediction results for each emotion category for EfficientNet.

Active Learning in Non-Iterative Approach

Shi-Jinn Horng[1, a], Sin-Jieh Chen [2]
[1] Department of Computer Science and Informaton Engineering,
Asia University, Taichuan Taiwan, E-mail: horngsj@yahoo.com.tw
[2] Department of Computer Science and Informaton Engineering, National Taiwan University of Science and Technology, Taipei Taiwan, E-mail: timmy10191998@gmail.com

With the rapid development of deep learning technology, deep learning has been widely adopted by many companies for various purposes and products. However, not all use cases have publicly available datasets to use. As a result, a significant amount of time and manpower is required for data labeling. In light of this, active learning techniques have emerged, which autonomously select valuable data for model learning and filter out data with low contribution to the model, effectively reducing the need for extensive data labeling and significantly lowering manpower and time costs.

However, traditional active learning frameworks require multiple iterations, involving repetitive processes of labeling, training, and data selection until the desired amount of data is selected. In this study, we propose a non-iterative active learning framework, eliminating the need for iterations. This framework utilizes a confidence correction model based on LSTM, which enables the confidence distribution generated by a model trained on a small amount of data to be comparable to the results produced by a model trained on a large amount of data. This method improves the accuracy of data selection using an entropy-based selection function.

We conducted experiments using the commonly used benchmark datasets in the active learning field, CIFAR10 and CIFAR100. The experimental results demonstrate that our proposed method can achieve accuracy comparable to that of models trained on complete datasets using only 50% and 63% of the data for CIFAR10 and CIFAR100, respectively. Moreover, compared to the traditional active learning framework, when aiming to select 50% of the data on the CIFAR10 dataset, our method achieves comparable accuracy while improving the overall execution speed by 7 times. Similarly, when aiming to select 50% of the data on the CIFAR100 dataset, our method improves the execution speed by 4.7 times compared to the traditional active learning framework.

Keywords: Active Learning, Labeled data, Data selection, LSTM, CIFAR10, CIFAR100

[a] Presenting Author

Modelling, Data Analytics and AI in Engineering

Muhammad Ahmad [1], Rohail Mali [2], Jari Vepsäläinen [1]
[1] Aalto University, E-mail: jari.vepsalainen@aalto.fi

There is an increasing number of requirements for machine design due to climate change. Engineers require more sophisticated tools to support in the design process to account for all possible solutions and their benefits and drawbacks. In addition to performance and cost, alternative solutions need to be evaluated in terms of emissions. Due to these factors, it is infeasible for the designer to consider and evaluate all possible solutions. A generative design approach could generate and evaluate feasible solutions. Generative design is an iterative approach, which aims to produce many different solutions for a given task and a set of limitations. In the existing literature, there are a multitude of use cases employing generative design in engineering design of electronics, mechanics, robots, and architecture. Based on the existing literature, there seems to be a lack of general approach to present and iterate over feasible solutions. Here we use a case example of powertrain design to lay the foundation for such a general generative design approach. The powertrain design is implemented using a limited component library consisting of electric and petrol-powered powertrain components. The given task is a driving cycle, which the design must complete with less than 5% MSE error. The hypothesis is that not only the generative design system generates purely electric and petrol-powered solutions but also series and parallel hybrids. Costs and emissions of components are considered. The control gains of each proposed powertrain is tuned automatically using a neural network and a genetic algorithm. The components are modelled in Simulink as input-output blocks with dependencies on other components and conditions. The developed generative design system lays a foundation for future research employing reinforcement learning to find the best solutions faster and developing the component presentation to a more unified format.

Keywords: Generative Design, Powertrain Design, Self-Tuning PID

MadeAI 2024 - Modelling, Data Analytics and AI in Engineering
2-5 July 2024, Porto, Portugal

On the hidden layer-to-layer topology of the representations of reality realised within neural networks

Peter Grindrod CBE [1,*]

[1]University of Oxford E-mail: grindrod@maths.ox.ac.uk

Abstract: Consider an information processing algorithm, such as a deep neural network, that is designed to process an input data object onto an output data object, usually making a discrete classification, via a number of successive internal *layers*, and mappings between them. Such algorithms are high-dimensional, often with millions of real parameters to be calibrated during training; they are non-linear, and the overall mapping from input space to output space may have some high gradients [**?**]. Whenever such an algorithm is applied to an input data object, each successive kth layer produces a set of observable, internal, real values that are usually called the "activations" of the layer's set of artificial neurons. These may be realised as a vector within a corresponding Euclidean space of high dimension, m_k say. We will refer to this space as the *embedding space*, E_k, and to m_k as the *embedding dimension*, which is also often called the *width* of the kth layer.and will be known. When the algorithm is applied to a large number, N, of input data objects it yields N vectors forming a point cloud within E_k. As we increase N we can think of the point cloud within E_k as more and more densely sampling a manifold $M_k \subset E_k$. Typically M_k will be curved and have a dimension that is much lower than m_k: it is the image of the input object space held at the kth layer. In [**?**] this exact situation was investigated for a well known image classifier algorithm possessing this type of layered neural network architecture. The authors estimated the *dimension*, D_k, of each of the M_k (k=1,2,...,K) using the two-nearest-neighbour algorithm [**?**] over the sampled points. This yields the fractal (Hausdorff) dimension of M_k. Although the embedding dimensions, m_k, were decreasing from the first layer to the final layer (by l design), the dimensions, D_k, were not always decreasing, For some transitions, it was possible that the dimension increased. Such a phenomenon occurs when M_k becomes folded over and over by φ_k and thus fills a manifold M_{k+1} of higher dimension (just as when we have familiar examples of space filling curves and volume filling surfaces). Of course any over intricate folding, that we will refer to as "pleating", means that there must be some points within the image clouds that are not close together in M_k yet are mapped by φ_k onto image points in M_{k+1} which are very close together. The perturbation distance between such points pairs thus becomes much smaller under φ_k, meaning that the local inverse must have a high gradient. When mapped backwards into input space, these perturbations were not represented and sampled within the input data object set, where they would be large and very possibly non-realistic deformations (not small data perturbations but large localised *semantic* perturbations). There is a possible relationship between this phenomenon and an algorithm's vulnerability to adversarial attacks, or *spoofing*, a growing threat for machine learning research, especially via *black box attacks* where the attacker has no access to the model's internal parameters (see the discussion and references in [**?**]). Typically AI classifiers are subject to input perturbations that appear negligible to humans yet causes miss-classifications. Hence the observable, put perhaps un-anticipated, occurrence of dimensional layer-to-layer increases (most likely due to pleating) is perhaps to be avoided. Ironically, given developers' full access to the internal activations, it is relatively inexpensive to make such calculations. This could become a standard performance check. The mere estimation of dimension is a very blunt tool though. In this paper we will deploy a more sophisticated method of analysis: computational topological data analysis, more specifically persistent homology, and the calculation of persistence diagrams of different degrees (see [**?**] and the references therein for a general

introduction). By doing so we gain further insights into the shape of the high dimensional point clouds (and the manifolds they are sampling), and to suggest a topological *loss term* that might penalise undesirable behaviour (pleating and so on) due to the latent layer-to-layer mappings, reducing the vulnerability of the calibrated algorithm to attacks and other miss-behaviour, and resulting in lower risk algorithms.

Keywords:

* Presenting author

References

[1] M. Raissi, P. Perdikaris, G.E. Karniadakis. 2019. Physics-informed neural networks: A deep learning framework for solving forward and inverse problems involving nonlinear partial differential equations. Journal of Computational Physics. Vol. 378, pp. 686-707.

[2] Huang, X., Kwiatkowska, M., Wang, S. & Wu, M. (2017) Safety verification of deep neural networks. In: Majumdar, R., Kunčak, V. (eds) Computer Aided Verification. CAV 2017. Lecture Notes in Computer Science(), vol 10426. Springer, Cham.

[3] Cui, Z., and Grindrod, P. (2022). Mappings, Dimensionality and Reversing Out of Deep Neural Networks, IMA Journal of Applied Mathematics.

[4] Facco, E., d'Errico, M., Rodriguez, A., & Laio, A. (2017) Estimating the intrinsic dimension of datasets by a minimal neighborhood information. Sci Rep 7, 12140.

[5] Singh, G., Mémoli, F., and Carlsson, G. E. (2007). Topological Methods for the Analysis of High-Dimensional Data Sets and 3D Object Recognition. In SPBG, pages 91–100.

[6] Otter, N., Porter, M.A., Tillmann, U., Grindrod, P., and Harrington, H.A., A roadmap for the computation of persistent homology. EPJ Data Sci. 2017;6(1):17. doi: 10.1140/epjds/s13688-017-0109-5. Epub 2017 Aug 9. PMID: 32025466; PMCID: PMC6979512.

Multivariable Automated Insulin Delivery Systems for People with Diabetes – A challenge in data interpretation, modeling and control

A Cinar[1, a], M Rashid [1], M Abdel-Latif[1], M Ahmadasas[1], M Park[2], L Sharp[2], L Quinn [2]

[1] Illinois Institute of Technology, E-mail: cinar@iit.edu, rashid@iit.edu, mabdella @hawk.iit.edu, mahmadasas@hawk.iit.edu

[2] University of Illinois Chicago, E-mail: {mpark61,sharpl,lquinn}@uic.edu

Diabetes is a chronic condition affecting one out of every eleven people around the world. People with Type 1 diabetes or advanced stages of Type 2 diabetes must inject insulin to regulate their blood glucose concentrations (BGC). An advanced diabetes treatment option is automated insulin delivery (AID), which uses a continuous glucose monitoring (CGM) system, an insulin pump and a control algorithm that manipulates insulin infusion from the pump to subcutaneous tissue. CGM data are reported every 5 minutes and insulin infusion rate can be adjusted at the same rate. Disturbances to BGC such as eating a meal and physical activity (PA) may cause hyperglycemia and hypoglycemia, respectively. Since 2018, AID systems called hybrid closed-loop AIDs are available commercially. Hybrid closed-loop indicates that meal and PA information must be manually entered by the user as inputs to the AID system for improving BGC regulation, causing a significant burden to them. Our research focuses on *multivariable* control algorithms for AID (mvAID) systems (Figure 1).

The mvAID system uses additional signals from wearable devices like wristbands as streaming data, interpretated in real time with data analytics and machine learning (ML) for detection and classification of disturbance-causing events (single or concurrent). This information is fed to adaptive models, control algorithms and AI-based decision-making modules, enabling fully-automated model predictive control of insulin infusion.

The mvAID system is focused on mitigating meal, PA, and acute psychological stress (APS) disturbances. PA and APS affect BGC in opposite directions, AP reduces BGC, and APS and meals increase it. The detection and classification of these disturbances enable feedforward (anticipatory) control, to reduce the delays in the control loop. CGMs detect glucose concentration in subcutaneous tissue that has 5-8 minutes of delay in reporting BGC. Worse, insulin infused to subcutaneous tissue has 40-50 minutes of delay in causing its effect on BGC.

The PA and APS detection, classification and estimation of their characteristics is based on data from 4 sensors that provide blood volume pulse, 3-axis accelerometer, galvanic skin response and skin temperature data reported by Empatica E4 wristband. ML techniques ranging from multivariate statistical methods to deep neural networks are used for detecting the occurrence, classifying and estimating the intensity of PA (sedentary state, stationary bike, treadmill running) and APS (no stress, mental stress, emotional anxiety stress). PA and APS can occur concurrently, for example during an athletic competition or in unexpected situations (Figure 2). The signals from sensors are noisy and have artifacts that affect the accuracy of heart rate estimation. Meals are detected and their carbohydrate content are estimated from CGM readings. There is tradeoff between the burden of entering meal information manually

[a] Ali Cinar *cinar@iit.edu*

and this automated delivery of meal occurrence and its carbohydrate content with a delay by using CGM data.

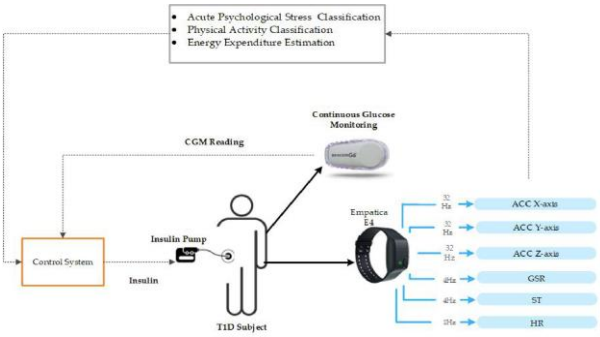


Figure 1. mvAID system information flow

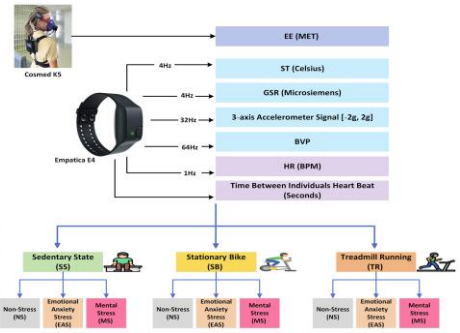


Figure 2. Concurrent PA and APS detection

Clinical experiments (34 subjects participated in 166 experiments) conducted at the University of Illinois Chicago where subjects undergo several PA, APS and meal events provide data to develop and test the algorithms proposed. Data filtering and artifact elimination uses several signal processing techniques and neural nets. Signal segmentation enables the trained models to be evaluated frequently. Random convolutional kernel transformation (ROCKET) is used to extract 1800 features from the time-series signals. Imputation of missing information is performed after extracting the feature variables by ROCKET to leverage the calculated feature maps and the relations among the features in estimating the missing samples. Probabilistic principal component analysis (PPCA) with 5 principal components is used to estimate the missing samples. Features with the highest co-linearity index are identified, followed by Partial Least-Squares Discriminant Analysis (PLS-DA) and PLS to extract the most informative features. Multi-Task recurrent neural networks (RNN) with LSTM models are developed to make simultaneous classification of APS (NS, EAS, MS) types and PA (SS, SB, TR) types. Weighted training and adaptive synthetic sampling (ADASYN) are utilized to handle the imbalanced classes. As an alternative to DNNs, multi-task Extreme Gradient Boosting (XGBoost) classification of PA Types and APS was also developed. F1 scores of both approaches range from 99.6% to 98%, with very few confusions in detection of PA and APS. To confirm that the appropriate measured variables are used in detection and classification of disturbances to glucose homeostasis SHAP (SHapley Additive exPlanations) are used to determine the most informative signals in APS detection. As expected, galvanic skin response and heart rate (blood volume pulse) were most informative. This illustrated the value of explainable AI in informing medical care providers about the relations between sensor data and detection of disturbances that affect BGC. Confusion matrices were also developed to confirm the low level of misclassifications.

The algorithms developed are being integrated to an mvAID prototype app working on a smartphone to illustrate the features to be considered in the next generation AID systems.

Keywords: Recursively updated adaptive models, disturbance detection and classification, neural networks, decision trees, SHAP, model predictive control, diabetes, explainable AI

Key Frame Selection for Personality Traits Recognition

NURRUL AKMA MAHAMAD AMIN [1, a], NILAM NUR AMIR SJARIF [2], SITI SOPHIAYATI YUHANIZ [3]

[1] University Technology Malaysia, E-mail: nurrulakma@graduate.utm.my

[2] University Technology Malaysia, E-mail: nilamnur@utm.my

[3] University Technology Malaysia, E-mail: sophia@utm.my

Personality traits recognition is a multidisciplinary field that brings together knowledge of psychology, computer vision and deep learning. The advancements of deep learning algorithms have significantly contributed to the research on recognizing human personality traits from video-based input data. A video is a series of images which are called frames, are captured, and eventually displayed at a given frequency. The number of frames for a video varies depending on the frame rate or frame per second (FPS) of the video. In general, default frame rate is 24 FPS, which means for 60 second video, it will consist of 1440 frames or images. Thus, it is computationally expensive to handle video processing for recognition process. In this paper, we address the issue of key frame selection to improve the accuracy of personality traits recognition. Key frame selection is the novel process of identifying and extracting the best frames from a video input that significantly differ from each other. Key frames encode the highest information compared to other frames in video input set. These key frames are considered the best frames that give a significant overview of content in video. Previous work on personality traits recognition has leveraged random and uniform frame selection with pre-determined number of selected frames.

However, in this work, we propose a method to select the best frames from video by finding the absolute difference between the pixels of each frame. Next, the best frames are selected based on the brightness and Laplacian score. In contrast to previous work, the number of frames selected in a video may vary depending on the video content including video length and video quality. The pipeline used to extract key frames consists of three main steps which are extract potential frames as candidate key frames, clustering similar candidate frames and selecting key frame from each cluster as a best frame. In detail, during the first step, the potential frames were identified and extracted from the video based on the frame pixel differences. Next, the second step involves generating clusters of similar frames, where frames that are close to each other are grouped together to form a single cluster. Finally, in the last step, the best frames from each cluster are selected and all other frames are discarded. With the aim of selecting the best top N frames from each video, the selection method considers the following criteria including brightness filtering, contrast/entropy filtering, clustering of frames and variance of Laplacian for non-blurred images selection. We show that the proposed method

[a] Nurrul Akma Mahamad Amin

of key frame selection improves the accuracy performance of personality traits recognition on ChaLearn dataset over the recent state-of-the-art models.

Keywords: personality traits recognition, video processing, key frames selection, frames clustering

Reconstruction of Core Power Distribution Using GMDH-Based Virtual Detectors

Ga-Hee Sim [1, a], Moon-Ghu Park [2]
[1] Sejong University, E-mail: gahe2S@sju.ac.kr
[2] Sejong University, E-mail: mgpark@sejong.ac.kr

This paper proposes a method to reconstruct the core power distribution of nuclear reactors using virtual detectors. The core power distribution is an essential parameter for the safe operation of nuclear reactors, as it determines the peaking factor, which indicates the ratio of the maximum power to the average power at any point in the core. A high peaking factor can cause local boiling or damage to fuel integrity; thus, the core power distribution must be controlled within a specific range. A three-dimensional power distribution is necessary to determine the peaking factor, and continuous measurement values from assemblies enable the creation of a 3D power distribution.

The nuclear reactors' fuel assemblies have ICI (in-core instrumentation) assemblies, which consist of five fixed in-core rhodium SPNDs (self-powered neutron detectors) axially. However, the ICI assemblies have limited and fixed installation locations in the core, which makes it difficult to obtain continuous values for the entire core. The virtual detector method solves this problem by assuming the existence of non-installed detectors and estimating the neutron flux in other parts of the core based on the signals from ICIs.

We adopt GMDH (Group Method of Data Handling), previously known as a polynomial neural network, to calculate the values of virtual detectors, employing a technique that generates a function to determine the optimal correlation between inputs and outputs. GMDH is transparent and complies with nuclear safety regulations, clearly expressing the functional relationship between inputs and outputs. Nuclear safety regulations are known for their strict and complex nature, presenting challenges in obtaining approval for AI (artificial intelligence) technologies like neural networks, which operate with obscure workings. In contrast, GMDH holds an advantage in the approval process due to its constructive representation of the functional forms.

To generate and evaluate GMDH functions for virtual detectors, we utilized 3417 data points. We created the function using 50% of the training data. We assessed the performance of the virtual detector by comparing the error between the power distribution generated by the existing installed ICI assemblies and using the virtual detector. The results indicated that the virtual detector method reconstructed the power distribution more accurately than the conventional approach. Plans involve a sensitivity analysis to reduce installed ICIs, potentially aided by virtual detectors to decrease existing SPND installations.

Keywords: nuclear reactor, virtual detector, GMDH, SPNDs, core power distribution

---

[a] Presenting Author

Optimizing Wind Turbine Energy Forecasts: A Hybrid Methodology of Clustering Analysis and Wind Speed-Sensitive Modeling

Mindaugas Jankauskas[1,*], **Artūras Serackis**[2]

[1]Department of Computer Science and Communications Technologies, Vilnius Gediminas Technical University, Saule˙tekio al. 11, Vilnius, LT-10223, Lithuania, E-mail: m.jankauskas@vilniustech.lt
[2]Department of Electronic Systems, Vilnius Gediminas Technical University, Saule˙tekio al. 11, Vilnius, LT-10223, Lithuania, E-mail: arturas.serackis@vilniustech.lt

Abstract: Accurate prediction of wind turbine energy production is crucial in the continually changing field of renewable energy. Wind power generation is becoming increasingly important in the global shift towards clean and renewable energy sources. Worldwide wind power capacity has increased from around 2.5 GW in 1992 to nearly 906 GW by the end of 2022. Compared with the 2030 global outlook released alongside the Global Wind Report last year, GWEC Market Intelligence has increased its forecast for total additions of wind power capacity for 2023-2030 by 143 GW (13% YoY). [1]. In our investigation, we propose an advanced methodology for forecasting wind turbine energy that integrates feature selection, data clustering based on wind speed, and Bayesian hyperparameter optimization for individual models. Initially, a comprehensive feature selection process was used to determine the key features that influence the generated power output of wind turbines. The data were then divided into three separate clusters, taking into account the key impact of wind speed on energy generation, with each cluster representing a certain range of wind speeds. A Bayesian hyperparameter optimization approach was used to fine-tune the hyperparameters of the forecasting models for each cluster, ensuring the development of the most precise and resilient model for each wind speed category. The models' performance was assessed using several key measures, such as the mean squared error, root mean squared error, mean absolute error, mean absolute percentage error, coefficient of determination, and normalized mean absolute error. Using real-world wind farm data, our customized method, which has been validated experimentally, not only outperformed traditional forecasting models, but also revealed the complex correlation between fluctuations in wind speed and energy production. The results highlight the ability of this advanced approach to significantly improve the operational efficiency of wind farms, providing a flexible structure to improve the integration of renewable energy into the power grid.

Keywords: Wind power generation, power generation prediction, recurrent neural network, BiLSTM

* Presenting author

References

[1] Global Wind Report 2023. https://gwec.net/globalwindreport2023. Accessed: 2024-02-14

Transient Simulations with Surrogate Elements

Markus Franke [1, a], Tom Krause [2], Marcus Wagner [3]
[1] OTH Regensburg, E-mail: markus.franke@oth-regensburg.de
[2] BMW Group, OTH Regensburg, E-mail: Tom-Janis.Krause@bmw.de
[3] OTH Regensburg, E-mail: marcus.wagner@oth-regensburg.de

Keywords: Surrogate modelling, Substructuring, Physics Informed Neural Network

Introduction

In finite element analysis substructuring is a widespread method for reducing computational costs [1]. One major restriction thereby is, that loads and supports have to be known prior to static condensation [2]. To overcome this issue, the emerging discipline of modelling the substructure with (physics informed) neural networks [3,4] can be employed.
We present a method for reducing the computational costs of linear transient finite element simulations. Thereby, regions of a physical domain are not discretized by several standard finite elements. Rather they are modelled with one single artificial *surrogate element (SE)*, which is generated by a physics informed neural network (PINN).

Surrogate Elements

To explain a *surrogate element*, we first introduce the physical domain Ω, which can be divided into a region of interest, Ω_{PR}, and a substructure region, Ω_{RR}, of no further interest. Nevertheless, Ω_{RR} is necessary to model Ω correctly. oor this, artificial SEs replace the subdomain Ω_{RR} by only just one element with less degrees of freedom (dof). Due to this, the dimension of the system of equations to solve, $\boldsymbol{K}\boldsymbol{u} + \boldsymbol{C}\dot{\boldsymbol{u}} + \boldsymbol{M}\ddot{\boldsymbol{u}} = \boldsymbol{f}$, is reduced, which leads to lower computational costs. Here, $\boldsymbol{K}$, $\boldsymbol{C}$ and $\boldsymbol{M}$ denote the stiffeness, damping and mass matrix, respectively. The vector $\boldsymbol{u}$ and its derivatives describe displacements, velocity, and acceleration, whereas $\boldsymbol{f}$ denotes the external force vector. The PINN creating the SEs consists of a single dense layer for the generation of the SEs mass matrix $\boldsymbol{M}^e_{SE}$, and an additional single dense layer for the calculation of the stiffness matrix $\boldsymbol{K}^e_{SE}$. These two layers are not connected. Next in the forward propagation of the PINN, the reduced matrices are built, and the system is solved for $\tilde{\boldsymbol{u}}$ by an implicit Newmark beta solver. To train the model, the first part of the training dataset is generated from standard static oE simulations of the fully discretized domain Ω. oor the training process of the reduced model, only Ω_{PR} is discretized, which results in $\boldsymbol{K}_{\mathrm{PR}}$. To fully model Ω with the reduced matrix $\tilde{\boldsymbol{K}}$, the SEs element matrix $\boldsymbol{K}^e_{SE}$ is added to the dofs of $\boldsymbol{K}_{\mathrm{PR}}$ connecting Ω_{RR} and Ω_{PR}. oonsequently, for optimization of the PINN, $\tilde{\boldsymbol{K}}\tilde{\boldsymbol{u}} = \tilde{\boldsymbol{f}}$ can be solved for $\tilde{\boldsymbol{u}}$, which enables the error calculation between $\tilde{\boldsymbol{u}}$ and the corresponding displacements of $\boldsymbol{u}$. After that, the surrogate element mass matrix, $\boldsymbol{M}^e_{SE}$, is trained in a similar process. oor this the second part of the training dataset, a transient dataset, is used. Due to the Rayleigh damping approach, $\tilde{\boldsymbol{C}}$ can be constructed from $\tilde{\boldsymbol{K}}$ and $\tilde{\boldsymbol{M}}$

[a] Presenting Author

Results

The SE stiffness and mass matrix are trained on datasets containing only simulations with a single beam, see oigure 1 a). This reduces training effort. In the static case, as well as in the transient case, the purple nodes are excited by random forces, whereas the orange nodes are fixed supported. oor validation purposes, the surrogate element is applied to a more complex model, see oigure 1 b). The schematic building is excited with forces at the purple nodes to schematically simulate an earthquake. Overall, 18468 dofs of the full model are reduced to 7776 dofs in the model with SEs. Therefore, computation time drops by the factor 10.

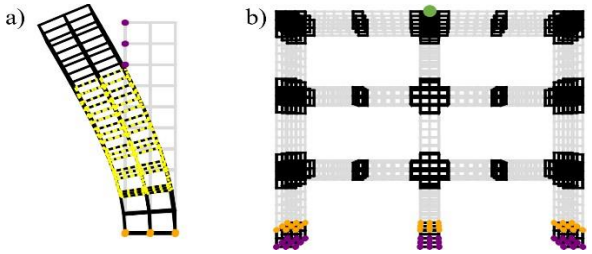


Figure 1: Model for training the SE, which region is marked yellow (a). In the validation model, (b), gray elements denote the full model, whereas the overlying black elements denote the reduced model.

oor a better assessment of the transient capabilities of the SEs, the displacement of the node marked green in oigure 1 b) is plotted in oigure 2. The displacement from the reduced model matches with the full solution, a maximum relative error of 1,7% can be calculated.

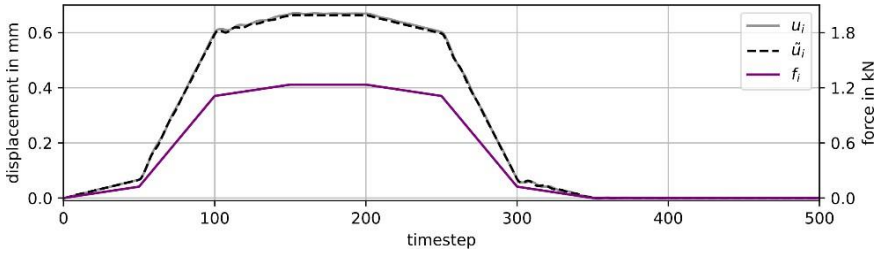


Figure 1: Displacement of the green marked node in Figure 1) over all timesteps.

Conclusion

In this work we show a method for boundary and load independent substructuring in transient analysis. The substructure is replaced by *surrogate elements*, which are generated by a physics informed neural network. With this method, computational times are reduced.

Literature

[1] Allen, M.S., Rixen, D., Seijs, M., Tiso, P., Abrahamsson, T., Mayes, R.L.: Model Reduction ooncepts and Substructuring Approaches for Linear Systems. Springer, oham (2020)

[2] K.-J. Bathe. oinite element procedures. Prentice-Hall of India, New Delhi, 2007.

[3] Koeppe, A., Bamer, o., Markert, B.: An intelligent nonlinear meta element for elastoplastic continua: deep learning using a new Time-distributed Residual U-Net architecture. oomput. Methods Appl. Mech.Eng. (2020)

[4] Huang, M., oui, T., Liu, o., Du, Z., Zhang, J., He, o., Guo, X.: A Problem-Independent Machine Learning (PIML) enhanced substructure-based approach for large-scale structural analysis and topology optimization of linear elastic structures. Extreme Mechanics Letters (2023)

Data Augmentation for Recorded Properties of Processed Materials in Industrial Production Processes for the Application of Machine Learning Models: A Case Study in an Automotive Press Shop

Tom Krause [1, a], Markus Franke [2], Ingo Heinle [3], Marcus Wagner [4]
[1] BMW Group, E-mail: tom-janis.krause@bmw.de
[2] OTH Regensburg, E-mail: markus.franke@oth-regensburg.de
[3] BMW Group, E-mail: ingo.heinle@bmw.de
[4] OTH Regensburg, E-mail: marcus.wagner@oth-regensburg.de

The digital transformation is driving significant advancements in both the economy and society. In industrial production, there is a growing trend of recording and processing data during the manufacturing process. Various solutions exist to seamlessly integrate sensors into process workflows, transmit the collected data to a database, and subsequently analyze it either centrally or on a computing unit located at the production facility e.g., an edge computer [1]. This enables data-driven decision-making before or during the production of goods. As a result, it becomes possible to reduce production downtime and optimize the quality of the manufactured products.

In this context, machine learning models can be employed to predict the quality of manufactured products based on the characteristics of the semi-finished product processed in the respective production process, or to suggest process parameters. The utilization of such models is economically significant, especially when the quality of the manufactured products is significantly dependent on fluctuating properties of the semi-finished product. However, in production processes, a challenge may arise where only a limited number of different values are available for each process parameter, as they are typically only adjusted when the required quality of the produced components necessitates it. Furthermore, the data or trained models may not always be transferrable from one production process to another. Changes in production processes can also render previously collected training data invalid, rendering the models unusable. Consequently, there may be a limited number of datasets available for training and validating such models, posing a risk of overfitting.

To address this issue, numerous techniques can be found in the literature, such as regularization [2] or data augmentation. The choice of machine learning model can also be crucial in this context. Our contribution demonstrates, using the example of car body part production in press shops, how the predictive accuracy of selected models to support plant operators can be enhanced by employing a data augmentation technique tailored to the specific challenges of model training in a production environment.

[a] Presenting Author

Keywords: Machine Learning, Data Augmentation, Recorded Material Properties, Press Shop, Industrial Production

Literature:

[1] Sit SKH, Lee CKM (2023) A Case Study on Data Analytics Based on Edge Computing for Smart Manufacturing System. Intelligent and Transformative Production in Pandemic Times: Proceedings of the 26th International Conference on Production Research (pp. 293-302). Springer International Publishing

[2] Bishop CM (2006) Pattern recognition and machine learning. Information science and statistics. New York: Springer, 2006

Harnessing ChatGPT Intelligence for Enhanced Aerodynamics Data Analysis in Aeronautics

E Andrés-Pérez[1], V Francés[1,4], J Nieto-Centenero[1,3] and R Castellanos[2]

[1] Theoretical and Computational Aerodynamics Branch, Spanish National Institute for Aerospace Technology (INTA). Ctra. De Ajalvir km 4.5, 28850 Madrid, Spain

[2] Subdirectorate General of Terrestrial Systems, Spanish National Institute for Aerospace Technology (INTA). Ctra. San Martin de la Vega km 10.5 , 28330 Madrid, Spain

[3] Universidad Politécnica de Madrid, Plaza Cardenal Cisneros 3, E-28040 Madrid, Spain

[4] Universidad Carlos III de Madrid, Avenida de la Universidad 30, 28911 Leganés, Spain

E-mail: eandper@inta.es, vfrabel@inta.es, jniecen@inta.es, rcasgar@inta.es

Machine learning (ML) has significantly impacted aeronautics, offering innovative solutions for aerodynamic analysis and optimization [1-2]. Key applications include aerodynamic shape optimization, predictive modelling, data-driven analysis, integration with computational fluid dynamics, management of aerodynamic databases, and uncertainty quantification [3]. These ML techniques have led to improvements in aircraft preliminary design process performance and efficiency while reducing development time and costs. Despite challenges such as data quality and model interpretability, the future of ML in aerodynamics is promising, with developments in hybrid models, automated optimization, and Explainable AI [4]. The advent of tools based on natural language processing, like ChatGPT, further highlights the potential for ML to revolutionize the field by streamlining analysis and extending its applications to broader scientific and engineering disciplines.

The potential of ChatGPT integration within the analysis pipeline for aerodynamic data within the context of aeronautics is explored in this study. Employing a conventional dataset containing the aerodynamic features of a NACA0012 airfoil (Fig. 1), ChatGPT stands in performing preliminary data analysis to detect intricate patterns and articulate nuanced relationships inherent in the data. Besides illustrating the effectiveness of ChatGPT in aerodynamic data analysis, we delve into the interpretability of its outputs and discuss the model's potential to automate certain aspects of the analysis, allowing researchers to focus on high-level interpretation and decision-making. In addition to preliminary data pre-processing and conventional data analysis, we exploit ChatGPT performance to develop and train ML models for regression purposes. Several regressors are tested to predict the lift coefficient (Fig. 2), highlighting the capabilities of ChatGPT to propose and train complex models such as deep neural networks (DNN). Nonetheless, the study also discusses the challenges related to the integration of a language model in the aeronautical field.

The outcomes suggest that ChatGPT exhibits potential as a valuable tool for aeronautical engineers and researchers, providing a novel dimension to aerodynamic preliminary data analysis. The synergy elucidated between NLP-AI and aerodynamics herein presented opens avenues for future research, with implications for enhanced design methodologies, performance optimization, and a deeper comprehension of aerodynamic phenomena. ChatGPT demonstrates its effectiveness in simplifying complex data analysis tasks by providing an accessible interface

for researchers and engineers. It streamlines data preprocessing, code generation, and exploratory analysis, reducing drastically the time and effort required for these critical tasks. The findings highlight the transformative potential of NLP models like ChatGPT in advancing aerodynamics data analysis and research.

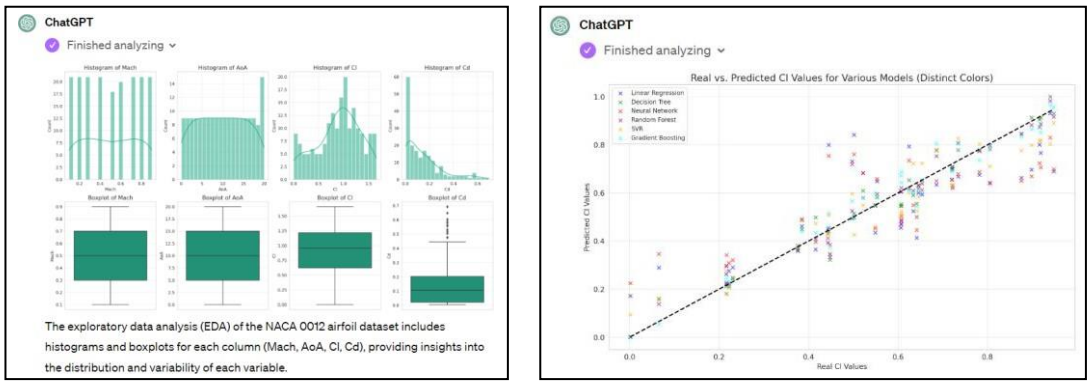


Fig. 1. Preliminary analysis on NACA0012 airfoil dataset. Visualization of dataset metrics (left) and the comparison of different regression models built with ChatGPT (right)

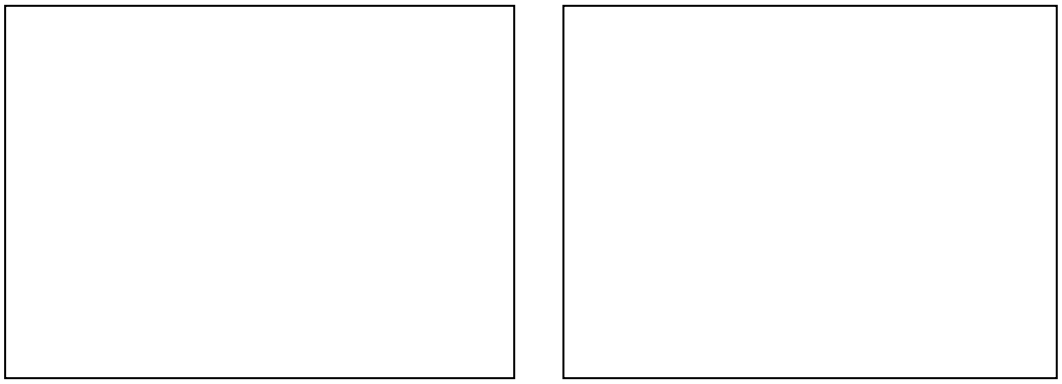


Fig. 2. DNN optimization with chatGPT for aerodynamic prediction: proposed model (left) and regression line plot (right)

References:

[1] Li, J., Xiaosong D., and Martin, J.R. (2022) Machine learning in aerodynamic shape optimization. *Progress in Aerospace Sciences*, **134**, 100849.

[2] Sabater, C., Stürmer, P., & Bekemeyer, P. (2022). Fast predictions of aircraft aerodynamics using deep-learning techniques. *AIAA Journal*, **60**(9), 5249-5261.

[3] Li, J., Liu, T., Zhu, G., Li, Y., & Xie, Y. (2023). Uncertainty quantification and aerodynamic robust optimization of turbomachinery based on graph learning methods. *Energy*, **273**, 127289.

[4] Wu, C., Wang, S., Zhang, X. L., & He, G. (2023). Explainability analysis of neural network-based turbulence modeling for transonic axial compressor rotor flows. *Aerospace Science and Technology*, **141**, 108542.

Keywords: Aerodynamics, machine learning, ChatGPT.

Prediction of Wing Aerodynamic Coefficients of an Unmanned Light Electric Aeroplane with ANN

Nihong Yang [a], Gebrihiwet Brhane, Yufeng Yao
E-mail: nihong2.yang@uwe.ac.uk, gabs.brhane@yahoo.com, Yufeng.Yao@uwe.ac.uk

Artificial Neural Network (ANN) is a powerful machine learning tool to establish a surrogated model for the prediction of aerodynamic performance in aeroplane wing design optimisation. The ANN network configuration should be optimised to avoid underfitting and overfitting to obtain the lowest prediction error and the highest accuracy. Once the optimal model is obtained, it can then be used to replace the conventional Computational Fluid Dynamics (CFD) simulations to predict the aerodynamic performance more efficiently.

In this study, 3D wing CFD simulation is first carried out to obtain aerodynamic performance data of unmanned light electric aeroplane wings at various Angles of Attach (AoA) and taper ratios. The effects of the neuron and hidden layer numbers on prediction accuracy are then investigated with a feedforward ANN method, using the simulated 3D wing aerodynamic data and the 2D NACA–0012 airfoil aerodynamic data taken from an open source. It can be seen that both prediction errors of the training set and validation set reduce with the increasement of neuron numbers or hidden layer numbers initially, but the prediction error of the validate set starts to increase at a number whereas the error of the training set continues to reduce. It is found that as many as 8 to 10 neurons in the hidden layers are needed to prevent underfitting while more than 2 hidden layers can cause overfitting, for the datasets in the applications. Use of more hidden layers likely causes overfitting than use of more neurons. For the 3D wing data, a feedforward ANN model with 1 hidden layer and 8 neurons in the hidden layer can achieve high prediction accuracy with the R value i.e. the square root of coefficient of determination being more than 0.98. This optimal model is then used for the prediction of the lift and drag coefficient ratios Cl/Cd of the unmanned light electric aeroplane wings.

Based on the data predicted by the optimal ANN model, it is found that at the design cruise speed the wing with a taper ratio of 0.1 has produced the best aerodynamic performance for the type of wings in consideration. Furthermore, this study provides a good overview of the ANN model training, validation, and the network configuration optimisation processes in MATLAB, with thorough details on how an ANN method can be used for the prediction of aerodynamic performance.

Keywords: Aerodynamic coefficients, Artificial neuron networks, Model training process, Optimal network configuration, Wing taper ratio optimisation.

[a] Presenting Author

Deep Learning techniques for modelling malware propagation on IoT environments

Angel Martin del Rey

Department of Applied Mathematics, Universidad de Salamanca, Spain, E-mail: delrey@usal.es

Abstract:

The technological development of our society since the end of the 20th century has been impressive. Thus, it is worth highlighting the development and establishment of the Internet of Things paradigm (Industry 4.0, smart cities, e-Health, smart agriculture, smart transportation, smart buildings, etc.) Our society is highly dependent on IT systems and services at both the individual and collective level. In this regard, IoT environments implemented in critical infrastructures or essential services are particularly important.

Obviously, this scenario is permanently subjected to cyber threats of all types [1, 2, 3]: from classic attacks to complex cyber attacks such those called Advanced Persistent Threats (APTs). In the vast majority of them, one of the main techniques employed is malicious code (malware) [4, 5, 6]. The "scientific" fight against it can be approached from two perspectives: either by developing algorithms to detect its presence in a given network, or by designing computational models to simulate its propagation through a device network. The first approach is the most common and countless works can be found in the scientific literature developing algorithms based on Deep Learning techniques [7, 8, 9]. Much less explored is the field of developing computational models to simulate the propagation of a given malware specimen [10, 11].

In this sense, there are very few works dedicated to the design of malware propagation models where Deep Learning tools are used both in their design and in their analysis. These proposals focus on the use of Physics-Informed Neural Networks (PINN), Differential Neural Networks (DNN) for the study of global models whose dynamics is mathematically described by means of differential equations [12, 13, 14], and Graph Neural Networks (GNN) in the case of the analysis of individual-based models [15].

The main goal of this work is to critically review the use of different neural network architectures to study the process of malware propagation on IoT networks. The attention is focused on their use in the design of individual-based models, which are the most suitable for simulating the dissemination of malicious code in IoT environments. In addition, a new model proposal is outlined taking into account the use of hybrid architectures.

Keywords: Malware propagation. IoT networks. Deep Learning. Mathematical Epidemiology. Physics-Informed Neural Networks. Differentiable Neural Networks. Cybersecurity.

* Presenting author

References

[1] I. Bibi, A. Akhunzada, N. Kumar. 2023. Deep AI-Powered Cyber Threat Analysis in IIoT. IEEE Internet of Things Journal. Vol. 10, pp.7749-7760.

[2] J.F.M. Cevallos, A. Rizzardi, S. Sicari, A.C. Porisini. 2023. Deep Reinforcement Learn- ing for intrusion detection in Internet of Things: Best practices, lessons learnt, and open challenges. Computer Networks. Vol. 236, Article number 110016.

[3] B. Nour, M. Pourzandi, M. Debbabi. 2023. A Survey on Threat Hunting in Enterprise Networks. IEEE Communications Surveys and Tutorials. Vol. 25, pp.2299-2324.

[4] A. Al-Marghilani. 2021. Comprehensive Analysis of IoT Malware Evasion Techniques. Engineering Technology & Applied Science Research. Vol. 11, pp. 7495-7500.

[5] A. Alharbi, A. Hamid, H. Lahza. 2022. Predicting Malicious Software in IoT Environment Based on Machine Learning and Data Mining Techniques. International Journal of Advanced Computer Science and Applications. Vol. 13, pp. 497-506

[6] A. Aldhaheri, F. Alwahedi, M.A. Ferrag, A. Battah. 2024. Deep learning for cyber threat detection in IoT networks: A review. Internet of Things and Cyber-Physical Systems. Vol. 4, pp. 110-128.

[7] M. Azeem, D. Khan, S. Iftikhar, S. Bawazeer, M. Alzahrani. 2024. Analyzing and comparing the effectiveness of malware detection: A study of machine learning approaches. Heliyon. Vol. 10, Article number e23574.

[8] A. Brown, M. Gupta, M. Abdelsalam. 2024. Automated machine learning for deep learning based malware detection. Computers & Security. Vol. 137, Article number 103582.

[9] P. Maniriho, A.N. Mahmood, M.J.M. Chowdhury. 2024. A systematic literature review on Windows malware detection: Techniques, research issues, and future directions. Journal of Systems and Software. Vol. 209, Article number 111921.

[10] J. Chen, S. Sun, C. Xia, D. Shi, G. Chen. 2023. Modeling and Analyzing Malware Propagation Over Wireless Networks Based on Hypergraphs. IEEE Transactions on Network Science and Engineering. Vol. 10, pp. 3767-3778.

[11] W. Yang, Q. Fu, Y. Yao. 2023. A Malware Propagation Model with Dual Delay in the Industrial Control Network. Complexity. Vol. 2023, Article number 8823080.

[12] R. Casado Vara, M. Severt, A. Diaz Longueira, A. Martin del Rey, J.L. Calvo Rolle. 2024. Dynamic Malware Mitigation Strategies for IoT Networks: A Mathematical Epidemiology Approach. Mathematics. Vol. 12, Article number 250.

[13] M. Sulaiman, A. Khan, A.N. Ali, G. Laouini, F.S. Alshammari. 2023. Quantitative Analysis of Worm Transmission and Insider Risks in Air-Gapped Networking Using a Novel Machine Learning Approach. IEEE Access. Vol. 11, pp. 111034-111052.

[14] Y. Yang, G. Liu, Z. Liang, H. Chen, L. Zhu, X. Zhong. 2023. Hybrid control for malware propagation in rechargeable WUSN and WASN: From knowledge-driven to data-driven. Chaos, Solitons and Fractals. Vol. 173, Article number 113703.

[15] T. Li, Y. Liu, Q. Liu, W. Xu, Y. Xiao, H. Liu. 2023. A malware propagation predic- tion model based on representation learning and graph convolutional networks. Digital Communications and Networks. Vol. 9, pp. 1090-1100.

Digital Twins for Spatio-temporal Long-term Temperature Dynamics Forecasting in Buildings

Leandro Von Krannichfeldt [1,2], Kristina Orehounig[3] and Olga Fink[1]
[1] EPFL, E-mail: leandro.vonkrannichfeldt@epfl.ch
[2] EMPA
[3] TU WIEN

Buildings are an essential part of everyday life. In the light of digitalization, building technology advancements increasingly focus on healthy and comfortable environments. Built-in systems to maintain desirable indoor conditions comprise heating, ventilation, and air conditioning system, water supply system, or the electrical infrastructure. However, most energy systems still depend on fossil fuels for operation. In 2020, construction and buildings were responsible for 36% of energy consumption as well as 37% of CO_2 emissions worldwide. Favorably, continuing digitalization and sensor employments facilitate advanced analytics and machine learning with the goal of optimizing system operation.

Real-time optimization of energy consumption requires a digital model of a building and its systems that is capable of reflecting the building's condition and allow for improved decision making. A promising framework for this task is the digital twin concept. By relying on spatially distributed sensors across the building, the digital twin permits continuous monitoring of the current state and prediction of future state trajectories. Based on these forecasts, optimal actions for the building management system or predictive maintenance suggestions can be recommended. Specifically, elaborate building management controllers rely on temperature dynamics forecasts to explore their action space. An important aspect in temperature dynamics forecasting is to account for long-term dependencies due to the building's physical properties, such as its thermal mass.

Different methods have been proposed for forecasting building temperature dynamics, including ARIMAX, Linear Regression, Resistance-Capacitance models, Feedforward Neural Networks or Long Short-Term Memory Networks. Typically, these models are employed to capture the temporal aspect of the building energy system dynamics. However, this focus introduces two main shortcomings. First, long-range dependencies may not be fully accounted for due to the model's architecture. Secondly, most of these methods do not explicitly consider spatial dependencies. However, accounting for both dependencies can be beneficial for building temperature forecasting, especially when long forecasting horizons are targeted. Recently, different Transformer architectures have been proposed for time series forecasting that can accurately model long-range and spatial dependencies in efficient ways.

In this work, we propose to leverage the learning of spatio-temporal dependencies in building temperature dynamics with Transformers. To this end, we employ the recently proposed Spacetimeformer, a sequence-to-sequence Transformer model for multivariate time series forecasting. It uses a spatiotemporal learning scheme and can model long-term dependencies in time and space in a principled way. The method has shown promising results

in other application areas, such as traffic and electricity demand forecasting. However, it has not yet been applied in building dynamics modeling. We showcase its performance and suitability in an extensive temperature forecasting study on a real-world dataset from a multi-zone building located in Switzerland. Our comprehensive analysis evaluates various approaches in terms of forecasting performance and method interpretability. Different types of state-of-the-art models commonly applied for building dynamics forecasting are included in the performance evaluation. The results show that Spacetimeformer significantly outperforms other compared approaches, and offers spatio-temporal interpretability through the attention matrix.

Keywords: Building dynamics, forecasting, Spacetimeformer

Modelling of Dynamic Pressure and Temperature Control at Successive Vacuum Infusion and Post-Infusion Molding Composite Parts

I. Zhilyaev [1], S.H. Chang [2], N. Snezhina [3], N. Kleymenov [3] and S. Shevtsov [4, a]

[1] 9T Labs, Zürich, Switzerland, E-mail: igor.zhilyaev@9tlabs.com

[2] National Kaohsiung University of Science and Technology Taiwan, E-mail: shchang@nkust.edu.tw

[3] Don State Technical University, Russia, E-mail: snezhina_nataly@mail.ru, ybr.rk@mail.ru

[4] South Center of Russian Academy of Science, E-mail: sergnshevtsov@gmail.com

Vacuum-infusion technology for the production of fiber- or fabric-reinforced polymer-composite structures is increasingly used in many industrial sectors, in particular in the aviation industry. However, along with such advantages of this process as the speed and low cost of preparing the production of new composite parts, these processes have a number of disadvantages that limit their use in highly loaded and critical structures. These include, first of all, an insufficiently high level and uneven distribution of the specific volume of reinforcement in the volume of the molded part, a high probability of the formation of areas not impregnated with resin (dry spots), especially in structures of complex shape, a local increase in porosity, which leads to a decline in strength properties. The most effective modification of the vacuum-infusion technology, studied on glass and carbon fiber simple specimens and retaining all its advantages, is the dynamic control of external pressures both during the actual infusion stage of molding and in the post-infusion stage, when the preform is completely filled with liquid resin. The article discusses the methodology and results of computer modeling of such a process using the example of an aircraft composite shell-shaped structure.

The computer model of the process used to simulate its evolution describes the propagation of liquid resin, the kinetic state and viscosity of which is controlled by temperature, as well as the distribution of pore pressure and its gradient, which determine the flow rate of the resin. and the ratio between the volume of resin-filled pores of the preform and the reinforcing fibers. A feature of the situations considered in the work is the use of a cyclic change in the external compressive pressure on the preform when it is filled with resin and the effect of elevated temperature at the post-infusion stage of the compressed preform until the resin gelatinizes and hardens in order to maintain a high content and ensure uniform distribution of the fiber volume fraction. The simulation results demonstrate the possibility of significantly accelerating and increasing the filling level of the preform with resin with the correct assignment of the pressure rate and pressure holding durations. Moreover, the capabilities of the system for modeling and post-processing the results make it possible to optimally assign the temperature regime at both stages of the process, ensuring uniform distribution of the

[a] Presenting Author

rheological state of the resin and eliminating the occurrence of increased residual stresses, which can result in warping of the cured part.

Surrogate Model-Based AI for Bearing State Estimation and Early Failure Detection in Marine Propulsion Shafts

G. N. Rossopoulos [1, a], I. Ioannidis [1], P. Bardavillia [1], C.I. Papadopoulos [1]

[1] National Technical University of Athens, School of Naval Architecture and Marine Engineering, Zografos, Greece, E-mail: georosso@mail.ntua.gr

Abstract

Bearing state estimation and early failure identification pose significant challenges in the maintenance of direct-drive marine propulsion shafts driven by two-stroke marine Diesel engines. While bearing failures are infrequent, they are catastrophic, making their early prediction crucial for ensuring the reliability and safety of marine vessels. However, due to the complex operational dynamics and environmental conditions, accurately predicting bearing failures in advance is extremely challenging. In the present study, we focus on addressing this problem through a comprehensive approach tailored specifically for an actual bulk-carrier ship. A detailed model of the ship propulsion system is developed to simulate a wide range of possible bearing offsets, representing various operating states. Leveraging artificial intelligence techniques, we establish a correlation between deflection measurements obtained from strategically placed LVDT sensors and the operational bearing offsets, along with the corresponding bearing loads. To validate our approach, we first apply it to a small-scale laboratory model of the shafting system of the vessel, where experimental results confirm the efficacy of our methodology in predicting bearing states and loads. Subsequently, we outline the procedure for upscaling this methodology to the full-scale propulsion train of the ship, emphasizing the practical applicability and scalability of our method. By enabling early detection and prevention of bearing failures, our approach offers significant benefits in terms of enhancing operational reliability, minimizing downtime, and ensuring the safety of marine propulsion systems.

Problem Description and objectives

In the present study, we propose a novel approach that combines surrogate model development and real-time data analysis from sensors embedded in the shafting system to address the challenges of bearing state estimation and early failure identification in direct drive marine propulsion shafts. These surrogate models serve as the foundational dataset for training machine learning algorithms essential for state identification and performance assessment. The AI-driven system utilizes machine learning models to identify the current operating state of the system, predict potential upcoming failures, and optimize overall performance by maximizing safety margins and minimizing power losses.

Furthermore, we discuss the integration of additional data sources such as strain gauges, vibration sensors, and lubricant oil temperature sensors to provide a comprehensive overview of the system's health state. The development and training of machine learning models tailored for the specific tasks and challenges of real-time performance assessment in this complex,

[a] Presenting Author

coupled system are analyzed. This includes considering the geometrical characteristics, different rotational speeds, and external loads to calculate performance-operation maps of the bearings and shafting system. Necessary simplifications are made to account for hull deflections and propeller eccentric thrust, ensuring a more realistic representation during surrogate model development and analysis.

The research includes a specific case study detailing the preliminary analysis and development of surrogate models for a bulk-carrier ship. A preliminary lab-scale evaluation utilizing dimensional analysis provides crucial insights into optimal sensor placement onboard the vessel and enables correlation of measured values with modeled system states. This methodology is extrapolated to a large-scale application, where strategically placed LVDT sensors enable identification of the current operating shaft deflection state during the ship's sea trials.

Key findings of this study include the identification of crucial factors during the preliminary analysis phase, definition of appropriate operational margins aligned with class rules, and proposal of a two-layered approach for optimal sensor placement. Additionally, the study examines and evaluates various metrics and objective functions to establish a robust solution for performance assessment. This comprehensive analysis enhances understanding of operational conditions and contributes valuable insights towards formulating a resilient methodology for powertrain performance assessment in marine propulsion systems.

References

Choi, S. P., Lee, J. U., & Park, J. B. (2021). Application of deep reinforcement learning to predict shaft deformation considering hull deformation of medium-sized oil/chemical tanker. *Journal of Marine Science and Engineering*, 9(7), 767.

Li, R., Wang, J., Chen, Z., Wang, F., & Liu, Y. (2023). Study on the methods of measurement, optimization and forecast of propulsion shaft bearing load of ships. *Journal of Marine Science and Engineering*, 11(7), 1324.

Magalhães, D. L., de SS Martins, D. H. C., Castro, B. M., Vaz, L. A., Monteiro, U. A., & Gutiérrez, R. H. (2023). Machine learning performance comparison for main propulsive shafting systems alignment. *Ocean Engineering*, 280, 114556.

Theofilis, P., Rossopoulos, G. N., & Papadopoulos, C. I. (2023, March). Solution Space and Optimality Concerns for the Shafting System Alignment of a Typical Bulk Carrier. *SNAME International Symposium on Ship Operations, Management and Economics* p. D021S006R002.

Acknowledgements

This research work was conducted in the framework of the research Project “sPRISMoID,” titled: “Ship Predictive Intelligent Sensor Model Integrated Digitally” (T2EDK-02405), within the framework of the National Recovery Plan and Resilience “Greece 2.0” funded by the European Union—NextGenerationEU.

Keywords: Marine Engineering, Marine Shafting Systems, Performance Assessment, Surrogate Models, ML&AI, State Identification

Data-driven models for classification of insomnia and healthy sleep including the effects of sedentary behaviour on sleep quality derived from multi-night actigraphy data

Sunita Rani[1], Sergiy Shelyag[2,1] and Maia Angelova [3,1,4,*]

[1] Deakin University, Data Analytics Research Lab, E-mail: ranis@deakin.edu.au
[2] Flinders University University, College of Engineering and Mathematical Sciences, E-mail: sergiy.shelyag@flinders.edu.au
[3] Aston Digital Futures Institute, Aston University, Email: m.angelova@aston.ac.uk
[4]InstituteofBiophysicsandBiomedicalEngineering, BulgarianAcademyof Sciences

Abstract: Sleep and sedentary behaviour are integral components of human life profoundly affecting physical and mental health. Insufficient sleep can lead to health complications such as insomnia while sufficient sleep facilitates physical regeneration, restoration and memory consolidation. Sedentary lifestyles prevalent in modern society may exacerbate sleep disturbances. The purpose of this study is to investigate the intricate relationship between sleep and sedentary behaviour in adults suffering from acute and chronic insomnia as well as in healthy individuals. Leveraging publicly available actigraphy data from two sleep studies con- ducted with different actigraphy devices, this study addresses four key research questions through statistical and fractal analysis, machine learning (ML) and association matrices.

To begin with, the first objective of this study is to develop a ML method for distinguishing chronic insomnia from acute insomnia. The second objective of this study is to examine the patterns of sleep of individuals with chronic insomnia and their partners during the working week and on weekends. The third objective is to examine the sedentary patterns of individuals with acute insomnia and healthy adults during the daytime. As a final objective, we examine the relationship between sleep quality of previous night and sedentary activities on the following day as well as the relationship between sedentary activities during the day and the sleep quality of the following night using seven nights of actigraphy data.

Our findings highlight the efficacy of ML models in distinguishing between acute and chronic insomnia achieving an impressive 81% accuracy. A significant difference was observed between chronic insomnia and healthy sleep, possibly reflecting psycho-physiological adaptations. As a second finding of the study, the sleep patterns of people with chronic insomnia and their healthy partners differed slightly between weekdays and weekends. Additionally, it has been found that those with chronic insomnia have similar sleeping patterns as their healthy partners, therefore healthy partners may also experience some sleep disturbances as a result of their partner's disrupted sleep patterns. Compared with healthy adults, individuals with acute insomnia spend a significant portion of their sedentary time engaging in medium (6 - 30 minutes) and long (over 60 minutes) duration bouts. As a final note, this study indicates that sleep quality influences the sedentary behaviour of the following day and the sedentary behaviour in the preceding day in turn impacts sleep quality in the following night.

In summary, this study delves into the significant correlation between sleep patterns and sedentary behaviour. It aims to elucidate the intricate connections between these two factors. Crucially, this research utilizes readily accessible objectively measured data from physical activities of the individuals, ensuring that the developed models and findings can be applied to future screening efforts with wearable devices in the comfort of homw environment. These evidence-based AI models have the potential to guide healthcare strategies and improve overall health by facilitating early detection and personalized interventions.

Keywords: machine learning, data-driven models, sleep, insomnia, sedentary activity

* Presenting author

Adaptive Feedback in Generative ML for Time-Varying Systems

Alexander Scheinker [1, a], Reeju Pokharel [2]
[1] Los Alamos National Laboratory, ascheink@lanl.gov
[2] Los Alamos National Laboratory, reeju@lanl.gov

Time-varying systems, or systems with distribution shift are challenging for Machine learning (ML)-based techniques. The typical approach to distribution shift is to re-train the ML model with new data once the shift is significant. For such re-training approaches, many methods have been developed for efficiently weighing new data relative to previously seen training data. However, there are many applications in which we do not have the luxury of collecting new data to re-train because collecting new data is too slow or because collecting new data requires an invasive procedure that disrupts the normal operation of the system of interest. For example, in charged particle accelerator-based user facilities approximately once per month researchers might get a few hours of dedicated experimental beam development time to gather invasive data, such as beam images based on destructive measurements. However, such measurements are not available for most of the operational time as such measurements would interrupt all users. Therefore, after the first training set is collected, if the initial conditions of the beam change, we cannot measure them to simply re-train the models.

This talk presents recent results on incorporating techniques from model-independent adaptive feedback control theory within the architectures of deep generative models, to make them more robust for time-varying systems without relying on re-training. These general methods add to the foundation and methods underpinning modelling, data analytics, and AI, for complex time varying systems.

We present several studies of the approach. We show how the method can be used as a virtual diagnostic for charged particle beams in accelerators. In particular, we use generative models to predict all 15 unique 2D projections of the 6D (x,y,z,p_x,p_y,p_z) phase space distribution of intense relativistic charged particle beams in particle accelerators and show that we can robustly track them as the beam's unknown initial condition changes with time. We also show how the method can be used to speed up 3D coherent diffraction imaging (CDI) reconstruction techniques by generating the 3D electron density phase and density fields of unknown objects based only on diffraction intensity measurements and show that we can uniquely robustly track an unknown time-varying object.

Keywords:
Generative Machine Learning, Deep Learning, Adaptive Control, Time-varying Systems

[a] Presenting Author

Hybrid adaptive finite elements-neural networks framework for the simulation of laser melting processes

Alexandre Caboussat[1,*], Maude Girardin[1,2], Marco Picasso[2]

[1]Geneva School of Business Administration (HEG), University of Applied Sciences and Arts Western Switzerland (HES-SO), E-mail: alexandre.caboussat@hesge.ch, maude.girardin@hesge.ch
[2] Institute of Mathematics, Ecole Polytechnique F´ed´erale de Lausanne (EPFL), E-mail: maude.girardin@epfl.ch, marco.picasso@epfl.ch

Abstract:

Direct physics-based, simulations of laser melting or laser polishing processes are computationally expensive [1]. The underlying multi-physics problem couples the Navier-Stokes equations with the tracking of free surfaces, together with the heat equation with solidification. The design of a digital twin thus allows to obtain real-time simulation results, or to solve a large number of occurrences, for instance when tackling inverse problems for parameters identification.

We present a hybrid framework involving adaptive finite elements and deep neural networks to ultimately design a digital twin for laser melting and laser polishing processes. We start by considering a generic parametric partial differential equation

$$F(u(x;\mu);\mu) = 0, \qquad x \in \Omega, \quad \mu \in P$$

where Ω denotes the physical domain and P the parameters domain.

We consider a hybrid method to approximate the parameter-to-solution map $(x;\mu) \mapsto u(x;\mu)$ that relies on deep neural network approximations using data generated from finite element simulations to build the training set [2]. We assess the errors coming from both the finite element and the neural network sources to estimate the accuracy of the finite element method and of the neural network approximation over both the physical space Ω and the parameter space P. Our aim is to try to balance both errors, and to quantify the numerical effort required to train the neural networks to reach a given total accuracy.

More precisely, denoting by u_h and u_N the finite element and the neural network approximations respectively, the error can be decomposed into

$$||u - u_N||_{L^2(\Omega\times P)} \leq ||u - u_h||_{L^2(\Omega\times P)} + ||u_h - u_N||_{L^2(\Omega\times P)},$$

with a first contribution coming from the finite element approximation, while the second term is the approximation introduced by the neural network trained on finite element-based data. Adaptive finite element techniques based on a posteriori error estimates are introduced in the physical space to increase the accuracy of the data in the training set, homogeneously for all values of the parameters in the parameters domain.

Numerical results are presented for an elliptic model problem that mimics the modeling of the temperature in laser melting process in two space dimensions. The strategy to generate an appropriate training set is discussed. A derivative-free framework to solve inverse problems based on this hybrid method is detailed and relies on a particle-swarm optimization (PSO) algorithm. It allows to identify parameters related to both the material and the laser processes. Finally we introduce a computational framework for the solution of the full multi-physics problem. Preliminary numerical results are discussed.

Keywords: Materials science; Laser melting; parametric PDEs; neural networks; adaptive mesh refinement; parameter identification; Error estimates; finite element method;

---

* Presenting author

References

[1] A. Caboussat, J. Hess, A. Masserey, M. Picasso. 2023. Numerical simula- tion of temperature-driven free surface flows, with application to laser melt- ing and polishing. Journal of Computational Physics: X. Vol. 17, pp. 100127. https://doi.org/10.1016/j.jcpx.2023.100127

[2] A. Caboussat, M. Girardin, M. Picasso. 2024. Error assessment of an adap- tive finite elements-neural networks method for an elliptic parametric PDE. Com- puter Methods in Applied Mechanics and Engineering. Vol. 421, pp. 116784. https://doi.org/10.1016/j.cma.2024.116784.

Enabling Real-Time Multiscale Microstructure Characterization Using Machine Learning

Reeju Pokharel [1, a]

[1] *Materials Science and Technology Division, Los Alamos National Laboratory*, E-mail: reeju@lanl.gov

We examine the challenge of non-destructive real-time characterization of complex mesoscale microstructures and their evolution under in situ loading conditions. Current bottlenecks in data analysis limit instant feedback during in situ experiments, hindering real-time guidance of multiscale measurements. Here, we present machine learning approaches to accelerate on-the-fly analysis, for enabling guided in situ experiments at advanced light sources. Towards this goal, we demonstrate accelerated reconstruction of crystal orientations from diffraction data using deep learning and further refined using model-independent adaptive feedback to improve accuracy. Additionally, we present our recent work towards developing deep learning surrogate models of crystal plasticity to efficiently predict orientation and strain fields of materials undergoing tensile deformation. By integrating physics-based principles, we strengthen model generalizability, robustness, and transferability to new material systems and loading conditions. These surrogate models provide initial guesses for reconstructing microstructure evolution, which will aid in real-time feedback during experiments. The goal is simultaneous multiscale characterization with continuous model-guided feedback. This integrated approach will enhance our understanding of material dynamics across scales by closing the analysis loop.

Keywords: Deep learning, materials microstructure, mechanical properties

[a] Presenting Author

Model-based Reinforcement Learning for Optimal Inspection and Maintenance Planning

Prateek Bhustali*, **Charalampos P. Andriotis**

Faculty of Architecture and the Built Environment, TU Delft, Netherlands
E-mail: {P.Bhustali,C.Andriotis}@tudelft.nl

Abstract: Recent advances in deep reinforcement learning (RL) have fostered uptake in sequential decision-making problems, such as inspection and maintenance planning of deteriorating systems. Real-world maintenance problems characterised by component multiplicity, partial observability of system states, stochastic degradation, risk/budget constraints, etc., can be formulated as partially observable Markov decision processes (POMDP) to obtain near-optimal policies using DRL. Most works in this area leverage model-free deep RL (MFRL) algorithms to learn optimal inspection and maintenance policies, wherein the agent learns to act optimally by probing a simulated environment in a black-box fashion. Although successful, MFRL approaches require many interactions with the environment and often struggle to exhibit good trans- fer capabilities, which could lead to high sample complexity and lack of robustness in policy deployment. Model-based RL (MBRL) algorithms aim to alleviate these limitations by building internal representations of the environment, also termed world models, to facilitate policy and value learning, exploration efficiency, and transferability to related tasks [1]. However, MBRL agents can suffer from model bias, i.e., overfitting policies and value functions on inadequately learned world models during training, thereby causing a degra- dation in online performance. Recently, recurrent state space models, such as in DreamerV3 [2], have shown promising results in building world models using action-observation histories when solving POMDPs [3]. This approach can maximally exploit the learned world model for continuous control tasks, owing to their differentiability. Differentiable world models can provide straight-through gradients, also known as value gradients, which have lower-variance (albeit biased) policy gradients than sample gradients used in MFRL for behaviour learning. However, the straight-through gradient approach has been less successful, specifically in DreamerV3, when applied to discrete control tasks via continuous re-parameterization of discrete actions. In contrast, approaches such as gradient-based planners [2], have been demonstrated to perform well using similar re-parameterization schemes. In this work, we investigate this gap and propose algorithmic solutions to this problem in the context of maintenance planning, where the action space is typically discrete. We examine this for a prototypical five-component system in a deteriorating environment and contrast it against MFRL approaches.

Keywords: Inspection and maintenance planning, Model-based deep reinforcement learning, Partially observable Markov decision processes

* Presenting author

References

[1] Moerland, T.M., Broekens, J., & Jonker, C.M. (2020). Model-based Reinforcement Learning: A Survey. Found. Trends Mach. Learn., 16, 1-118.

[2] Hafner, D., Pa˘sukonis, J., Ba, J., & Lillicrap, T.P. (2023). Mastering Diverse Domains through World Models. ArXiv, abs/2301.04104.

[3] Lambrechts, G., Bolland, A., & Ernst, D. (2023). Informed POMDP: Leveraging Additional Information in Model-Based RL. ArXiv, abs/2306.11488.

Predicting Premature Failure in Quantum Cascade Lasers Using a Support Vector Machine Classifier

A. Cagri Aydinkarahaliloglu [1], Arifin Nur Alif [1], Xiaojun Wang [2], Mariano Troccoli [3], and Anthony J. Hoffman [1, a]

[1] University of Notre Dame, Notre Dame IN USA
[2] Adtech Photonics Inc., City of Industry CA USA
[3] Evolution Photonics, Inc., Pasadena, CA USA

Laser lifetime impacts the total cost of ownership of quantum cascade lasers (QCLs). Previous studies of these mid-infrared (/∴ ~ 3 – 30 μm) electrically injected lasers estimate the lifetime as longer than 800,000 hours [1-3]. However, these device lifetimes are only for lasers that survive an initial operation period that is typically on the order of hundreds of hours. Failure within this period is referred to as premature failure, and establishing processes for identifying devices that fail prematurely is essential for further development, commercialization, and integration of QCLs.

One strategy to identify QCLs that exhibit premature failure is to develop a process where the lasers are operated and monitored for sufficiently long times to detect the actual failures. In this so-called burn-in process, a trade-off exists between the length of the process and the likelihood of identifying devices that exhibit premature failure. Long burn-in processes are expensive and can limit the production rate of QCLs. Short burn-in times however will not identify enough of the devices that fail prematurely. An alternative approach is to *predict* premature failure using standard electrical and optical measurements of the QCL during the burn-in process.

In this work, we show how a classifier based on a support vector machine (SVM) can be used to predict premature failure. SVMs are one approach to supervised machine learning [4, 5]. The objective of a SVM is to build and train a two-class model using training data consisting of an input data set that is labeled with the correct class. The trained SVM is then used to classify unknown data into one of the two classes. The SVM we train classifies light-current-voltage (LIV) measurements as coming from a device that is operational or inoperative after 400 hours. Using the SVM as a classifier, we predict premature failure as much as 319 hours before the actual failure of a QCL. By identifying the devices likely to fail early in the burn-in process, the total cost of ownership can be reduced. Furthermore, identifying devices before the failure event can enable additional research on the physical mechanisms influencing premature failure in QCLs.

In total, 50 QCLs undergo an accelerated burn-in process where the QCL is operated at an elevated temperature and an SVM-based classifier is used to predict the status of the device after 400 hours of operation. We emphasize that the accelerated burn-in process can be significantly shorter than 400 hours. The QCLs are designed to emit at 4.6 μm and are from two epitaxial wafers grown via metal organic chemical vapor deposition. The QCLs wafers have distinct active region and waveguide designs. The lasers vary in length from 3.8 to 5.0 mm and have ridge width varying between 9 and 14 μm. During the

[a] Presenting Author Email: ajhoffman@nd.edu

burn-in process, the lasers are operated at a heat sink temperature of 30 °C in continuous-wave (CW) mode at 80% of their peak optical power. The CW LIV characteristics of the QCLs are measured throughout the burn-in process with intervals between measurements from 2.5 to 48 hours. The QCLs are tested for 400 hours or until the device fails. Fig. 1 shows every LIV measurement recorded for nine QCLs, over 500 measurements. Here, the green curves are from devices that are operational after 400 hours of testing and the red curves are from devices that fail before 400 hours of testing. There are no readily apparent features that indicate the status of the device after 400 hours. Similar to these nine devices, no trends are observed across the full data set of 50 QCLs.

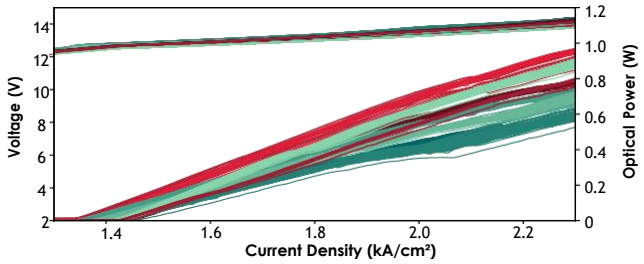


Fig. 1. Measured voltage and optical power versus current density curves for nine QCLs. The green curves are for devices that are operational at the end of testing (five devices) and the red curves are for devices that are inoperative (four devices).

A SVM classifier is trained and tested using the LIV measurements obtained during the burn-in process. We treat each LIV as an independent measurement—there are no relationships between LIV measurements from the same device. For each LIV, we extract 14 features that describe the measurement. These features include the threshold current density, applied voltage at lasing threshold, slope efficiency, peak optical power, and more.

The LIVs are divided into training and testing groups by device. We emphasize that all the LIVs from a single device are assigned exclusively to the training or testing group—LIVs from a single device are never mixed between the groups. During training and testing, the LIVs of a single device are classified according to the operational status of the device at the end of the 400-hour testing period. For a device that fails during testing, all the LIVs are classified as belonging to an inoperative device. Likewise, for a device that is operational at the end of testing, all the LIVs for that device are assumed to come from an operational device.

We use a radial basis function kernel with two hyperparameters in our SVM. The hyperparameters are determined using a grid search method where we create 504 different pairs of hyperparameters for the SVM. We define our SVM classifier to label QCLs that have at least one LIV categorized as belonging to a failing device as a laser that will exhibit premature failure.

We evaluate the SVM classifier by calculating the true positive rate (TPR) and true negative rate (TNR) versus the hypothetical burn-in time. The TPR is the ratio of the number of devices predicted to be operational after 400 hours of operation to the number of operational devices at the conclusion of 400 hours of operation. The TNR is the ratio of the number of devices predicted to fail before 400 hours of operation to the number of devices that fail within the 400 hour testing period. Fig. 2 shows the TPR

and TNR when the SVM is trained on devices from both quantum designs. When all the LIV

measurements are included (dashed curves), the TPR approaches ~60% for long hypothetical burn-in periods. We attribute this drop in the TPR to temporal changes in the device electrical and optical characteristics early in the device testing. The time scale for these significant and rapid changes is approximately 20 hours, which can potentially be attributed to annealing of defects inside the QCL or annealing of the electrical contacts. When we exclude the first 20 hours of LIV measurements from the data set (both training and testing), the TPR improves significantly and remains 100% until approximately 40 hours of operation. The TNR at 40 hours is approximately 50%, which is 7x greater than the TNR for conventional burn-in processes. While these results are obtained by training on both quantum designs, we observe similar results when training the SVM on a single quantum design, which could be used to identify potential mechanisms of premature failure in the lasers.

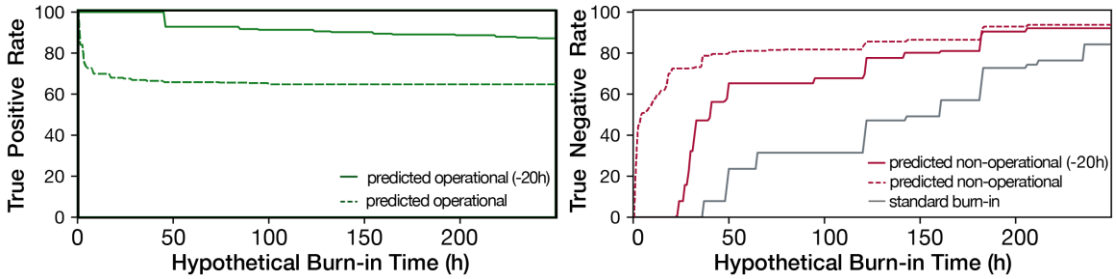


Fig. 2. Calculated true positive rate (blue) and true negative rate (red) for the QCLs classified using the SVM. The results for a standard burn-in process are shown in gray. The dashed curves are when all LIVs are included in training and testing sets. The solid curves are when the first 20 hours of testing are excluded.

In this work we demonstrate a classifier for predicting premature failure in QCLs using a supervised learning algorithm. Our approach the accelerated burn-in testing significantly outperforms conventional approaches which rely on observing the failure of the device. We show that after 40 hours of accelerated burn-in testing, the TPR is 100% (i.e. no good devices are misclassified) and the TNR is 7x greater than conventional approaches. The ability to predict premature failure 10's to 100's of hours in advance can reduce the cost of ownership of QCLs and enable additional studies on the mechanisms leading to premature failure.

References

[1] F. Xie, H.-K. Nguyen, H. Leblanc, L. Hughes, J. Wang, D. J. Miller, and K. Lascola, *Novel In-plane Semicond. Lasers XVI* 101231J (2017).
[2] A.A. Lyakh, R. Maulini, A.G. Tsekoun, C.K.N. Patel, Opt. Eng. **49**, 11105 (2010).
[3] T. Myers, B. Cannon, C. Brauer, M. Phillips, M. Taubman, and B. Bernacki, SPIE Proc. 9836, 98362J (2016)
[4] C. Cortes and V. Vapnik, *Mach. Learn.* **20**, 273–297 (1995).

Natural Language Querying for Spatio-Temporal Data Analytics

Yuri Bogomolov[1,*], **Stanislav Sobolevsky**[1,2]

[1]Masaryk University, E-mail: 533441@mail.muni.cz
[2]New York University

Abstract: Urban datasets, characterized by their complex spatial and temporal components, are crucial for city planning and management. The analysis of these datasets provides insights into urban dynamics, enabling planners to make informed decisions regarding infrastructure development, environmental sustainability, and public services optimization. However, the complexity and volume of urban data pose significant challenges for non-technical users, such as city planners, in accessing and interpreting this information effectively. This paper introduces an innovative approach to building a natural language interface for complex urban datasets.

With the advances in Large Language Models (LLMs) text-to-SQL solutions became the main direction of Natural Language Interfaces for analytical systems. Prior research primarily focused on extracting question- to-SQL patterns and training encoder-decoder models using Text-to-SQL corpora. However, the recent paradigm shift towards LLMs, such as GPT-4, has presented a new set of challenges, primarily centered around prompt engineering, to elicit accurate SQL queries from these models [1].

The core problem in LLM-based Text-to-SQL solutions lies in prompt engineering, encompassing question representations, example selection, and organization. Previous studies have made notable progress but lack a systematic exploration of these components [2]. Other challenges include adapting large language models to understand SQL syntax and semantics, handling variability in database schemas, designing effective prompts, incorporating database knowledge, and achieving generalization across different domains [3, 4].

Applying Text-to-SQL approaches to spatial analysis poses several challenges due to the unique nature of spatial data and the complexities involved in processing and querying such data within databases. Some of the challenges include:

- Spatial Data Representation: Spatial data often includes complex geometries and spatial relationships. Converting natural language queries into SQL queries requires representing spatial concepts in a structured format understandable by SQL. Designing a suitable representation for spatial entities, such as points, polygons, or spatial relationships like containment or proximity, in natural language poses a significant challenge.
- Handling Geometric Operations: SQL queries for spatial analysis often involve complex geometric operations (e.g., spatial joins, buffers, overlays). Expressing these operations in response to natural language queries and ensuring accuracy in their execution through Text-to-SQL models is challenging due to the intricate nature of these operations.
- Limited Training Data for Spatial Queries: Obtaining large and diverse training datasets for spatial queries in natural language is challenging. Training Text-to-SQL models to understand and generate SQL queries for spatial analysis accurately requires extensive and varied data, which might not always be readily available.

Our previous paper proposed a specialized data model for networks with spatial and temporal dimensions [5]. In this paper, we present a generic approach to building Natural Language Querying capabilities for domain-specific data models. The specialized data model approach provides multiple advantages:

- The data retrieval API provides a way to identify the right data source automatically.
- Domain-specific filtering and aggregation API simplifies the code generation step.
- The ability to convert a dataset into a standard network, a time series, or a geospatial object functions as a common denominator and bridges the gap between different types of analytical queries.
- Rich visualization functionality provides an intuitive way to explore the data.

The combination of these items enables building an end-to-end analytical system that can process queries, like: ”plot a New York choropleth map by the number of outgoing yellow taxi passengers in December 2023” and a few seconds later receive an interactive map presented in figure 1. We also compare our solution with the state-of-the-art solutions for generic Natural Language Querying (Data Analyst based on GPT4).

Keywords: Natural language querying, Spatio-temporal transactional networks, Urban networks

* Presenting author

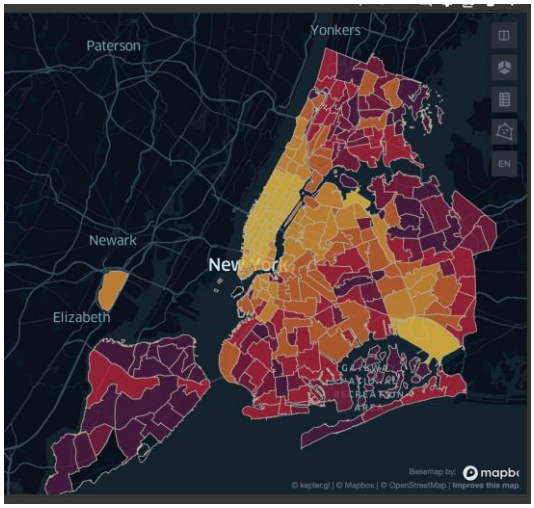


Figure 1: New York City districts by the number of outgoing taxi passengers in December 2023.

References

[1] Mohammadreza Pourreza and Davood Rafiei. Din-sql: Decomposed in-context learning of text-to-sql with self-correction. arXiv preprint arXiv:2304.11015, 2023

[2] Shuaichen Chang and Eric Fosler-Lussier. How to prompt llms for text-to-sql: A study in zero-shot, single-domain, and cross-domain settings. arXiv preprint arXiv:2305.11853, 2023

[3] Linyong Nan, Yilun Zhao, Weijin Zou, Narutatsu Ri, Jaesung Tae, Ellen Zhang, Arman Cohan, and Dragomir Radev. Enhancing few-shot text-to-sql capabilities of large lan- guage models: A study on prompt design strategies. arXiv preprint arXiv:2305.12586, 2023

[4] Chunxi Guo, Zhiliang Tian, Jintao Tang, Pancheng Wang, Zhihua Wen, Kang Yang, and Ting Wang. A case-based reasoning framework for adaptive prompting in cross-domain text-to-sql. arXiv preprint arXiv:2304.13301, 2023.2

[5] Yuri Bogomolov and Stanislav Sobolevsky. A Scalable Spatio-Temporal Analytics Framework for Urban Networks. Fifth Networks in the Global World Conference. Cham: Springer International Publishing, 2022.

Last-piece exploring model operator networks

Suguru Shiratori[1,*], So Yamashita[2], Kakeru Ishizawa[2], Taisei Kato[1], Hideaki Nagano[1], Kenjiro Shimano[1]

[1]Tokyo City University, E-mail: sshrator@tcu.ac.jp
[2]Graduate School, Tokyo City University

Abstract: This study proposes a new architecture of neural networks, that learns an operator for missing parts of governing equations (GE) for physical systems. The proposed network is composed of physics-informed neural networks (PINNs) and DeepONets. The prescribed part of GE is calculated by the automatic differentiation with PINNs, and the remaining part of GE is predicted through DeepONets. The loss function is defined as the sum of the unsupervised loss of GE and the supervised loss of observation. It is confirmed that the proposed method can predict the hidden convective term in the Burgers equation.

Keywords: Missing physics inferring, PINNs, DeepONets

* Presenting author

1 Motivation

In the process of modeling and simulation of complex nonlinear physical systems, the governing equation (GE) is preliminary formulated, and part of the GE is reformulated for a better prediction of the real-world observation. For learning the physical model from the observed data, some methodologies have been proposed, for instance, Neural ODE [1] or Hamiltonian Neural Networks [2]. However, these methods are designed to learn the physical model that describes the total system. In many engineering problems, it is rare that nothing is known about the GEs, and it is also rare that the GEs are completely known. Since dominant physics can be identified through some easy observations, the actual task is to find the remaining missing physics. For learning of operators for a missing part of GE, this study proposes a new architecture of neural networks, named as *last-piece exploring model operator networks* (LEMON).

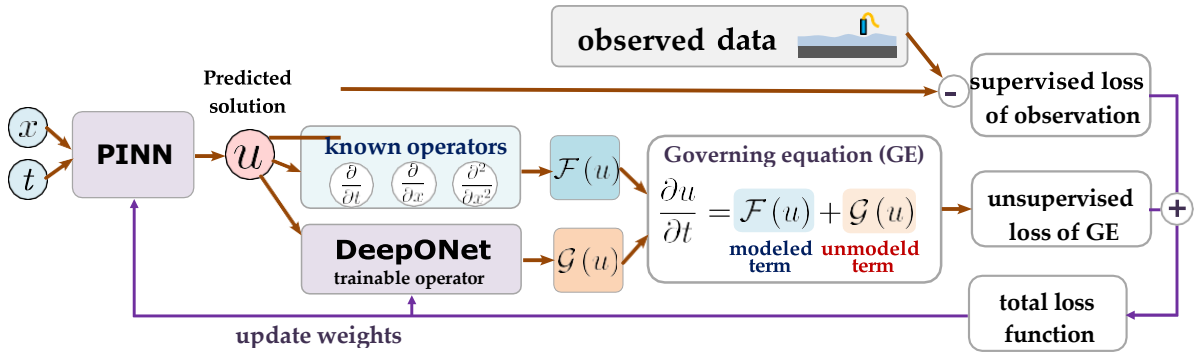


Figure 1: Architecture of proposed LEMON that learns missing part of governing equations.

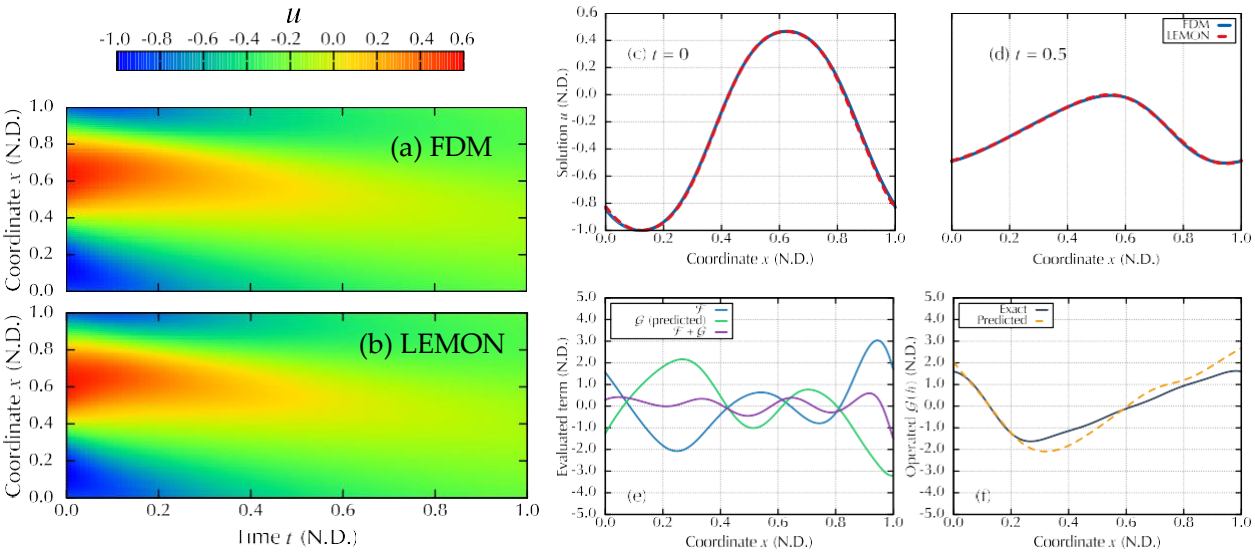


Figure 2: How the LEMON predicted hidden convective term in Burgers equation. (a) The spatio-temporal variation of the solution u(t, x) predicted by (a) finite difference methods and (b) LEMON. The selected snapshots of the instantaneous spatial distribution at (c) t = 0 and (d) t = 0.5. (e) The prescribed part (blue) F, hidden part G (green) and total (violet) of the governing equations. (f) The exact (dark blue) and predicted (orange) hidden part G for the data not involved in the training data.

2 Proposed architecture for missing physics learning

As shown in **Fig. 1**, the LEMON is composed of mainly physics-informed neural networks (PINNs) [3] and DeepONets [4]. The prescribed part of GE is calculated by the automatic differentiation with PINNs, and the remaining part of GE is predicted through DeepONets. The total loss function is defined as the sum of the unsupervised loss of GE and the supervised loss of observation.

The proposed method was validated through the one-dimensional Burgers equation

$$F(u) + G(u) = 0, \qquad F(u) = \frac{\partial u}{\partial t} - D\frac{\partial^2 u}{\partial x^2}, \qquad G(u) = u\frac{\partial u}{\partial x},$$

where the convective term $G(u) = u\partial u/\partial x$ is treated as a missing term. The results are summarized in **Fig. 2**.

References

[1] Ricky T. Q. Chen, Yulia Rubanova, Jesse Bettencourt, and David Duvenaud. Neural ordinary differential equations. In *NeurIPS*, 2018.

[2] Yuhan Chen, Takashi Matsubara, and Takaharu Yaguchi. Kam theory meets statistical learning theory: Hamiltonian neural networks with non-zero training loss. *Proc. AAAI Conference on Artificial Intelligence*, 36(6):6322–6332, June 2022.

[3] M. Raissi, P. Perdikaris, and G.E. Karniadakis. Physics-informed neural networks: A deep learning framework for solving forward and inverse problems involving nonlinear partial differential equations. *J. Comp. Phys.*, 378:686–707, 2019.

[4] Lu Lu, Pengzhan Jin, Guofei Pang, Zhongqiang Zhang, and George Em Karniadakis. Learning nonlinear operators via deeponet based on the universal approximation theorem of operators. *Nat. Mach. Intell.*, 3(3):218–229, March 2021.

L1-Approximation of supply curves

Andrés M. Alonso [1, a], Zehang Li [2]

[1] Universidad Carlos III de Madrid, E-mail: andres.alonso@uc3m.es

[2] Universidad Carlos III de Madrid, E-mail: zehang.li@alumnos.uc3m.es

In liberalized electricity markets, production companies offer blocks of energy at different prices, generally related to their marginal costs, at specific times of the day. The system operator brings together all the offers (energy blocks) and their corresponding prices to form the supply curve from which the marginal price of each hour will be obtained. These curves are step and non-decreasing functions, with as many steps as there are different prices in the set of offers for each hour.

In this project, we illustrate the computation of the approximation of the supply curves using a one-step basis. We study the L1 approximation and propose two procedures for the selection of nodes of the approximation. The L1 approximation is formulated as a linear programming problem and the selection of nodes is formulated as a mixed–integer programming problem. We provide a simple procedure to solve this linear programming problem that, as a byproduct, allows us to propose a dyadic search for nodes.

We illustrate the use of this approach using the supply curves from day-ahead Spanish electricity market. It is shown that the proposed approach obtains a better, much more parsimonious approximation than other alternatives that assume smoothness of the supply curves.

Keywords: electricity market, supply curve, approximation, linear programming, mixed-integer programming.

[a] Presenting Author

Step-by-step Learning

Andrés M. Alonso [1, a]
[1] Universidad Carlos III de Madrid, E-mail: andres.alonso@uc3m.es

The natural or generational learning process consists of building models based on available experiences. Each generation learns from the models obtained by its predecessors and gets a new model for its own batch of experiences. In this project, we discuss this step-by-step learning procedure for supervised classification and regression problems on large datasets.

We assume that the learning procedure is performed in G steps or generations. The g-th generation has its own data set, $D_g = \{X_{i,g}, Y_{i,g}: i = (1,2, \ldots, n_g)\}$, and also knows the models, $\{M^{(1)}, M^{(2)}, \ldots, M^{(g-1)}\}$, estimated by the preceding generations. The result of training the step-by-step learning model is a set of estimated models, $\{M^{(1)}, M^{(2)}, \ldots, M^{(G)}\}$. The set of features of the model $M^{(g)}$ has, at least, one more feature than model $M^{(g-1)}$, since the prediction obtained with that model was incorporated.

Using eight large real data sets, we show that the stepwise learning procedure performs competitively with respect to the approach using a single model for the entire data set.

Keywords: Machine learning, batch processing, federated learning, regression, supervised classification.

[a] Presenting Author

Robustness and Variability Analysis for Hardware Neural Networks

Zhihao Chen[1,a], Amin Farjudian[2], J. C. Greer[1,3]
[1] Department of Electrical and Electronic Engineering,
University of Nottingham Ningbo China E-mail: zhihao.chen@nottingham.edu.cn
[2] School of Mathematics, University of Birmingham
E-mail: a.farjudian@birmingham.edu.uk
[3] Nottingham Ningbo China Beacons of Excellence Innovation and Research Institute
E-mail: jim.greer@nottingham.edu.cn

Hardware neural networks (HNNs) offer advantages for applications requiring high energy efficiency, fast compute time, and a small circuit footprint [1]. On the other hand, HNNs suffer from lower levels of accuracy compared to software NNs largely due to component variability at the physical level. A HNN design is studied using a standard crossbar topology for multiply and accumulate (MAC) operations with a novel two-transistor (2T) circuit originally introduced to provide a RELU activation function (AF) [2]. The 2T circuit is generalized to allow generation of a set of AFs that can be approximated by a piece-wise linear (PWL) function $\alpha(v_i; v_-, v_+)$ given by

$$\alpha(v_i; v_-, v_+) = \begin{cases} v_- & v_i \leq v_- \\ v_i & v_- < v_i < v_+ \\ v_+ & v_+ \leq v_i \end{cases}$$

with v_i the input to circuit, v_i, v_+ are lower and upper saturation limits, respectively. The circuit is capable of approximating a variety of activation functions such as ReLU, ReLU6, and a hard-hyperbolic tangent ($\tanh_H$). However, unlike the PWL model, the circuit activation provides a differentiable transition near the saturation limits. The circuit's approximation to a $\tanh_H$ AF is considered in this work with $-v_- = v_+$.

A digitized version of the hardware AF from the 2T circuit is used to compare to ideal AFs used in identical neural networks (NNs)[i]. The HNN is implemented as a NN software model as well as by explicit circuit simulation. Training with the MNIST database using an ideal NN with ReLU, hyperbolic tangent, and hard hyperbolic tangent AFs, as well as the digitized hardware AF, is performed. From the simulations, it is found that the 2T circuit performs well compared to all three of the ideal AFs for training loss. For accuracy loss, it is found that the tanh, $\tanh_H$, and digitized hardware AF perform at a comparable level whereas ReLU performs poorly. Hence with ideal components, the HNN can achieve comparable performance to a software implementation of the NN.

[a] Presenting Author

Next, simulations using the NN model are performed by varying the weights and biases by gaussian distributed random variables selected corresponding to resistor variations in the MAC circuit due to component tolerances. In a similar fashion, simulations are performed to model variability in the hardware AFs throughout the network. From the simulations, the allowable component variation in the MAC and AF, as well as their interplay, versus acceptable values of test loss and accuracy is quantified for simple characterization and regression examples.

Variability of the hardware components needs to be accounted for during the design of a network architecture, and for the training phase selection and development of training algorithms capable of responding to uncertainties in the hardware-defined weights, biases, and circuit AF is needed.

[1] Measuring the algorithmic efficiency of neural networks, D. Hernandez and T. B. Brown, arXiv preprint arXiv:2005.04305 (2020)

[2] A CMOS rectified linear unit operating in weak inversion for memristive neuromorphic circuits, B. Li and G. Shi, Integration, **87,** pp. 24-28 (2022)

[i] The NN consists of 784 input neurons, 28 and 14 neurons in the first and second hidden layers, respectively with ten Softmax output neurons after the logits layer [784 × 28 × 14 × 10].

A surrogate model for the design of offshore monopile foundations

Y. Yang [1, a], P. Tantivangphaisal [1], A. Ruiz López [1], D.M.G. Taborda [1]
[1] Imperial College London, London, UK, E-mail: yunxiang.yang22@imperial.ac.uk

Keywords: Offshore geotechnics; machine learning; surrogate model; Support Vector Regression

1 INTRODUCTION

Despite significant advances in computational power, engineering design processes can still be constrained by the large simulation times involved in 3D Finite Element (FE) analysis. This is certainly the case in geotechnical engineering, where FE analysis tends to be highly nonlinear due to the complex constitutive models that are required to simulate soil behaviour realistically. In this context, surrogate models offer a powerful alternative to streamline design processes in geotechnical engineering. Through the adoption of machine learning techniques, these models can approximate the behaviour of an underlying FE model with sufficient accuracy to be employed in design while being orders of magnitude faster to run than numerical models. This study demonstrates the feasibility of using surrogate models for the predesign of offshore monopile foundations, at the stage where the geometry is optimised based on the monopile's load-displacement response. To this end, a Support Vector Regression (SVR) model is adopted to mimic the load-displacement response of the monopile foundation.

2 DESCRIPTION OF THE NUMERICAL MODEL

The numerical analysis consisted of a lateral pushover test on a monopile adopting the Dunkirk site characteristics; the analysis was conducted in PLAXIS 3D. The setup of the 3D model followed that outlined by Taborda et al. (2020) with Dunkirk sand being simulated with the state-parameter dependent small-strain stiffness sand model proposed by Taborda, Pedro & Pirrone (2022). The lateral load in all analyses was continuously increased up to a displacement at mudline level of 15% of the pile diameter. A total of 500 analyses were carried out adopting different pile geometries (embedded length, diameter and thickness); Latin Hypercube Sampling was used to define the dimensions to be adopted by each of the analyses adopting bounds for each dimension informed by design experience.

3 GENERATION OF THE SURROGATE MODEL

Prior to any training, the displacements were normalised by the pile diameter and all the load-displacement curves were represented by 20 discrete points located at the same normalised displacements for all curves, ensuring a consistent dataset.

The SVR model from the scikit-learn library (Pedregosa et al., 2011) was employed in this study. The model was trained to predict the load at a normalised displacement at mudline

[a] Presenting Author

level given the diameter, embedded length and thickness of the monopile; the inputs were scaled before training using MaxAbsScaler (Pedregosa et al., 2011). The dataset was divided into an 80:20 ratio for training and testing purposes, respectively. The SVR hyperparameters were fine-tuned adopting an optimisation algorithm along with cross-validation. The final SVR hyperparameters were determined as: $CC = 19989.524$; $\epsilon\epsilon = 0.496$; $ggggmmmmgg =$ '$ssssggssss$'; and '$rrrrrr$' kernel. Figure 1 shows that both training and testing results are remarkably similar, with a coefficient of determination R^2 reaching 0.9998 for both cases. A learning curve generated during training of the model showed that, with approximately 170 analyses, the SVR model provided a satisfactory level of accuracy. Additionally, parametric studies were performed to gain deeper insights into the contribution of each input to the pile behaviour.

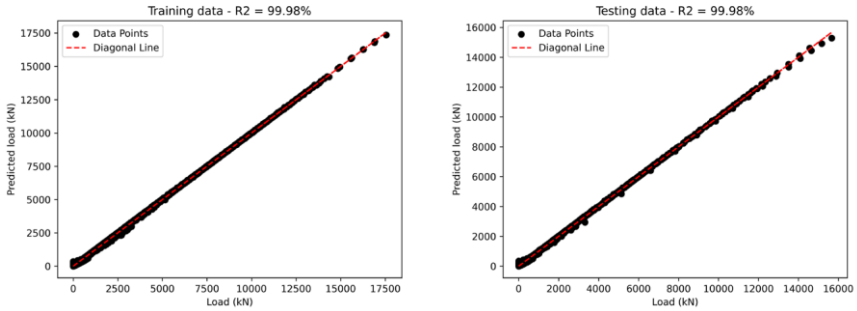


Figure 1: Comparison of the predicted results from training & testing dataset

4 CONCLUSIONS

This study investigates the feasibility of applying a SVR model to simulate the monopile load-displacement curve. The developed surrogate demonstrates its promising potential for practical application in real design scenarios.

5 ACKNOWLEDGEMENTS

The authors gratefully acknowledge the financial support provided by the Department of Civil and Environmental Engineering at Imperial College London, through a Dixon scholarship for the first author's PhD research.

REFERENCES

Pedregosa, F., Varoquaux, G., Gramfort, A., Michel, V., Thirion, B., Grisel, O., Blondel, M., Prettenhofer, P., Weiss, R. & Dubourg, V. (2011) Scikit-learn: Machine learning in Python. *The Journal of Machine Learning Research.* 12 2825-2830.

Taborda, D. M., Pedro, A. M. & Pirrone, A. I. (2022) A state parameter-dependent constitutive model for sands based on the Mohr-Coulomb failure criterion. *Computers and Geotechnics.* 148 104811.

Taborda, D. M., Zdravković, L., Potts, D. M., Burd, H. J., Byrne, B. W., Gavin, K. G., Houlsby, G. T., Jardine, R. J., Liu, T. & Martin, C. M. (2020) Finite-element modelling of laterally loaded piles in a dense marine sand at Dunkirk. *Géotechnique.* 70 (11), 1014-1029.

Towards producing innovative engineering design concepts using AI

Imelda Friel[1a], Andrew R. Colligan[1], Simon Hickinbotham[2], Rahul Dubey [2], Trevor Robinson[1], Mark Price[1], Andy Tyrrell[2]

[1] Queen's University Belfast, E-mail: i.friel@qub.ac.uk

[2] University of York, E-mail: simon.hickinbotham@york.ac.uk

Introduction

The discovery of innovative engineering design concepts is difficult and costly. Typically, a design is created, modelled and simulated by skilled engineers who make design decisions based on simulation results. Experience and subject knowledge play a major role in interpreting these results and making the decisions, and consequently, as the same knowledge, experience and tools are used to develop new designs, each new generation is similar to the last, and so stagnates innovation. Artificial intelligence (AI) is beginning to inform engineering design processes [1-3]. A promising technology is generative design (GD) which allows engineers to explore and select more innovative designs through the use of processes such as topology optimisation. Evolutionary algorithms (EAs) are a form of AI that can produce innovative design concepts by creating a population of possible designs and updating these over many generations through permutations of the design's parameters, mimicking nature's processes of evolution such as selection and mutation. Alongside EAs, neural networks (NN) are layers of connected neurons, each with different weights and biases relating inputs to outputs, where the mapping from inputs to outputs are refined through learning processes. The NN can be seen as a decision process where inputs (results of engineering simulations) are intepreted to create an output (design changes), and thus have the potential to control design.

This paper examines the application of a novel Evolutionary-Development (Evo-Devo) system that integrates AI tools within the conceptual design process to produce populations of innovative design options. The aim is to allow the behaviours of designs to be learned and then exploited later in the design process. Here a design concept (referred to as an organism) is constructed from cells, which have an evolving NN architecture controlling each cells'parameterisation. The following work demonstrates the application of the Evo-Devo process on a volume-to-point heat transfer problem, returning design concepts with a network of heat channels that direct heat built up in the plate to a point at ambient temperature.

Evolutionary-Development Design System

The Evo-Devo system consists of a development cycle embedded within an evolutionary loop. The evolutionary loop uses NSGA II [4], a multi-objective EA, creating populations of genomes which encode rules and policies and are evolved using typical evolutionary processes, including selection, crossover, and mutation. These rules describe the design behaviours given a set of input values or cell state. Specifically, an extended version of NEAT [5] represents the genome as real value encoded networks, as well as supporting both model complexity and being computationally efficient. The genome acts on the parameters of a cell it is associated with, the

[a] Presenting Author

topology and geometry of which represents the physical form of the design and hence are used to build a simulation model for performance evaluation. Simulation results are inputs to the network, the outputs of which are directly applied to the cell's parameters, creating geometric or topological changes. An instance of these changes is a development step, of which multiple become the development cycle of the Evo-Devo system.

In the following example, the organism is a volume, modelled as a flat plate, discretized into triangles. The volume is modelled using 2D shell elements (cell) with thickness (parameter), and the channels as 1D beam elements (cell) with a circular cross-section and area (parameter). The two are connected via the shared nodes of the beams and shells. The environment includes two distributed heat fluxes of different magnitude applied to different zones of the plate, with the sink temperature at a point, P on one outer edge, shown with the resulting temperature distribution in Figure 1(a). The design goal was to create design options with minimal average temperature across the plate and minimal channel volume within the plate, i.e., maximize cooling with minimal intrusive conductive volume. Figure 1(b) shows two organisms produced by the system. It can be seen that; 1) the organisms have developed to include a connected channel network; 2) the thickness of the channels increases towards the sink point, reflecting the accumulation of thermal load and 3) the channel volume is directed toward the hottest area of the plate. It should be noted that the neural network has learned to direct the design in this way, i.e., develop channels towards areas of higher temperature whilst distributing volume across the network from high to low, away from the heat sink.

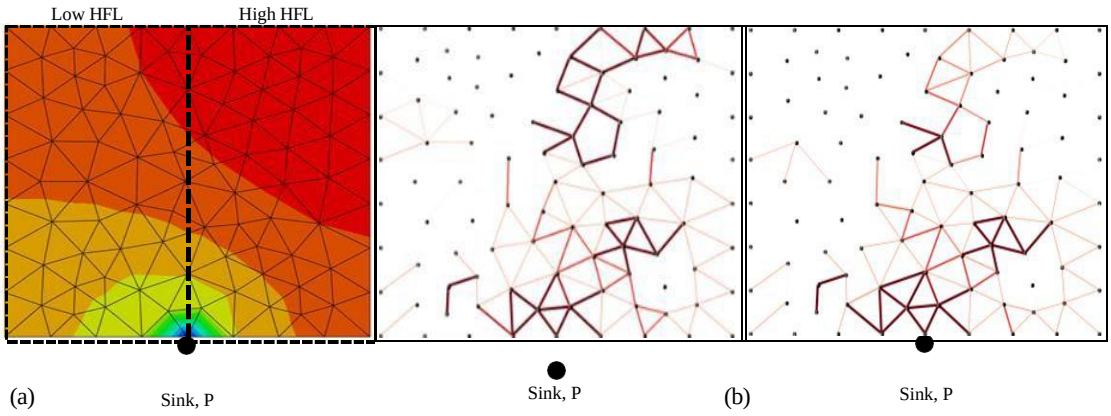


Figure 1 (a) Organism without channels, showing heat flux application, sink point and temperature distribution (b) Channel network in evolved organisms, showing sink point. (Darker colour represent thicker cross-section)

For the system to perform in this way, there are numerous considerations to be made when setting up the GRN, defining the evolutionary criteria and selecting the modelling parameters and simulation variables. The success of the genome, the rules and knowledge of the organism's behavior within the environment, which this work intends to capture, are beholden to the definition of these parameters and variables. This work successfully demonstrates the Evo-Devo system in a volume-to-point thermal conduction problem as a step towards capturing innovation during the conceptual design phase.

Keywords: Evolutionary Development, Engineering Design

References

[1] https://www.autodesk.co.uk/products/fusion-360/features#generative-design

[2] https://www.ntop.com/software/capabilities/generative-design/

[3] https://www.ptc.com/en/technologies/cad/generative-design

[4] Deb, A. Pratap, S. Agarwal and T. Meyarivan, "A fast and elitist multiobjective genetic algorithm: NSGA-II," in IEEE Transactions on Evolutionary Computation, vol. 6, no. 2, pp. 182-197, April 2002, doi: 10.1109/4235.996017

[5] Stanleyandm K.O., Miikkulainen, R., “Evolving neural networks through augmenting topologies.” Evol. Comput., vol.10, no.2, pp.99–127,2002. [Online]. Available: http://dx.doi.org/10.1162/106365602320169811

Development of a Hybrid Model to improve the Scale-Up of Decanter Centrifuges

Ouwen Zhai [1, a], Hermann Nirschl[2], Marco Gleiss[3]
[1] Karlsruhe Institute of Technology, E-mail: ouwen.zhai@kit.edu
[2] Karlsruhe Institute of Technology, E-mail: hermann.nirschl@kit.edu
[3] Karlsruhe Institute of Technology, E-mail: marco.gleiss@kit.edu

Continuous solid bowl centrifuges such as decanter centrifuges are widely used in the chemical and mineral processing industries to separate finely dispersed particles from a continuous liquid phase. The state-of-the-art method of designing decanter centrifuges is based on steady-state models that are highly simplified. Dynamic events within the apparatus, such as the sediment build-up and compaction or the hindered settling phenom, are not considered by these models. As a result, manufacturers must perform time-consuming pilot scale experiments and derive their own correction factors to compensate for the inaccuracies of the models.

A promising alternative modeling approach is the use of a hybrid model. In general, three primary modeling approaches exists: White Box Models (WBMs), Black Box Models (BBMs) and Grey Box Models (GBMs). WBMs are fully transparent parametric models. Aside from computationally intensive, high-fidelity simulation methods such as Computational Fluid Dynamics, Reduced Order Models can produce comparably accurate predictions with significantly lower computational times. However, the lower computational effort is often achieved by making assumptions in the model that can lead to inaccuracies. In contrast, BBMs, such as Artificial Neural Networks (ANNs), can be used without having a priori knowledge of the process. Given the absence of physical information, the predictive accuracy of BBMs relies solely on both the amount and quality of data available. In addition, BBMs are not suitable for extrapolation tasks. GBMs are hybrid models which combine a WBM and a BBM. This can lead to several advantages.

This talk presents a GBM that combines an established Reduced Order Model with an ANN. The Reduced Order Model uses empirical material functions derived by laboratory scale centrifuges to describe the settling and the compaction behavior in decanter centrifuges. However, uncertainties due to the experimental design or procedure and missing effects (e.g., shear compaction) can lead to an inadequate description of the material behavior. To counteract this, the ANN adapts the material functions to better reflect reality. This approach offers significant advantages, such as better prediction quality while maintaining low computational times. Furthermore, the GBM presented in this study is considerably more stable for extrapolation tasks than pure data-driven approaches, while requiring less data, leading to a

[a] Presenting Author

wider range of applications. In addition, the developed GBM can be trained in laboratory scale to predict decanter centrifuges of larger scales, making it a promising tool to reduce experimental effort during scale-up, thus reducing costs for manufacturers.

Keywords: Solid-Liquid Separation, Decanter Centrifuge, Grey Box Model, Scale-Up

Data assimilation based on pretrained physics-informed neural networks

Kakeru Ishizawa[1,*], So Yamashita[1], Suguru Shiratori[2], Hideaki Nagano[2], Kenjiro Shimano[2]

[1]Graduate School, Tokyo City University [2]Tokyo City University, E-mail: sshrator@tcu.ac.jp

Abstract: This study proposes a new data assimilation (DA) method based on physics-informed neural networks (PINNs). The use of the PINNs for DA has been proposed in the original paper on the PINNs, where the physical parameters are trained together with the weights of the neural networks. This training process requires many computational costs that are not suitable for online instruments. The original point of this study is that the PINNs are pre-trained. In this way, the DA procedure can be fastly executed. The validity of the proposed DA method is confirmed through twin experiments.

Keywords: PINNs, data assimilation, physical properties

* Presenting author

1 Background and purpose

In the modeling and simulation of complex physical systems, physical properties must be preliminarily obtained. For instance, in the coating of the liquid films, multiple physical properties are required and they are dependent on the concentration of the resin involved [1]. Measuring all the physical properties takes extreme effort. This effort can be reduced by introducing data assimilation (DA). This study proposes a new DA method using learned Physics-informed neural networks (PINNs) [2].

In the DA procedure, uncertain model parameters, such as physical properties, are identified by minimizing errors between simulation results and observed data. By applying DA, multiple physical properties can be identified through only one type of observation data, for example, thickness distribution. In the conventional variational adjoint method, one of the representative methods of data assimilation, the gradient of the loss function is calculated by solving the adjoint problem, which requires discretizations, program coding, and numerical time integration. The cost for this work is a bottleneck in the application of DA. To solve this problem, we propose a new DA framework based on PINNs. By use of pre-trained PINNs, the gradient can be calculated efficiently using automatic differentiation (AD), thus it enables a fast and effective data assimilation. Moreover, the proposed DA method does not require the interpolation procedure, that is needed in the conventional adjoint method since the grid points and observed points are not necessarily colocated. In the following, the proposed DA procedure is described, then it is validated through the identification of physical properties.

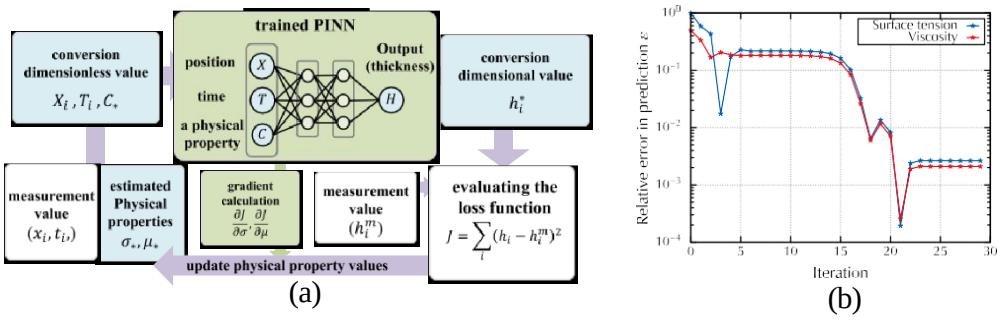


Figure 1: (a) Architecture of Data assimilation methods using learned PINNs. (b) History of the relative error in prediction of physical property during iteration of data-assimilation.

2 Proposed data assimilation methods based on the pretrained PINNs

Fig. 1(a) shows the architecture of DA proposed in this study. First, the PINN is trained with physical properties c within the assumed range. In the DA procedure, the pre-trained PINN is used to predict the solution $h_i(c)$ for the given c. The physical property c is determined by minimizing the loss function J defined as

$$J = \sum_i (h_i(c) - h_i^m)^2 , \quad (1)$$

where h_i^m is the observed data. The use of the PINNs for DA methodology has been proposed in the original paper of the PINNs [2], where the physical parameters are trained together with the weights of the neural networks. This training process requires many computational costs that are not suitable for online instruments. The original point of this study is that the PINNs are pre-trained. In this way, the DA procedure can be fastly executed.

3 Validation results

The proposed DA method was validated through the twin experiment. In this experiment, the surface tension and viscosity are assimilated in the same procedure. The loss function J is successfully reduced and both physical properties are sufficiently reconstructed to the prescribed values as shown in **Fig. 1**(b).

References

[1] Suguru Shiratori and Toru Kubokawa. Double-peaked edge-bead in drying film of solvent-resin mixtures. *Phys. Fluids*, 27(10):102105, 2015.

[2] M. Raissi, P. Perdikaris, and G.E. Karniadakis. Physics-informed neural networks: A deep learning framework for solving forward and inverse problems involving nonlinear partial differ- ential equations. *J. Comp. Phys.*, 378:686–707, 2019.

Enhancing Electric Vehicle Battery Thermal Management through Real-Time Temperature Prediction Using Machine Learning

Hanwen ZHANG [1,a], Abbas FOTOUHI [1,*], Daniel J. AUGER [1]
[1] School of Aerospace, Transport and Manufacturing, Cranfield University,
* Email: a.fotouhi@cranfield.ac.uk

Effective thermal management is vital for optimising the performance and longevity of electric vehicle (EV) batteries [1]. Maintaining the battery within a specific temperature range is critical for safety and efficiency. Current Battery Thermal Management Systems (BTMS) focus on real-time temperature monitoring but cannot predict the temperature even shortly ahead of time as a useful element for proactive control [2]. This study proposes an innovative hybrid system designed to enhance BTMSs by integrating a Machine Learning-based battery temperature prediction model with an online battery parameter identification unit. The proposed Machine Learning (ML) model, employing an Adaptive Neuro-Fuzzy Inference System (ANFIS), utilises historical battery charge/discharge data and its internal parameters to predict surface temperature within a set time frame. Additionally, an online parameter identification unit continuously updates the battery model by adjusting its thermal and electrical parameters based on battery state variations such as state of charge, temperature, and internal resistance. A precise battery temperature prediction can support the battery cooling system, allowing it to anticipate temperature fluctuations caused by high discharge rates or other factors, thereby ensuring robust and efficient operation of the battery.

Figure 1 depicts the configuration of the battery surface temperature prediction system. The data is split into two groups: directly measured data and the data collected from the battery parameter identification unit. Direct measurements are from battery sensors, including current, terminal voltage, and surface temperature. The online identification unit processes the measured data to obtain required parameters such as internal resistance and open-circuit voltage. These parameters are then used to calculate the battery heat generation rate and estimate the expected change in battery temperature within the prediction horizon. Experimental tests are carried out on two types of battery to validate the proposed system: (i) Lithium Nickel Cobalt Aluminium Oxides (NCA) battery, and (ii) Lithium Iron Phosphate (LFP) battery [3]. A thermal chamber maintains a consistent ambient temperature during the tests, covering from -10°C to 40°C. A power supply is controlled via MATLAB software to automate the battery charge/discharge rates and to log the measured signals.

Figure 2 demonstrates an example validation test result in which the NCA battery surface is predicted 30 seconds ahead and at an ambient temperature of 10°C. The figure compares the predicted temperature versus the reference temperature obtained from a sensor. There is a considerable overlap between the predicted and the reference temperature values, indicating a high level of accuracy for the proposed system. A mean absolute error (MAE) of 0.04°C is

[a] Presenting Author

obtained in that case, which proves the overall accuracy of the prediction model. Additionally, a maximum error of 0.77°C is observed which provides an insight into the worst-case scenario. Notably, the results indicate that the temperature predictions closely follow the reference values with no significant outliers. The proposed battery temperature prediction system has demonstrated great performance in other validation cases as well, such as longer prediction horizons of up to 2 minutes and for other battery types, such as the LFP battery. In conclusion, the proposed system delivers high accuracy across various battery types, which is crucial for diverse applications such as electric vehicles, renewable energy storage, and consumer electronics. Indeed, by combining the benefits of the model identification unit and the ANFIS model, the proposed system offers robust and efficient temperature prediction in real-time applications. These findings promise to enhance battery safety and functionality across industries, mitigating the risk of thermal runaway.

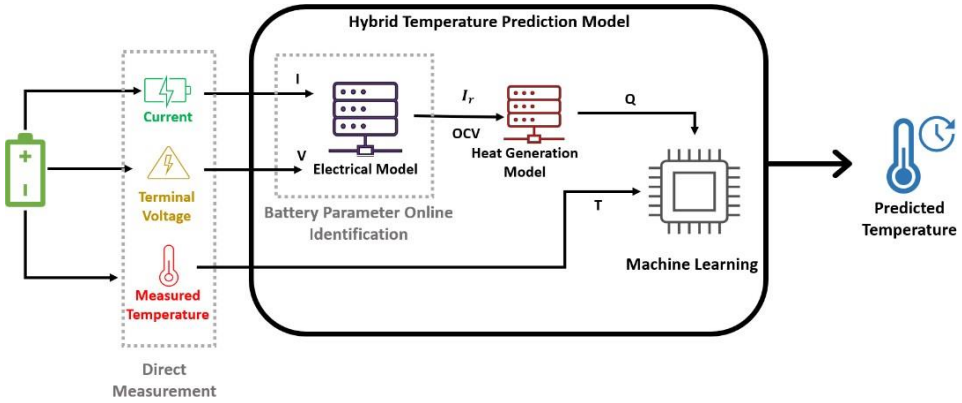


Figure 1 The concept of battery temperature prediction using machine learning and system identification

Figure 2 An example battery surface temperature prediction 30 seconds ahead

References

[1] Shahid, S., & Chaab, M. A. (2022). A review of thermal runaway prevention and mitigation strategies for lithium-ion batteries. Energy Conversion and Management: X, 16, 100310.
[2] Jaguemont, J. (2016). A comprehensive review of lithium-ion batteries used in hybrid and electric vehicles at cold temperatures. Applied Energy, 164, 99-144.
[3] Editorial board, EV Markets Reports (2023). Retrieved 11 22, 2023, from https://evmarketsreports.com/lfp-batteries-transforming-ev-market-dynamics-globally/

Artifical neural networks based surrogate modelling of finite element simulations of steel components' mechanical behavior

Ela Marković[1, a], Tea Marohnić[2], Robert Basan[3]

[1] University of Rijeka, Faculty of Engineering, Croatia, E-mail: ela.markovic@riteh.uniri.hr

[2] University of Rijeka, Faculty of Engineering, Croatia, E-mail: tea.marohnic@riteh.uniri.hr

[3] University of Rijeka, Faculty of Engineering, Croatia, E-mail: robert.basan@riteh.uniri.hr

The advancement of computer technology and computer-aided engineering has revolutionized the product development process by enabling early-stage simulations of component behavior. When dealing with components of complex geometries or material properties, such as heat-treated engineering components, obtaining precise analytical solutions for mechanical behavior is not feasible. Therefore, computer simulations are conducted, most commonly using the finite element analysis (FEA). However, the iterative nature of FEA slows down the process of fine-tuning model parameters for even minor geometric or material adjustments when exploring various scenarios and determining the most effective solutions.

To address these challenges, a novel methodology leveraging artificial neural networks (ANNs), is presented in this study. A parametrized numerical model adaptable to diverse component geometries and material variations is developed. This model is utilized to simulate the behavior of component-like steel specimens under various load conditions. Extracted simulation results, such as deformations and stresses, across predefined parameter ranges, are used to develop and train a parametric surrogate artificial neural network model which aims to reduce computational costs while maintaining same accuracy.

Creating ANN based surrogate model from FEA simulation results, offers a faster and more efficient alternative to traditional FEA simulations, especially in components with complex geometry or complex material properties.

Keywords: Finite element analysis, Artificial neural networks

Acknowledgments: This work has been supported by Croatian Science Foundation under the project IP-2020-02-5764 and by the University of Rijeka under the project uniri-tehnic-18-116. The work of doctoral student Ela Marković has been fully supported by the „Young researchers' career development project – training of doctoral students" of the Croatian Science Foundation.

[a] Presenting Author

Numerical homogenization using a PINN-based LOD for the solution of multiscale problems

Mehdi Elasmi[1,*], **Felix Krumbiegel**[1], **Roland Maier**[1]

[1]Institute for Applied and Numerical Mathematics
Karlsruhe Institute of Technology

Abstract: For the simulation of multiscale problems with arbitrary coefficients, we propose a numerical homogenization technique based on Localized Orthogonal Decomposition (LOD) [1] and Physics-Informed Neural Networks (PINNs) [2].
The LOD method relies on the construction of a low-dimensional solution space that exhibits high approximation properties with respect to the solution. In its classical version, this is achieved by adapting the finite element basis functions, e.g., nodal basis functions, to the problem's coefficients. To this end, the resolution of several localized sub-problems, referred to as correction problems, is needed. Obviously, this process can pose computational difficulties when dealing with rough and unstructured materials or for time-dependent coefficients. To overcome this challenge, we associate a neural network to each patch configuration and learn in an offline step the corresponding multiscale basis functions associated to a sample of relevant coefficients using PINNs. By incorporating the governing equations of a correction problem into the loss function, PINN allows the reduction of the sample's dimension needed for the training procedure, and guarantees if success- ful physically and mathematically consistent results. In the present work, the learning procedure is solely model-based and does not necessitate supplementary data.
Thanks to the generalization property of deep learning techniques, this hybrid offline-online scheme reveals to be a promising alternative to classical LOD, particularly in the presence of material uncertainties, and for solving inverse and time-dependent multiscale problems.

Keywords: LOD, PINNs, multiscale problems, numerical homogenization, offline-online schemes.

* Presenting author

References

[1] A. Målqvist and D. Peterseim. 2020. Numerical homogenization by localized orthogonal decomposition. Society for Industrial and Applied Mathematics (SIAM), Philadelphia. SIAM Spotlights, Vol. 5.

[2] M. Raissi, P. Perdikaris, G.E. Karniadakis. 2019. Physics-informed neural networks: A deep learning framework for solving forward and inverse problems involving nonlinear partial differential equations. Journal of Computational Physics. Vol. 378, pp. 686-707.

Application of artificial neural networks in estimation of mechanical behavior of steels

Tea Marohnić [1, a], Robert Basan [2], Ela Marković [3]

[1] University of Rijeka, Faculty of Engineering, E-mail: tmarohnic@riteh.uniri.hr

[2] University of Rijeka, Faculty of Engineering, E-mail: robert.basan@riteh.uniri.hr

[3] University of Rijeka, Faculty of Engineering, E-mail: ela.markovic@riteh.uniri.hr

Early in the product development process, when various materials and design solutions are being evaluated, simulations of the behavior of parts and structures and the determination of load carrying capacity are made possible by the growing advancements in computer technologies and computer-aided engineering. Therefore, computer modeling of material behavior is an essential tool so these activities could be carried out, since the chosen material and its monotonic, cyclic, and fatigue behavior play a significant role in the new product development process. As a result, one of the key requirements for effective material modeling is an understanding of the mechanical behavior of materials, or models, as well as the related material properties and parameters that characterize their behavior.

The most precise way to determine a material's behavior, properties, and parameters is through experimental determination. However, this method is costly, time-consuming, and – most importantly – experimental testing is limited during the early stages of design, when a variety of candidate materials and design solutions are being considered. Empirical methods that estimate complex nonlinear cyclic and fatigue behavior of materials from readily available monotonic material properties are available in literature and are widely used in industrial practice (Bäumel & Seeger, 1991; Li et al., 2016; Lopez & Fatemi, 2012; Roessle & Fatemi, 2000), which reduces the volume of required experiments (Blackmore, 2009; Williams et al., 2003). The analytical nature of these estimation techniques is still in use today because of their applicability, ease of use, and fast available results, as demonstrated by Derrick & Fatemi, 2022, who establish correlations between the hardness and defect size and fatigue strength of additively manufactured metals. Nevertheless, closed mathematical forms cannot (accurately) describe many of the material properties and parameters. As a result, as published material data from simulations and experiments becomes more readily available, the focus is shifting to more complex computer-based (data-driven) models based on machine learning (Marohnić et al. 2018, 2023), i.e. the fourth paradigm of material science, as stated by Stoll & Benner, 2021.

Availability of quality data sets in material science, although increasing can still be relatively low in context of data analytics and machine learning. High dimensionality data mixed with a small number of datasets might negatively influence the behavior and performance of machine learning algorithms (Stoll & Benner, 2021), as can low quality data.

[a] Presenting Author

Here, our efforts in application of artificial neural networks for estimation of cyclic and fatigue behavior of steels, by considering their monotonic properties and/or heat treatment and related microstructure, are presented.

Acknowledgments: This research has been supported by Croatian Science Foundation under the project IP-2020-02-5764 and by the University of Rijeka under the project number uniri-tehnic-18-116. The work of doctoral student Ela Marković has been fully supported by the „Young researchers' career development project – training of doctoral students" of the Croatian Science Foundation.

Keywords: artificial neural networks, small datasets, mechanical behavior of steels

Merging metabolic networks with deep neural networks under the SBML standard

José Pinto[a], João R. C. Ramos, Rafael S. Costa, Rui Oliveira
LAQV-REQUIMTE, Department of Chemistry, NOVA School of Science and Technology, NOVA University Lisbon, Campus da Caparica, Caparica, 2829-516, Portugal

The integration of mechanistic knowledge with artificial neural networks (ANN) in a hybrid workflow has found wide application in process systems engineering since the early 1990s. Psichogios and Ungar (1992) described one of the first applications of hybrid mechanistic/ANN models to bioprocess engineering. The proposed hybrid model consisted of dynamic material balance equations of bio-chemical species (system of ordinary differential equations (ODEs)) connected with a shallow feed-forward neural network in a common mathematical structure. Ever since, hybrid models were applied to a wide array of biotechnological processes such as wastewater treatment, clean energy, biopolymers, and biopharmaceutical manufacturing (Agharafeie et al., 2023).

With a significant lag, hybrid modeling is currently receiving a lot of attention in the systems biology scientific community, with Machine Learning (ML) gaining popularity in all fields of biological sciences. A large number of systems biology models (of mechanistic basis) have been developed and stored in databases in the Systems Biology Markup Language (SBML) format (Hucka et al., 2003). SBML is a free and open standard based on XML to encode computational models of biological processes with widespread use in the systems biology scientific community. The SBML standard is, however, not commonly adopted in ML software tools. This significantly hinders the interlink between both modeling approaches in a hybrid workflow.

Here, we propose a hybrid modeling framework that combines both modeling approaches and obeys the SBML standard. A previously published python package, SBML2HYB, is used (Pinto et al., 2023). The so-formed hybrid models are trained with a deep learning algorithm based on ADAM, stochastic regularization and semidirect sensitivity equations. The final (trained) hybrid models are uploaded in SBML databases, where they may be further analyzed as regular SBML models. This procedure was applied to three well-known models: the E. coli threonine pathway model (Chassagnole et al., 2001), the P58IPK signal transduction pathway model (Goodman et al., 2011) and the yeast glycolytic oscillations model (Dano et al., 2006). Figure 1 illustrates a hybrid metabolic network for the yeast glycolytic oscillations. In this example, the FFNN has seven inputs corresponding to the concentrations of the seven species (ADP, AMP, ATP, BPG, DHAP, FBP, GAP), three hidden layers (10 × 10 × 10) with hyperbolic tangent activation functions, and 11 outputs corresponding to the kinetic rates (v_1r, v_2r, v_3r, v_4r, v_5r, v_6r, v_7r, v_8r, v_9r, v_10r, v_11r). Despite the limit cycle stability being a challenging problem, the hybrid deep model was capable of faithfully reproducing the

[a] Presenting Author: jmm.pinto@campus.fct.unl.pt

oscillatory behavior of the original model even when exposed to conditions outside of its training dataset. The shown model obtained a noise free WMSE for the test partition of 0.11.

Keywords: hybrid modeling, deep neural networks, deep learning, SBML, systems biology, computational modeling

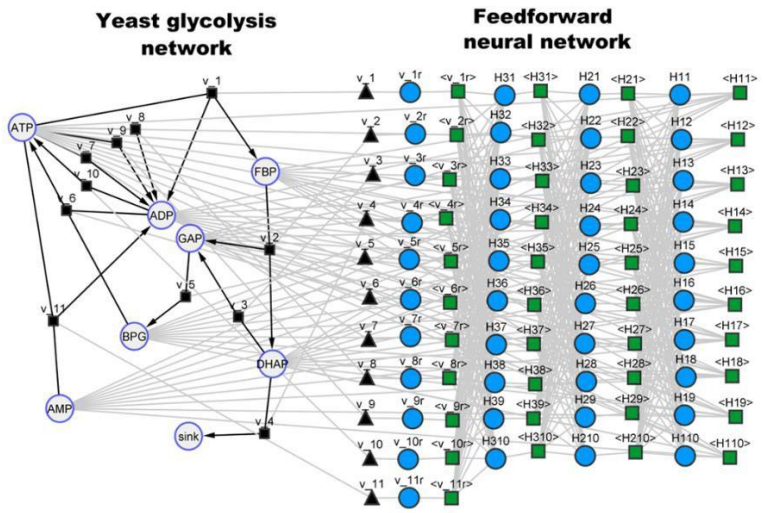


Figure 1: Hybrid metabolic network for the yeast glycolytic oscillations model (Dano et al., 2006).

References:

Psichogios, D. C., & Ungar, L. H. (1992). A hybrid neural network-first principles approach to process modeling. AIChE Journal, 38(10), 1499-1511.

Agharafeie, R., Oliveira, R., Ramos, J. R. C., & Mendes, J. M. (2023). Application of hybrid neural models to bioprocesses: A systematic literature review. Authorea Preprints.

Hucka, M., Finney, A., Sauro, H. M., Bolouri, H., Doyle, J. C., Kitano, H., ... & Wang, J. (2003). The systems biology markup language (SBML): a medium for representation and ex-change of biochemical network models. Bioinformatics, 19(4), 524-531.

Pinto, J., Costa, R. S., Alexandre, L., Ramos, J., & Oliveira, R. (2023). SBML2HYB: a Python interface for SBML compatible hybrid modeling. Bioinformatics, 39(1), btad044.

networks. Computers & Chemical Engineering, 165, 107952.

CHASSAGNOLE, C., FELL, D. A., RAÏS, B., KUDLA, B., & MAZAT, J. P. (2001). Control of the threonine-synthesis pathway in Escherichia coli: a theoretical and experimental approach. Biochemical Journal, 356(2), 433-444.

Goodman, A. G., Tanner, B. C., Chang, S. T., Esteban, M., & Katze, M. G. (2011). Virus infection rapidly activates the P58IPK pathway, delaying peak kinase activation to enhance viral replication. Virology, 417(1), 27-36.

Danø, S., Madsen, M. F., Schmidt, H., & Cedersund, G. (2006). Reduction of a biochemical model with preservation of its basic dynamic properties. The FEBS journal, 273(21), 4862-4877.

Bioprocess Hybrid Modeling: A Comparative Study of Physics-Informed Neural Networks and Traditional Semiparametric Hybrid Modeling

Monesh Kumar [1, a], Bernardo Ribeiro[2], José Pinto[3], Rui Oliveira[4]

[1, 2,3,4] NOVA Science and Engineering School, NOVA University of Lisbon, Portugal
mokuth@campus.fct.unl.pt[1], bmp.ribeiro@campus.fct.unl.pt[2], jmm.pinto@campus.fct.unl.pt[3], rmo@fct.unl.pt[4]

In the realm of bioprocess technology, bioreactors play a central role. The intrinsic mechanistic complexity of cell cultivation systems due to population heterogeneity in cell size, reproduction cycle, genetic stability as well as intracellular composition poses a formidable challenge for process digitalization. The development of predictive models for optimization and control at an acceptable cost is still challenging in the bioprocessing industries[1].

Traditional mathematical modeling, such as mechanistic or first principles relying on prior knowledge often have a low benefit/cost ratio due to the effort of developing a very complex mathematical model that in the end poorly describes the process. On the other side, data-driven approaches relying on process data face constraints due to limited data availability as big data infrastructure is lagging in the bioprocess industries. To address these challenges, a hybrid modeling concept was introduced, and a plethora of studies underwent it in the early 1990s. Hybrid modeling is a synergistic approach that combines the first principles/mechanistic modeling with data-driven approaches to overcome the limitations of each approach individually[2 3].

Physics-informed neural network (PINN) is an emerging technique that incorporates known physical knowledge governing the system, usually partial differential equations or ordinary differential equations (PDE or ODE), into the loss function of a deep neural network during the training process[4]. This PINN framework enables the capture of complex physics even with limited data, and this unique approach is standalone from traditional hybrid modeling. In this study, we compare for the first time physics-informed neural networks (PINN) to traditional semiparametric hybrid modeling and evaluated its application to a fed-batch bioreactor synthetic dataset. We aimed to incorporate governing equations into the deep neural network and predict its accuracy.

---

[a] Presenting Author

Throughout the study, we used the adaptive moment estimation (ADAM) algorithm, the *tanh* activation function, three hidden layers with 32 nodes each (pre-optimized), 50000 epochs for the PINN model topology. However, these training hyperparameters must be validated on a case-by-case basis. The key conclusion is that embedding physics knowledge in the neural network during the training process has achieved a higher prediction accuracy than the deep neural network (Fig. 1). This work demonstrates that by adopting the governing equations during the training process, enhances the predictive capabilities of PINN comparatively to the deep neural network.

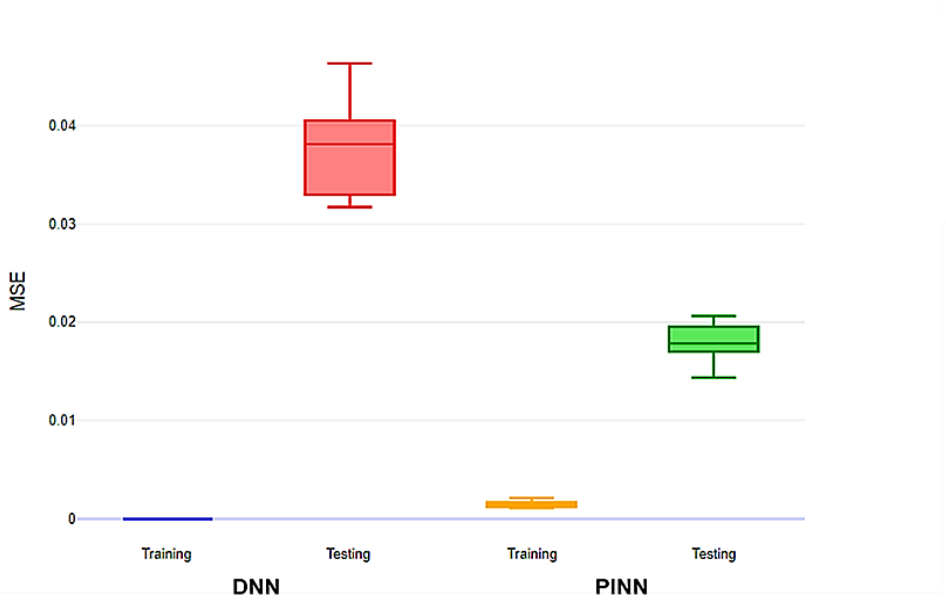


Fig 1. Boxplot of training and testing MSE for 10 training repetitions by the deep neural network and by the PINN

Keywords: Physics-informed neural network, Bioprocess technology, Deep neural network

References:

(1) Hong, M. S., & Braatz, R. D. (2021). Mechanistic modelling and parameter-adaptive nonlinear model predictive control of a microbioreactor. Computers & Chemical Engineering, 147, 107255.

(2) Psichogios, D. C., & Ungar, L. H. (1992). A hybrid neural network-first principles approach to process modeling. AIChE Journal, 38(10), 1499-1511.

(3) Bradley, W., Kim, J., Kilwein, Z., Blakely, L., Eydenberg, M., Jalvin, J., ... & Boukouvala, F. (2022). Perspectives on the integration between first-principles and data-driven modeling. Computers & Chemical Engineering, 166, 107898.

(4) Raissi, M., Perdikaris, P., & Karniadakis, G. E. (2019). Physics-informed neural networks: A deep learning framework for solving forward and inverse problems involving nonlinear partial differential equations. Journal of Computational physics, 378, 686-707.

MadeAI 2024 - Modelling, Data Analytics and AI in Engineering
2-5 July 2024, Porto, Portugal

Last-piece exploring model operator networks –validations through various terms and equations–

So Yamashita[1,*], Kakeru Ishizawa[1], Taisei Kato[2], Suguru Shiratori[2], Hideaki Nagano[2], Kenjiro Shimano[2]

[1]Graduate School, Tokyo City University
[2]Tokyo City University, E-mail: sshrator@tcu.ac.jp

Abstract: This study addresses *a Last-piece Exploring Model Operator Network* (LEMON), which is proposed in another paper presented at MadeAI [1]. The LEMON is neural networks that learn an operator for missing parts of governing equations (GE) for physical systems. In this paper, we report additional verifications of the LEMON by applying to the diffusion term in the Burgers equation, and the convective and 3rd-order derivative terms in the Korteweg-de Vries (KdV) equation.

Keywords: Missing physics inferring, PINNs, DeepONets

* Presenting author

1 Motivation

In the modeling and simulation of unsteady physical phenomena, all the related physics must be formulated preliminary as governing equation (GE). The predicted solutions generally differ from the observed data, thus the model is required to be reformulated. Carrying this reformulation is a hard task since it requires wide knowledge and experience for the computational science and the physics. For learning the physical model from the observed data, some methodologies have been proposed, for instance, Neural ODE [2]. These methods attempt to identify a physical model that describes the entire phenomenon. When the partial information on physical models is known in advance, it is sufficient to learn the remaining part of GE and its training process is expected to be efficient. However, no method has been proposed for such purpose. The author's research group proposes new architecture of neural networks, named as *a Last-piece Exploring Model Operator Networks* (LEMON), that discovers unmodeled terms in physical systems.

As shown in another paper [1], the network of the LEMON is mainly composed of a combination of physics-informed neural networks (PINNs) [3] and DeepONets [4]. The governing equations to be solved consist of a modeled term $\mathsf{F}(u)$ and an unmodeled missing term $\mathsf{G}(u)$, where $\mathsf{F}(u) + \mathsf{G}(u) = 0$ is total GE that must be satisfied. First, the solution $u(x, t)$ for given x and t is predicted by the PINNs, and the modeled operator $\mathsf{F}(u)$ can be computed through automatic differentiation of the PINNs. The unmodeled operator $\mathsf{G}(u)$ is predicted by the DeepONet, which learns the functional operator from input-output relationships. The total loss function consists of the unsupervised loss of GE and the supervised loss of the observed data. In another paper Ref.[1], the basic architecture is described, whereas the validation of the proposed method is only shown for the case of the convection term in the Burgers equation. In this work, the LEMON is validated for the other terms and equations.

Table 1: Cases for validations. F is prescribed term and G is hidden missing term.

Name	Equation form	Modeled term F(u)	Unmodeled term G(u)
Burgers equation	$\frac{\partial u}{\partial t} + u\frac{\partial u}{\partial x} - D\frac{\partial^2 u}{\partial x^2}$	$\frac{\partial u}{\partial t} + u\frac{\partial u}{\partial x}$	$-D\frac{\partial^2 u}{\partial x^2}$
Korteweg-de Vries equation	$\frac{\partial u}{\partial t} + u\frac{\partial u}{\partial x} - D\frac{\partial^3 u}{\partial x^3}$	$\frac{\partial u}{\partial t} - D\frac{\partial^3 u}{\partial x^3}$	$u\frac{\partial u}{\partial x}$
		$\frac{\partial u}{\partial t} + u\frac{\partial u}{\partial x}$	$-D\frac{\partial^3 u}{\partial x^3}$

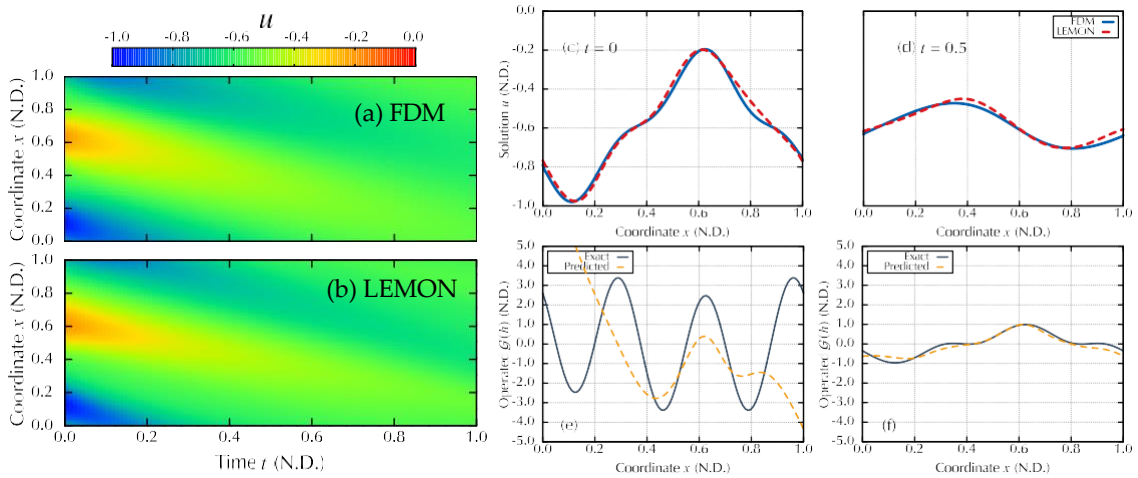


Figure 1: How the LEMON predicted hidden diffusion term in Burgers equation. (a) The spatio-temporal variation of the solution u(t, x) predicted by (a) finite difference methods and (b) LEMON. The selected snapshots of the instantaneous spatial distribution at (c) t = 0 and (d) t = 0.5. (e) and (f) The exact (blue) and predicted (orange) hidden part G for the data not involved in the training data.

2 Validations

Table 1 shows the modeled term F(u) and the unmodeled terms G(u) that are responsible for this validation, and a total of three patterns are applied to LEMON to investigate the accuracy. Fig. 1 shows the results when the LEMON is applied to the diffusion term in the Burgers equation. The sub-figures (c,d) in Fig. 1 are selected snapshots for the instantaneous solution, that showed good agreement with the result calculated by the finite difference method (FDM). Fig. 1(e,f) are exact (dark-blue) and predicted (orange) terms.

References

[1] Suguru Shiratori, So Yamashita, Kakeru Ishizawa, Taisei Kato, Hideaki Nagano, and Kenjiro Shimano. Last-piece exploring model operator networks. In *Proceedings of MadeAI*, 2024.

[2] Ricky T. Q. Chen, Yulia Rubanova, Jesse Bettencourt, and David Duvenaud. Neural ordinary differential equations. In *NeurIPS*, 2018.

[3] M. Raissi, P. Perdikaris, and G.E. Karniadakis. Physics-informed neural networks: A deep learning framework for solving forward and inverse problems involving nonlinear partial differential equations. *J. Comp. Phys.*, 378:686–707, 2019.

[4] Lu Lu, Pengzhan Jin, Guofei Pang, Zhongqiang Zhang, and George Em Karniadakis. Learning nonlinear operators via deeponet based on the universal approximation theorem of operators. *Nat. Mach. Intell.*, 3(3):218–229, March 2021.

Enhancing Precision and Efficiency in Hot Forging Processes through Advanced Machine Learning Models: CrystalMind and DeepForge

Jan Petrik[1,*], **Markus Bambach**[1]

[1]Advanced Manufacturing Laboratory, ETH Zurich, Switzerland

Abstract:

The advancement of material processing techniques is a critical objective within the manufacturing sector, with the aim of improving product quality and operational efficiency. This paper focuses on the application of two machine learning models, CrystalMind and DeepForge, to the hot forging process, a line of research that has shown potential for significant improvements in both accuracy and efficiency. The motivation be- hind this work is to explore innovative approaches to overcome the challenges associated with traditional hot forging processes, including optimisation of forging strategies and microstructure control.

CrystalMind is a surrogate model designed to accurately reconstruct 3D models after hot forging deforma- tion using a dual input system consisting of a 3D model of the pre-stroke workpiece geometry and a detailed forging vector. This model incorporates MLP (Multi-Layer Perceptron) based and PointNET++ based ar- chitectures for comparison, and demonstrates their ability to predict recrystallisation and deformation with a margin of error limited to less than 2 % for recrystallisation and less than 0.9 % for deformation. In par- ticular, the MLP architecture achieves a computational speed that is 36 times faster than its counterpart, with an average of 5 ms per run, providing significant efficiency gains for optimisation purposes.

In addition, DeepForge introduces a machine learning-based model suitable for microstructure control in closed die hot forging, integrating Model Predictive Control (MPC) with a machine learning model that combines 1D convolutional neural networks and gated recurrent units. Despite using only such a limited input as the surface temperatures of a workpiece, DeepForge is able to predict microstructural changes with a mean absolute error of 0.4 0.3 %±The model's use of MPC facilitates the adjustment of inter-stroke wait times, counteracting temperature variations to target a grain size of less than 35 microns within a specified 2D area of the workpiece.

In summary, these two models enrich the state of the art in metal forming by replacing FE simulations with machine learning approaches. CrystalMind outperforms previous models by providing accurate and detailed 3D predictions of deformation and recrystallisation using a point cloud of 7,808 nodes refined from a dataset of more than 1200 strokes with varying parameters. Furthermore, DeepForge extends its innovation by introducing an MPC framework tailored for microstructure control, which has been experimentally verified. Specifically, it uses only surface temperature - a parameter that can be measured in real time by an IR camera during the manufacturing process.

Keywords: Metal Forming, Forging, Artificial Intelligence, Multilayer Perceptron, Finite Element Simulation, Optimization

* Presenting author

Surrogate Solutions to Partial Differential Equations and the Inverse Problem with Symbolic Regression

Benjamin Cohen[1], Burcu Beykal[1,2], George M. Bollas[1,*]

[1]University of Connecticut, Department of Chemical and Biomolecular Engineering
[2]University of Connecticut, Center for Clean Energy Engineering

Abstract: Symbolic regression (SR) sits at the junction between machine learning and traditional modelling paradigms. Unique in its ability to learn interpretable models automatically from data, SR is well-poised to aid scientists and engineers in uncovering models that simultaneously predict future states and elucidate the underlying phenomena driving change [1]. Of particular interest across science and engineering is the modelling of dynamical systems most concisely represented using partial differential equations (PDEs). PDEs adeptly capture spatial and temperature changes, but are often difficult to solve, requiring specialized tools and skillets.

Machine learning techniques, like Physics-informed neural networks (PINNs) [2], have emerged as alternatives to traditional PDE solvers, enabling the automatic discovery of surrogate solutions for fast and accurate state estimates. These neural networks can also combine data and physics to solve the inverse problem. Inherent in their structure however, the surrogate solutions learned using tools like PINNs are opaque, lacking interpretability.

In this work, SR is used in place of neural networks to generate interpretable surrogate solutions of PDEs while solving the inverse problem from small datasets. These surrogate solutions offer representations of PDE solutions that resemble, and sometimes embody, analytical solutions. By leveraging SR, the learned surrogates are more trustworthy and interpretable compared to their neural network counterparts, requiring many fewer parameters to capture observed dynamics. This reduced model complexity, defined as number of parameters in the surrogate solution, facilitates a clearer understanding of each parameter's impact, promoting the transparency of the models produced.

The search of a surrogate model which approximates the solution to a PDE while learning unknown parameter values of that PDE began with three ingredients: data, the known structure of a PDE, and an argument and primitive set to be used in model building. SR, implemented in the open-source tool SymbolicRegression.jl [3], then searched the symbol space for an optimal expression which minimizes the maximum likelihood estimation (MLE) between the surrogate model and the data while satisfying the known PDE. Derivatives of the analytical surrogate solution were taken using automatic differentiation to check for the solution's consistency with the known PDE. During this process, the parameter values of the known PDE were estimated.

The overall objective of the SR can be represented as the optimization problem of Eq. 1. In this problem, h is the known PDE, y are the measured data, $s \in S$ is the surrogate solution to the PDE in the symbol space defined by the primitive and argument sets, $\boldsymbol{\theta} \in \mathbb{R}^{n_p}$ is the vector of n_p parameters in the PDE model, λ is a regularization term, x is space, t is time, and s_i indicates the derivative of s with respect to i.

$$s^*, \boldsymbol{\theta}^* \in \operatorname{argmin}_{s \in S, \boldsymbol{\theta} \in \mathbb{R}^{n_p}} (1 - \lambda)\mathrm{MLE} + \lambda h(y, s_x, s_{xx}, s_t; \boldsymbol{\theta}) \quad (1)$$

Performance of the proposed method was evaluated by testing the capacity of SR to discover the advection and Burgers' equations (shown in Eqs. 2 and 3), where u represents the states and grid data for both systems, generated in space, $x \in [-5, 5]$ and time, $t \in [0, 2]$ with 500 points taken in each dimension. Data for the advection equation was generated using an analytical solution, and data for the Burgers' equation was generated by solving the PDE using a numerical differential equation solver.

$$u_t + 0.5u_x = 0 \quad (2)$$

$$u_t - 0.1u_{xx} + 0.5u_x = 0 \quad (3)$$

Experiments to test the proposed method were run with varying levels of noise and amounts of data randomly sampled across the domain. As a benchmark for comparison, the experiments were also conducted using PINNs, implemented using PyTorch. All experiments were run on an Intel Xeon CPU.

When tasked with the discovery of the advection equation, SR was able to identify the parameter of the PDE very well, even in high noise, low data environments. This is, in part, because the SR can learn the closed-form analytical solution to the PDE. Compared to PINN estimates, SR is better at estimating PDE

parameters, especially as noise grows and data becomes scarce. This improved performance comes at a slight cost of time, as SR takes longer to return good parameter estimates and an analytical solution to the PDE.

To test the SR method on a slightly more complex system, a small amount of diffusion was added to the advection equation resulting in Burgers' equation. When SR attempted to discover good surrogate solutions to Burgers' equation, it struggled. Despite this difficulty, the parameter estimates for the convection term in Burgers' equation uncovered by SR still were close to the ground truth. SR failed to capture the diffusion term. Because the complexity of the system grew, the PINN approach outperformed the SR approach, although the SR method still learns a much less complex (and much less accurate) surrogate solution to the PDE than PINNs.

Establishing trust and understanding in models is essential across disciplines in science and engineering. SR is well aligned with this objective, learning models that can be interpreted with complexities much less than those of other types of machine learned models. In the discovery of surrogate solutions to PDEs and optimization of PDE parameters, SR can be an effective tool when dynamics can be captured relatively simply. A small change in a system that results in difficult to capture phenomena, like shock-waves, however, can become a significant hurdle to using SR as an alternative to PINNs. When SR does work, it is able to learn very understandable surrogate or exact solutions to PDEs and perform PDE parameter estimation from very scarce and noisy data. These results warrant continued investigation into methods that are better suited to leverage SR for the discovery of surrogate solutions to PDEs for use in modelling, control, and optimization.

Keywords: Symbolic Regression, Partial Differential Equations, Modelling, Machine Learning

* Presenting author, E-mail: george.bollas@uconn.edu

References

[1] B. Cohen, B. Beykal, G.M. Bollas. 2024. Physics-Informed Genetic Programming for Discovery of Partial Differential Equations from Scarce and Noisy Data. Journal of Computational Physics. Under Review.

[2] M. Raissi, P. Perdikaris, G.E. Karniadakis. 2019. Physics-informed neural networks: A deep learning framework for solving forward and inverse problems involving nonlinear partial differential equations. Journal of Computational Physics. Vol. 378, pp. 686-707.

[3] M. Cranmer. 2023. Interpretable Machine Learning for Science with PySR and SymbolicRegression.jl. arXiv. eprint 2305.01582.

Deep Neural Network Modelling in Supercritical CO2 Extraction Process

R.Agharafeie [1,2] [a], J.Pinto [1], P.C.Simões[1], J.M.Mendes [2,3], R. Oliveira[1]

[1] LAQV-REQUIMTE, Nova School of Science and Technology (NOVA-SST), NOVA University Lisbon, E-mail: rmo@fct.unl.pt (R.O.)

[2] NOVA Information Management School (NOVA IMS), NOVA University Lisbon, Campus de Campolide, E-mail: d20200461@novaims.unl.pt (R.A.)

[3] NOVA Cairo at The Knowledge Hub Universities, New Administrative Capital, Cairo, Egypt, E-mail: jmm@isegi.unl.pt

Deep learning and big data are wide-spreading across various industries to enhance production efficiency. However, in the biomanufacturing sector the development of big data infrastructure is lagging compared to other industries. To address this, a promising strategy involves integrating deep neural networks (DNN) with prior knowledge in hybrid neural networks (HNN), which are less reliant on the quality and quantity of data[1].

In this study we develop a HNN for Supercritical fluid extraction (SFE) in industrial chemical plants. SFE offers several immediate advantages compared to traditional methods. As an example, SFE eliminates the need for harmful organic solvents and costly post-processing to remove solvents from extracts. Carbon dioxide stands out as the preferred solvent for SFE due to its safety, accessibility, and affordability. Its relatively low critical temperature (304.25 K) enables the extraction of heat-sensitive substances without causing degradation. Notable examples include the extraction of lipids from cyanobacteria [2].

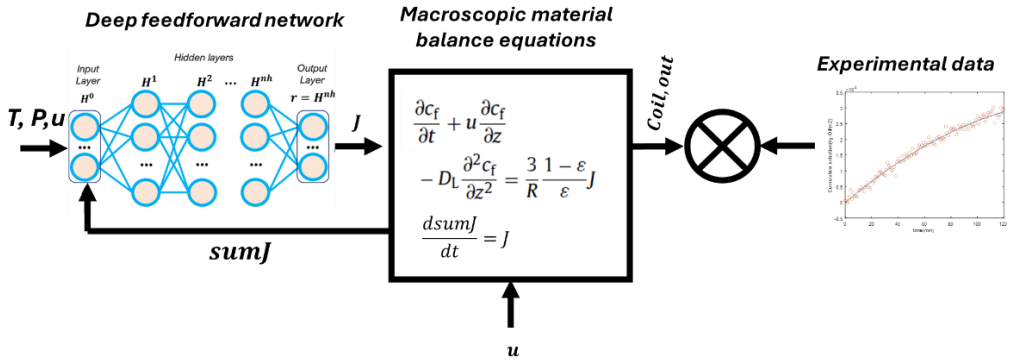


Figure 1- Schema the Deep Hybrid Model

A deep HNN model for the supercritical carbon dioxide (SCCO2) extraction process was developed to predict the optimal extraction rate by considering critical process parameters (CPPs) such as temperature, pressure, gas flow rate, and specification of the raw material. The deep HNN model is a combination of a deep neural network model with three hidden layers

[a] Presenting Author

and five nodes in each of the layers, and the mechanistic model has been developed based on the macroscopic material balance equations and physical and chemical properties of the raw material (Fig.1).

The result showed that the model prediction and synthetic data in training and testing datasets completely cover each other, and it means that the model has a good capability to predict the efficiency of the extraction process for the synthetic data (Fig.2). For the next step we will train the model with the experimental data to check its prediction capability.

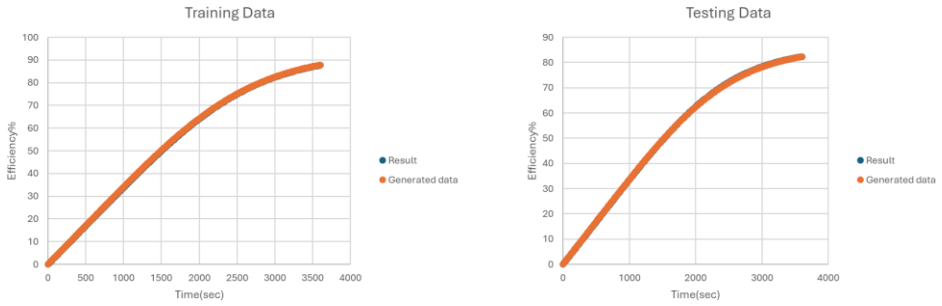


Figure 2-The comparison between the output of the model and the synthetic data

Keywords:
Deep Neural Network, Hybrid Neural Network, Supercritical Carbon Dioxide Extraction, Bioprocess Optimization, Bioprocess prediction

References:

1- Agharafeie, R., Ramos, J. R. C., Mendes, J. M., & Oliveira, R. M. F. (2023). From Shallow to Deep Bioprocess Hybrid Modeling: Advances and Future Perspectives. Fermentation, 9(10), 1-22. Article 922
2- Couto, Ricardo M., Joao Fernandes, MDR Gomes Da Silva, and Pedro C. Simoes. "Supercritical fluid extraction of lipids from spent coffee grounds." *The Journal of Supercritical Fluids* 51, no. 2 (2009): 159-166.

Generative Adversarial Networks for SHM: a short experimental study

Evangelos Papatheou [1, a], Konstantinos Agathos [1], Raja Sekhar Battu[1], Keith Worden[2]

[1] Dept. of Engineering, Faculty of Environment, Science and Economy, University of Exeter, UK, E-mail: e.papatheou@exeter.ac.uk

[2] Dynamics Research Group, Dept. of Mechanical Engineering, University of Sheffield, UK, E-mail: k.worden@exeter.ac.uk

Structural Health Monitoring (SHM), is a very active research field, aimed at producing methodologies for the periodic, and often online, assessment of structures. While there are different approaches to SHM, they can largely be divided into model-based and data-based methods. The former tend to rely on physics-based, commonly numerical methods while the latter favour machine learning (ML). There has been success in the use of ML in SHM, especially when combined with probabilistic approaches. However, SHM with ML relies heavily on data from structures to create the models for their monitoring.

Especially, if supervised learning approaches are employed, then data from all possible damaged states of the structure will be required. For inexpensive structures, destructive means of acquiring those data under laboratory conditions may be possible, but for more expensive structures it may become prohibitively expensive, and other approaches will be required. Experimental approaches in the form of damage metaphors, such as added masses is one proposed solution, and they have been shown to work, but they have practical limitations. Numerical models may offer another possible solution, but they are very costly to develop and difficult to validate in different damage scenarios. Recently, generative machine learning models have been used to create synthetic data to create or augment databases and provide an alternative solution to the lack of training data. The current work explores the use of Generative Adversarial Networks for the creation of synthetic data for SHM. The approach is applied on a laboratory structure.

Keywords: Synthetic data, Generative Adversarial Networks, Structural Health Monitoring

[a] Presenting Author

Gaussian process priors for parameters of a physically based model for the CCT-diagram

Juho Luukkonen

University of Oulu, E-mail: juho.3.luukkonen@oulu.fi

Abstract: The continuous cooling diagram (CCT-diagram) is a convenient representation of how austenite decomposes into different microstructures. It can be applied for designing suitable cooling paths in order to achieve desired mechanical properties. Since the decomposition of austenite depends on the chemical composition of the steel, understanding how different components affect the time and temperature of the transformation provides a valuable tool in choosing a suitable composition. Because construction of CCT-diagrams by empirical methods is expensive and time consuming, there exists a demand to create them by means of mathematical modelling where the model is fitted to previously known available experimental data. Several studies have previously tackled this task. In [1] a regression model was constructed based on analysing the steel isothermal time-temperature-transformation (TTT) diagrams, which could be used for calculating the austenite decomposition. Regression models and more sophisticated data-driven models have also been fitted directly to CCT-diagrams. In this study we extend on the approach taken in [1], and combine rigid parametric physically based modelling with a non-parametric approach to fitting parameters and in this way hope to gain the best of both worlds.

Keywords:

* Presenting author

References

[1] KIRKALDY, J. S. Prediction of microstructure and hardenability in low alloy steels. In: Proceedings of the International Conference on Phase Transformation in Ferrous Alloys, 1983. AIME, 1983.

Physics Informed Neural Networks as a Surrogate for Empiricism in the Seperated Flow Boiling Model

Logan M. Pirnstill[1, a], Chirag Kharangate [2]
[1] Case Western Reserve University, E-mail: logan.pirnstill@case.edu
[2] Case Western Reserve University, E-mail: chirag.kharangate@case.edu

Flow boiling and flow condensation are multi-phase fluid flow regimes that couple the complexities of turbulent fluid flow and liquid-vapor/vapor-liquid phase change. These flow regimes are important as they combine the heat exchange capabilities of both sensible and latent heat. As a result, two-phase flows offer themselves as a viable alternative to traditional heat exchange components for high heat flux devices such as high energy lasers, next generation computers, and nuclear power generation. We address the complexities of two-phase flows by utilizing simplified models derived from control volumes. These types of models average over part of the domain and this integration helps alleviate some of the complexity issues at the expense of resolution. Still, these models are useful for predicting bulk quantities of interest such as pressure drop and heat transfer coefficient. To close these models, we typically invoke empirical or semi-empirical parameters that account for difficult to measure quantities. For the separated flow boiling model, the empirically derived quantity of interest is the interfacial shear stress between the vapor and liquid. Typically, this shear stress is computed through the Wallis correlation, which relates the interface shear to the square difference between the liquid and vapor fluid velocities which is also the dynamic pressure as computed by the relative velocity. However, this relation tends to yield inaccurate results as the friction factors that scale this dynamic pressure rely heavily on correlation and may not apply directly to the system in question. In this paper we use physics informed neural networks (PINNs) as a surrogate for this empirical relation. The PINN infers the interfacial shear directly from the data and uses it to fit a set of control volume equations. In general, we find that the PINN outperforms these empirical fits as the PINN is able to adjust itself locally whereas the Wallis correlation is predetermined by the a priori estimate of the liquid and vapor velocity.

Objectives

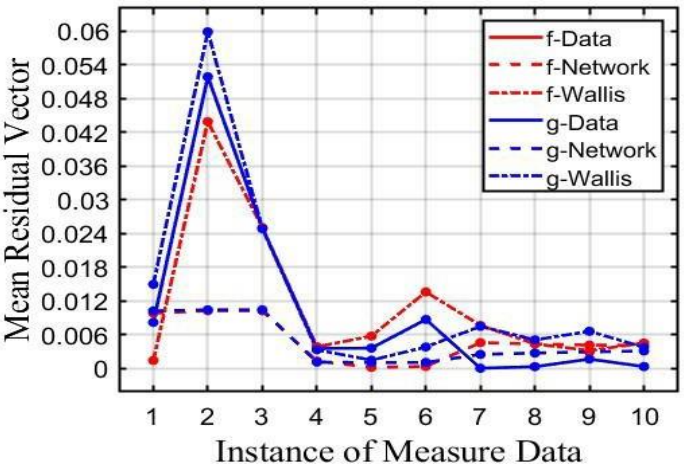
In this study we aim to:

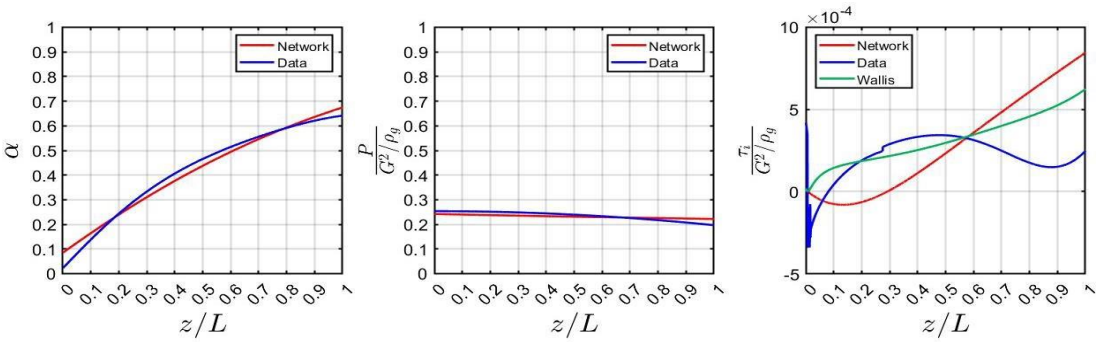
1. Learn the void fraction and pressure curve as collected from experimental measurements.
2. Sufficiently solve the separated flow boiling model using a PINN
3. Infer the interfacial shear stress between the liquid and vapor phases directly from the experimental data using physics informed machine learning.

[a] Chirag Kharangate

Key Results

We demonstrate the effectiveness of PINNs as a surrogate for empiricism by comparing how empirically derived interfacial shear, as well as numerically computed interfacial shear compares to the PINN solution.





The PINN solution for the interfacial shear is capable of minimizing the residual forms of the governing equations more effectively than the semi-empirical correlations as well as the interfacial shear as computed directly from the separated flow model equations. We are also able to effectively learn the void fraction and pressure drop across the channel to a high degree of accuracy. We demonstrate that the PINN is not only effective at learning the relevant physical parameters, but is also a sufficient surrogate for traditional empirical methods for predicting interfacial shear stress.

Data-driven Modelling of Cyclic Plasticity

Burcu Tasdemir [1, a], Vito Tagarielli [2], Antonio Pellegrino [2]
[1] University of Bristol, E-mail: burcu.tasdemir@bristol.ac.uk
[2] Imperial College London , E-mail: v.tagarielli@imperial.ac.uk
[1] University of Bath, E-mail: ap3551@bath.ac.uk

Accurate predictions of the elastic-plastic response of engineering materials are fundamental in structural design and failure analysis. For solids undergoing cyclic loading, involving the sequential application of positive and negative strains, it is fundamental to capture in detail the strain-hardening characteristic of the material to obtain accurate predictions. The theoretical models available to engineers often rely on simplifying assumptions or combinations of these assumptions.

In this study, the complex strain hardening of commercially pure Titanium is modelled using exclusively the results of carefully designed measurements, by applying supervised machine learning. The complex strain hardening characteristic of this material is captured for arbitrary non-monotonic uniaxial loading, without relying on any theoretical description. The data-driven model is based on feed-forward neural networks, trained with data obtained from uniaxial cyclic experiments with variable random amplitude. Uniaxial tests were conducted in strain control, applying random histories of axial strain in the range [-0.04,0.04], to prevent the occurrence of significant damage. The corresponding stress versus strain histories were subdivided into a finite number of increments, and supervised machine learning was applied to predict the change in stress in each increment. The predictions of the surrogate model were validated by comparing with experimental data from unseen experiments. The comparison between the experimental measurements and the predictions of the surrogate model shows that these are in excellent agreement.

Keywords: Machine learning; plasticity; strain hardening; surrogate models; constitutive model.

[a] Presenting Author

Statistics-Informed Neural Network: Performance Analysis

Zihan Xu [1], Roummel Marcia [2], Changho Kim [3, a]

[1] University of California, Merced, E-mail: zxu64@ucmerced.edu

[2] University of California, Merced, E-mail: rmarcia@ucmerced.edu

[3] University of California, Merced, E-mail: ckim103@ucmerced.ed

The statistics-informed neural network (SINN) has been proposed as a machine-learning-based stochastic trajectory generator [1]. With the capability of learning stochastic dynamics from time trajectory data and reproducing stochastic time trajectories faithfully and efficiently, this methodology is considered a promising tool for surrogate modeling.

SINN has the following unique features. First, SINN is built on a deterministic recurrent neural network (RNN) that takes an input stream of white noise sequences to generate an ensemble of stochastic trajectories that has statistical properties similar to the original stochastic dynamics (see Figure 1). This new type of neural network was theoretically inspired by a universal approximation theorem for stochastic systems [1] and the projection-operator formalism for stochastic modeling. Second, to capture memory effects that the underlying stochastic system may have, SINN employs a standard long short-term memory (LSTM) architecture as the building block for SINN (see Figure 2). Third, instead of seeking a path-wise approximation to the stochastic dynamics, SINN compares the statistical properties of the ensemble of simulated trajectories with those for the original trajectories. The total loss function is given as the weighted sum of loss functions defined in terms of statistical properties, including the auto- and cross-correlation functions and marginal probability density functions (PDFs).

While the capabilities of SINN have been demonstrated using various one-dimensional non-Markovian processes [1], for this methodology to be a useful tool for real applications, it is necessary to extend SINN to reproduce multidimensional stochastic processes. To this end, we add the following features to SINN. First, since many cross terms are to be included in the total loss function to capture the complex statistical properties of a multidimensional process, we employ a self-adaptive loss-balanced technique to effectively balance various loss terms. Second, since the estimation of a multidimensional PDF is computationally inefficient, instead of adding these to the total loss function, we include a set of one-dimensional PDFs of some linear combinations of component processes. Third, we allow multidimensional white noise sequences.

In this presentation, after describing our efforts to extend SINN to multidimensions, we present our analysis on the performance of SINN. More specifically, for each development (i.e. self-adaptive loss-balancing, additional one-dimensional PDFs for linear combinations, multidimensional white noise sequences), we analyze the improvement of training speed and quality and the computational overhead. In addition, we will also consider alternative architectures where LSTM units are replaced by gated recurrent units (GRUs) or transformers

[a] Presenting Author

and compare their performance. As application examples, we present simulation results of the Langevin dynamics of the Fermi-Pasta-Ulam chain and the kinetic Monte Carlo simulation of surface chemistry.

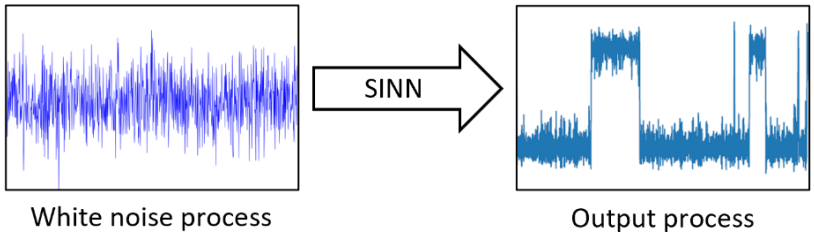


Figure 1. SINN (statistics-informed neural network) as a stochastic time-trajectory generator.

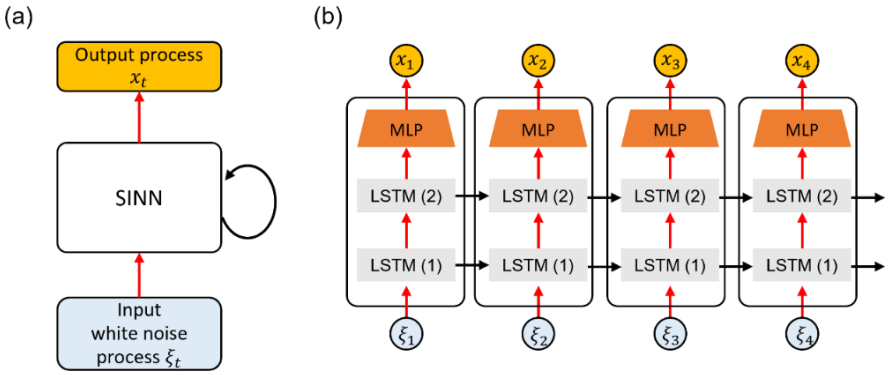


Figure 2. The recurrent neural network structure of SINN. The compressed form is shown in panel (a), whereas SINN is unfolded in time in panel (b). Here we consider a case where SINN is composed of two LSTM (long short-term memory) layers with one MLP (multi-layer perceptron). Note that both the input white-noise process and output process can be multi-dimensional although the vector notations are dropped.

Reference.

[1] Y. Zhu, Y.-H. Tang, C. Kim, “Learning stochastic dynamics with statistics-informed neural network”, *J. Comput. Phys.* 474, 111819 (2023). https://doi.org/10.1016/j.jcp.2022.111819

Keywords: Recurrent Neural Network, Stochastic Processes, Long Short-Term Memory, Gated Recurrent Units, Transformer, Kinetic Monte Carlo

Development of Data based Digital Twinning Framework for Integrated Vehicle Health Management of Aircrafts

Fahad Farid [1, a], Ankur Agarwal [2, a], V Sudhakar [2, b], N S Vyas [1, b]
[1] Indian Institute of Technology Kanpur, India, E-mail: erfahad28@gmail.com
[2] Aeronautical Development Agency (ADA), India, E-mail: sudhakarv.ada@gov.in

Modern aircraft demands efficient maintenance strategies to ensure operational readiness while minimizing downtime and costs. Innovative approach using Digital Twining Framework has been being explored to capture inter system behaviors and assessing health of systems which will help in planning the maintenance aspects. This approach employs advanced Deep Learning Protocols to analyze the intricate interactions among various systems using the data collected from various systems.

The research involves extensive Data Collection from sensors within Aircraft, followed by Data Preprocessing and Feature Selection using domain knowledge and correlation analysis. Neural networks are designed for individual systems, and hyper parameter tuning is performed to optimize their performance. By using the available sensors data, during the model integration phase, an overall health assessment of the aircraft has been generated. This assessment enables advanced fault identification and further, isolation, at the system level by identifying subtle deviations in system behaviors, expediting troubleshooting and corrective actions.

This research lays a framework for advancing Condition-based Maintenance in aircraft using deep learning techniques. Further enhancement, for exploring multi-system interactions, real-time health monitoring, anomaly detection, root cause analysis and the incorporation of emerging deep learning methodologies for long-term performance evaluations, are possible. Results obtained for the digital twins for identified systems and their integration are presented in detail. The paper highlights the case studies with the testing of digital twin models developed on the aircraft data.

Keywords:
Digital Twin, Deep Learning, Integrated Vehicle Health Management, Condition Based Maintenance, Aircraft

Fahad Farid,
Department of Mechanical Engineering,
Indian Institute of Technology Kanpur, India

[a] Presenting Author

Non-intrusive model order reduction for structural dynamics using deep operator inference

Konstantinos Agathos[1,*], **Konstantinos Tatsis**[2]

[1]University of Exeter, E-mail: k.agathos@exeter.ac.uk
[2]ETH Zurich, E-mail: konstantinos.tatsis@sdsc.ethz.ch

Abstract: Reduced Order Modelling (ROM) is one of the main tools for the construction of efficient sur- rogates for computationally expensive models of physical systems governed by partial differential equations, with a wide array of applications, including digital twinning and uncertainty quantification. Among such methods, projection based approaches, such as the Proper Orthogonal Decomposition, are perhaps the most popular. They rely on pre computations to form subspaces of reduced dimensions that approximate the solution space of high dimensional models. Subsequently, the governing equations of these models are pro- jected into and solved in these low dimensional spaces at a reduced numerical cost. However, for problems involving nonlinear operators, the aforementioned projection cannot be performed efficiently online, requir- ing an additional step, termed hyper-reduction, where the projection of these operators in the reduced space is approximated. Hyper-reduction techniques, typically require access to the high-dimensional model to approximate the reduced nonlinear operators, thus limiting the applicability of the method. In the present work, the use of Deep Learning (DL) models is proposed for learning these operators non-intrusively, based only on output data from the high-dimensional model. In particular, Fully-Connected feed-forward Neural Networks (FCNN) are employed to learn the operators by minimising sequences of residuals with respect to the high-dimensional model, allowing the identification of underlying non-linear models, whose evaluation is highly accelerated. The structure of the learned model further allows the use of automatic differentiation to compute jacobian matrices, which are necessary for the solution of the governing equations in the reduced space. The efficacy of the proposed approach is tested through a series of applications from the field of structural dynamics.

Keywords: Neural networks, model order reduction, structural dynamics

---

* Presenting author

Unravelling the Atomistic Mechanisms Underpinning the Morphological Evolution of Al-Alloyed Hematite and Its Catalytic Activity for Hydrogen Production

Jinxing Gu, [1] Jefferson Zhe Liu, [2] Lian Zhang [1,*]

[1] Department of Chemical and Biological Engineering, Monash University, Vic 3800, Australia, E-mail: lian.zhang@monash.edu

[2] Department of Mechanical Engineering, The University of Melbourne, Vic 3156, Australia Email: zhe.liu@unimelb.edu.au

Hydrothermal synthesis upon the use of Al^{3+} as the dopant and/or ethanol as the solvent is effective in promoting the growth of hematite into nanoplate rich in (001) surface, which is highly active for a broad range of catalytic applications. However, the underpinning mechanism for the flattening of hematite crystals is still poorly comprehended. To close this knowledge gap, in this work, we have attempted intensive computational modelling to construct a binary phase diagram for Fe_2O_3-Al_2O_3 under typical hydrothermal conditions, as well as to quantify the surface energy of hematite crystal upon the coverage of Al^{3+} and ethanol molecules. An innovative coupling of density functional theory calculation, cluster expansion and Monte Carlo simulations in analogy to machine learning and prediction was attempted. Upon a successful validation by experimental observation, our simulation results suggest an atomic dispersion of Al^{3+} within hematite in case its concentration is below 4 at.%. Otherwise, the phase separation occurs, and discrete Al_2O_3 nano-clusters can be preferentially formed. Computations also revealed that the adsorption of ethanol molecules alone can reduce the specific surface energy of the hematite (001) surface from 1.33 to 0.31 J m^{-2}. The segregation of Al^{3+} on the (001) surface can further reduce the specific surface energy to 0.18 J m^{-2}. Consequently, the (001) surface growth is inhibited, and it becomes dominant after the disappearance of other surfaces upon their continual growth. This work provides atomistic insights into the synergistic effect between the aluminum textural promoter and the ethanol capping agent in determining the morphology of hematite nanoparticles.

Additionally, we will also here report the in-situ transform of the Al-doped hematite into a Fe_3O_4@$Fe(Fe_{1-x},Al_x)_2O_4$ core-shell structure during the H_2-reduction. The resultant catalyst is superior over those with larger Al contents including the broadly claimed 5 wt% for hydrogen production from water-gas shift reaction, reaching 77% CO conversion at 450 ^oC as well as an activation energy of ~41 kJ/mol that is much lower than the high-Al counterparts and other catalysts reported in the literature. The combined use of machine learning and density functional theory modelling is critical in engineering the amount of Al substitute on the atomic level for a tunable design of

iron oxide-based core-shell catalyst and maximizing its perofmrnace in the catalytic applications.

Keywords: Hydrogen production; Al promoter; DFT calculation, cluster expansion, and active machine learning.

Physics-Informed Graph Convolutional Networks for Ice Thickness Prediction

Maryam Rahnemoonfar [1,2,a], Ben Zalatan [1]
[1] Deaprtment of Computer Science and Engineering, E-mail: maryam@lehigh.edu
[2] Deaprtment of Civil and Environmental Engineering, E-mail: bjz222@lehigh.edu

In response to rising global atmospheric temperatures and evolving climate patterns, the accurate tracking and prediction of polar snow accumulation and ice thickness have become imperative. Understanding the variability of polar snow accumulation is crucial for refining climate models, particularly in estimating sea level rise. Studying the internal ice layers of polar ice sheets is essential for forecasting snow mass balance, extrapolating ice age, and inferring challenging-to-observe processes.

Traditional methods like ice core drilling and shallow pits fall short in reliably capturing catchment-wide accumulation rates due to their sparsity, accessibility challenges, high costs, and depth limitations. Attempts to interpolate these in-situ measurements introduce uncertainties, especially given the high variability in local accumulation rates. Airborne measurements using nadir-looking Synthetic Aperture Radar (SAR) sensors offer a complementary approach, mapping ice sheet topography and monitoring accumulation rates with broad spatial coverage and the ability to penetrate deep ice layers.

To enhance predictive accuracy, we developed a physics-informed geometric deep learning model. This model employs a supervised, multi-target, adaptive long short-term memory graph convolutional network to predict the thicknesses of multiple deep ice layers within an ice sheet based on known thicknesses of shallow ice layers. Physical parameters, including snow mass balance (SMB), surface temperature, meltwater refreezing, height change due to melting, and snowpack height, are integrated as node features alongside layer thickness. Notably, the inclusion of snow mass balance, meltwater refreezing, and height change due to melting as node features significantly improve the model's performance.

Our proposed model outperforms state-of-the-art techniques, showcasing the efficacy of integrating geometric deep learning and Physical models for enhanced prediction of polar ice dynamics.

Keywords: Physics-informed Machine Learning, Graph Convolutional Network, Ice Dynamics, Climate change, Snow mass balance

[a] Presenting Author

Airborne Snow Radar Data Simulation via Deep Generative and Physics-Driven Methods

Masoud Yari [1, a], Maryam Rahnemoonfar [2]
[1] Lehigh Uinversity, E-mail: yari@lehigh.edu
[2] Lehigh Uinversity, E-mail: maryam@lehigh.edu

Monitoring the properties of ice sheets in the polar regions is a major challenge in glaciology. Although a significant amount of radar data is available from the polar regions, it is heterogeneous and has been collected through expensive missions. It is still a great challenge to extract meaningful information from this large volume of data. In recent years, with the advancement of machine learning techniques, many scientists have been interested in using these algorithms and techniques to explore and mine Arctic and Antarctic data. However, these advancements have mostly happened in supervised learning where the models are data-hungry and require large amounts of annotated data. Generating simulated data can be an effective and affordable way to provide large labeled datasets for training machine learning models. In this study, we explore two approaches to simulate Arctic snow radar echogram images: a physics-based approach combined with statistical measures, and a data-driven approach based on a generative network. We use several image comparison metrics to analyze the usefulness of both methods for simulating echograms. Our results demonstrate that the physics simulator generates images with good structural similarities, while the purely data-driven approach achieves better textural similarities for simulated images. Finally, we show that by augmenting our real dataset with the simulated echograms, we can enhance our deep-learning model for tracking internal layers of snow.

Keywords: deep generative models, physics-informed machine learning, simulation, radar, arctic, ice sheet, climate change

[a] Presenting Author

Computed tomography based finite element modelling of femur to predict fracture risk: Age-related Variations

Rahul A. Gujar[1], Kirtibala V. Shinde[2], Neeta Mandhare[3]
[1,3] Pimpri Chinchwad College of Engineering, Pune (MH), India, rahul.gujar@pccoepune.org
[2] ValueDX Technologies, Pune (MH), India, kirtibalashinde@gmail.com

This study endeavors to comprehensively investigate the stress-strain distributions in order to predict the fracture risk of the femur bone utilizing advanced finite element analysis. Employing state-of-the-art techniques, a meticulously constructed 3D model of the femur bone was generated from high-resolution computed tomography image data, utilizing the cutting-edge capabilities of Simpleware ScanIP software. This sophisticated femur bone 3D model, incorporating realistic heterogeneous material properties, was further subjected to rigorous analysis utilizing the powerful Altair Hypermesh software. The investigation involved the application of boundary conditions, subjecting the femur head to an incremental compression loading, ranging from 1000 N to 8000 N, at selected inclinations of 0°, 8°, and 15. The ensuing analysis evaluated the von Mises stress and strain distributions for each distinct tilting condition, thereby successfully finding the precise scenarios exhibiting the highest risk of femur fracture. Eighteen human femur bone samples were employed and classified into four distinct age groups: 21-35 years, 36-50 years, 51-65 years, and 66 years above. Subsequently, finite element modelling were performed and assessing the influence of age, bone tilt, and compressive load on the fracture risk of the femur bone. The comprehensive study successfully unveiled that the von Mises stress and strain distributions exhibited notable variations, intrinsically linked to the age of the subjects, the tilting of the bone, and the magnitude of the applied loading. Strikingly, the highest risk of fracture was consistently observed at a higher inclination under identical loading conditions across all age groups. Furthermore, the analysis revealed a pronounced trend, with individuals belonging to the higher age groups exhibiting the maximum fracture risk, emphasizing the critical role of age in determining susceptibility to femur fractures.

These groundbreaking findings possess profound implications for the realm of clinical practice, as they offer immense potential in terms of fracture risk prediction and the formulation of personalized treatment strategies. This study represents a significant leap forward in our understanding of femur fracture risk assessment, paving the way for enhanced clinical decision-making and improved patient outcomes.

Keywords: von mises; computed tomography; stress; strain; fracture risk; finite element modelling; femur; heterogeneous.

Cognitive Modelling of Human Translation Production: Eliciting Mental Translation Processes through Translation Data Analytics and an Active Inference Agent

Michael Carl
mcarl6@kent.edu

What makes human translation difficult? Why do translators produce sometimes flawless fluent translations, while at other times they encounter uncertainty, hesitation and engage in extended revision? Which parts of a translation are accomplished "automatically" with little apparent effort, and which sections require reflective thought and human experience?

The talk addresses these questions from an empirical angle by exploring how translators distribute their cognitive resources in their work. I draw on a large database of translation behavioral data that consists of recorded translation sessions - keystrokes and eye movements (gaze data) in time - suited to elicit the underlying mental processes that generate the observed translation behavior. The structure of typing-pausing and the eye-hand (keystrokes) coordination, as retrieved from the recorded data, suggests that translations unfold on (at least) three embedded layers of concurrent sensorimotor, cognitive, and phenomenal processes. I suggest modelling these embedded processing layers as an artificial agent within a hierarchical architecture in which each of the processing layers realizes a different timeline, overviewing more fine-grained or larger stretches of temporal coordination. The agent is based on the Free Energy Principle (FEP, Friston 2009, 2010) and Active Inference (AIF, Parr et al 2023), drawing on principles of Bayesian inference and predictive coding. It aims at modelling the temporal dynamics of human translation production, delving into the interplay between the execution of entrenched translation routines, reflective thought and human experience.
Understanding these intrinsic mental mechanisms and interdependencies is critical for advancing cognitive translation studies (CTS) and it has implications for research in broader fields related to human language production, cognitive sciences and creativity studies in general.

It is trained and evaluated on empirical translation process data.

The agent will be instrumental to model and thus increase our understanding of coordination and interaction of translation and the translation effort.
Through simulation experiments, the ACTIMODE agent will reproduce actions and events of human translators as they type, monitor, and reflect on their translation outcomes.

is able to reproduce the temporal structure of translation processes. The agent

It investigates how, where and why translators invest their mental resources during translation production by

It investigates the hidden mental mechanisms and processing strata that bring about those performance parameters, assuming that the interplay between translators' expertise, source text complexity, and expected translation quality cause the observed fluency effects. Within an Active Inference framework, ACTIMODE examines different forms of linguistic anticipation at different levels in the ACTIMODE architecture that best explains translators’ behavior.

ACTIMODE will develop

Keywords:

Total Energy Consumption for the UAV Swarm Based on Temporal Energy Demand Models in Different Flight States

Micahł Duda [1, a], Krzysztof Falkowski [2]

[1] Military University of Technology in Warsaw, E-mail: michal.duda@wat.edu.pl

[2] Military University of Technology in Warsaw, E-mail: krzysztof.falkowski@wat.edu.pl

Increasing interest in Unmanned Aerial (UAV) vehicles prompts scientists to research new rapid prototyping methods and develop such systems. While working with physical devices grants satisfying results, new technologies allow to perform a significant part of the research in virtual reality. In such a case, the UAVs are modeled, and their performance is simulated in given conditions. This method is advantageous when not a single but an entire swarm of UAVs is considered. Then, the ability to simulate large amounts of such objects accelerates the research without needing to build or buy numerous physical devices.

Swarms of UAVs are often referred to rotary-wing drones, which are used in a large variety of tasks due to their properties, the main one being the ability to remain in a hover state. They are also capable of precise flight in all directions. However, such capabilities come with a significant drawback, which is limited flight time. The battery capacities are often low; hence, any optimization of energy consumption can contribute to better swarm performance. Although there is a high interest in UAV swarms, much research neglects this aspect of those systems.

Mathematical modeling of dynamics for rotary-wing UAV is a complex task as it involves few independent propellers and their impact on the drone's motion. The more precision is considered, the more complicated the formulas and calculations. The task is even more complex when energy consumption needs to be described analytically. The number of steps that need to be described to transform the energy stored in the battery to the propeller's thrust is significant, even if efficiencies and energy losses are neglected.

The other approach allows us to skip the mathematical apparatus and determine the relations between the given physical values. If experimental data is available, it is possible to identify dynamic models, that describe the time characteristics of dynamic processes. Later, such models can be implemented into simulations, allowing us to imitate the physical processes with convincing precision. The drawback of this approach is that the inside of the process is not defined; therefore, the partial parameters cannot be determined by it.

Our research focuses on the rotary-wing UAV swarm performing Coverage Tasks using a stochastic sweep coverage algorithm. In this method, drones scan the task area, moving randomly and independently of each other. Due to the stochastic nature of the coverage, the

[a] Presenting Author

optimal solutions are represented by the best number of drones in the swarm, which allows them to perform the task in the least time but consume the least amount of energy. For the simulations to be precise, it is necessary to implement proper UAV models.

The physical UAV was built, and flight data was collected during experimental real-life flights. The dynamic models for different flight states were identified based on the collected data. The models described movement dynamics and temporal power while performing the maneuvers. Such an approach allowed us to simulate the swarm behavior closely mimicking the real-life system. Also, it was possible to evaluate the total energy consumption while performing the mission based on the power models.

This paper presents the method of determining the total energy consumption of the swarm using the identified models of the temporal power during different flight states. The power consumption chart during flight can be recreated for every UAV based on the flight states chart. Later, by integrating and summarizing it for the entire swarm, the total energy consumed can be evaluated. It is also possible to compare the amount of energy consumed to hover and what part of it was spent on the maneuvers. Optimal solutions regarding the number of drones in the swarm can be drawn from the results.

Keywords: UAV Swarms, modeling, energy consumption,

Smart Project Analytics:

Leveraging AI in VUCA Environments for Project Risk Management

Byung-Cheol Kim [1, a]

[1] Penn State University, the Behrend College, Erie, PA, USA. E-mail: buk70@psu.edu

Abstract: The rise of Artificial Intelligence (AI) technologies, particularly those powered by large language models (LLMs), introduces unprecedented challenges and opportunities for both engineers and business decision-makers. The traditional view of engineering projects as straightforward endeavors with clear goals is evolving into complex and dynamic systems subject to the whims of VUCA (Volatility, Uncertainty, Complexity, and Ambiguity) environments. In this new reality, the role of project analytics becomes crucial, offering a range of tools that extract valuable insights from limited data and provide actionable intelligence.

This study investigates the emerging potential and early indicators of AI technology's impact on project risk analytics, particularly as a cornerstone in managing complex, large-scale projects in VUCA conditions. We demonstrate that AI technologies extend beyond providing simple tools for improving efficiency in everyday tasks, fundamentally reshaping how analytics are defined and utilized in project management. Our focus is on how technology, specifically LLMs like ChatGPT, can serve as an invaluable asset for beginners, facilitating detailed risk assessments by identifying, defining, organizing, and prioritizing potential risks. Moreover, we discuss how AI enhances our perspective, offering sophisticated approaches for the integration of expert insights into quantitative risk analysis using Monte Carlo simulation. The key insights from our investigation include:

- The intricate practice of project analytics under VUCA conditions.
- The end-to-end enhancement of project risk planning through AI.
- AI techniques for gathering and fine-tuning expert input for risk simulations.
- The broad application of AI in achieving a comprehensive project risk assessment.

Keywords: Artificial Intelligence (AI); Large Language Models (LLMs); Project Risk Analytics; VUCA (Volatility, Uncertainty, Complexity, Ambiguity); Monte Carlo Simulation

[a] Presenting Author

Author Biography:

Dr. Byung-Cheol Kim is an Associate Professor of Project and Supply Chain Management at the Black School of Business at Penn State Behrend. He earned his Ph.D. degree at Texas A&M University, TX. He served as an Assistant Professor at Ohio University and has seven years of industry experience in heavy highway construction. Dr. Kim has published one book on project management, and more than a dozen research articles in top-quality management journals such as the European Journal of Operational Research, IEEE Transactions on Engineering Management, Production Planning and Control, the Journal of Construction Engineering and Management, the Journal of Management in Engineering, and the Engineering Economist. His current research interests include project analytics, stochastic project control, risk visualization, forecasting, simulation modeling, Kalman filter forecasting, Bayesian decision making, and risk-based EVM systems. Dr. Kim is a registered Professional Engineer in Ohio, a registered Structural Engineer in South Korea, and a Project Management Professional.

Dataset Modelling Effect on Internal Thread Defect Detection

You-Rui Lai [1], Lih-Pying Huang [2], Thanh-Cong Nguyen [3], Quang-Cherng Hsu [4, a]

[1] National Kaohsiung University of Science and Technology, E-mail: F110142178@nkust.edu.tw

[2] National Kaohsiung University of Science and Technology, E-mail: I111142102@nkust.edu.tw

[3] National Kaohsiung University of Science and Technology, E-mail: I111142108@nkust.edu.tw

[4] National Kaohsiung University of Science and Technology, E-mail: hsuqc@nkust.edu.tw

The fastener industry is trending toward high quality and customization. The methods and requirements for fastener inspection are becoming increasingly stringent, especially for detecting surface defects in the internal threads. The traditional AOI detection methodology is no longer sufficient to meet the current demand. The rapid development of Deep Learning in recent years has led to numerous industries trying to use Deep Learning for detection, and the results have been excellent. Therefore, in this paper, deep learning is used to detect various defects on the surface of internal threads.

In this paper, the object detection method in YOLOv5 is used to detect the images of internal threads photographed by an industry camera with a tilt-shift lens. Figure 1 depicts the developed hardware, including an image-captured device with a lighting system and a position and rotation platform for detected components. The detection defects include extensive damage to the thread edges and crests, broken, as well as subtle burrs and granule defects. Table 1 lists the labeling images for internal thread defects. By utilizing several kinds of defects discovered on the surface of internal threads provided by various vendors, this study aims to validate the capability of models to train and detect internal thread defects with diverse or similar characteristics from several producers. The study also strives to observe the influence of the bounding box method for featuring defects on model training. The effect of the data augmentation hyperparameters and the number of model parameters is further explored. Finally, a transfer learning approach is employed to investigate the possibility of similar model training features across suppliers' internal thread defects.

The research results show that different bounding box strategies significantly impact the model training for internal thread defects, with a 5.5% difference in mAP (mean average precision) for the same dataset using YOLOv5. With the same amount of data, adjusting the data augmentation parameter increases the AP of burr defect from 63.6% to 72.9%, an increase of 9.3%, the AP of granule defect from 79.8% to 87.2%, an increase of 7.4%, and the mAP increases by 2.1%. Finally, the result of pre-training weights has a mAP of 81.6%, which is 11.2% higher than without pre-training weights for 80% training – 20% validation. The findings of this study demonstrate that the bounding box strategies positively impact model convergence during defect training. It was observed that adjusting the data augmentation parameters led to

[a] Presenting Author

a notable improvement in model performance. Additionally, the results suggest that mixing the datasets can enhance the model's ability to generalize and effectively train on new data.

Keywords: YOLOv5, Metal surface, Defect detection, Internal threads, Transfer learning, Data Augmentation

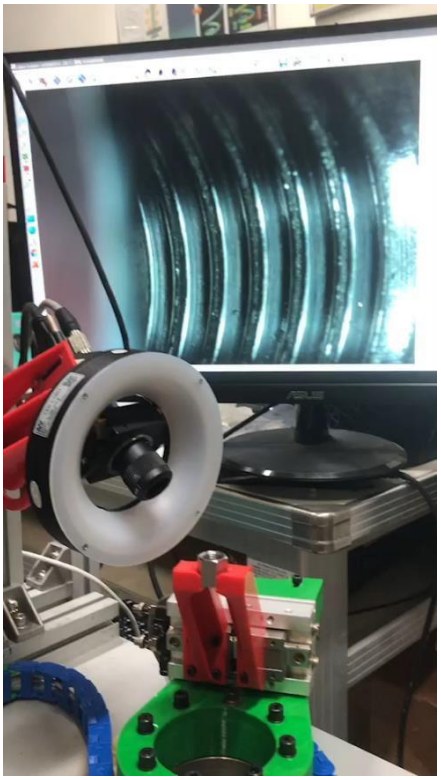
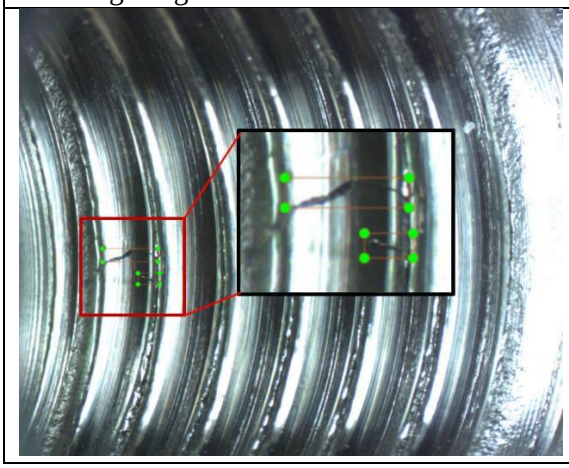


Fig. 1 Inner thread defect detection hardware including a position and rotation platform, industry camera with tilt-shift lens and lighting system, and computer with monitor.

Table 1 Labeling image and defect definition for inner threads only showing burr defect.

Labeling image	Defect definition and description
	Burr: strip with a length larger than 1/3 of the width of thread root or top; material can be stainless steel or carbon steel.

Multi-scale design and optimization of PC/ABS polymer blends

A. Francisca Carvalho Alves[1,*], Bernardo P. Ferreira[2], F. M. Andrade Pires[3]

[1]DeMec, Faculty of Engineering of University of Porto, Porto, Portugal, afalves@fe.up.pt
[2]School of Engineering, Brown University, 184 Hope St, Providence, RI 02912, U.S.A., United States, bernardo_ferreira@brown.edu
[3]DeMec, Faculty of Engineering of University of Porto, Porto, Portugal, fpires@fe.up.pt

Abstract: The PC/ABS polymer blend is one of the most successful commercial polymer blends, finding its main applications in automotive and consumer electronics. The relevance of this blend lies in the combination of both the excellent thermal and mechanical properties of polycarbonate (PC), and the improved toughness, processability and usually lower price and weight of acrylonitrile-butadiene-styrene (ABS) – itself a binary blend of styrene-acrylonitrile (SAN) and polybutadiene (rubber).

Depending on the loading conditions and the morphology of the blend, different deformation mechanisms control the response of the material, such as the internal particle cavitation of the rubber particles in the ABS and the debonding at the interface between the PC matrix and ABS particles [1]. While PC exhibits high toughness in some applications, it loses its toughness and becomes brittle in the presence of notches, small defects or scratches. In contrast, ABS has a high toughness and high notch resistance resulting from the cavitation of the rubber particles and the growth of voids. In this context, modelling the response of the PC/ABS blend and optimizing the design of its microstructure is a challenging task.

In the present contribution, a multi-scale framework is proposed to model the response of different PC/ABS blends and to optimize the design of their microstructure. This framework includes (i) the efficient generation of suitable representative volume elements for the PC/ABS microstructure [2], (ii) the establishment of accurate constitutive models for the blend phases [3], and (iii) the development of an efficient and unsupervised framework for optimizing the design of the blend's microstructure [4]. Within this setting, the open-source software CRATE [5] is employed to compute the response of several PC/ABS blends. CRATE performs multi-scale nonlinear analyses of heterogeneous materials at reduced computational cost by leveraging a suitable coupling between first-order computational homogenization and clustering-based reduced-order modeling. Several microstructure descriptors of the PC/ABS blends are then optimized by embedding the CRATE software in the open-source package piglot [6], tailored for the automated optimization of responses stemming from numerical solvers. With this framework, which can easily be extended to different materials and models, we find the optimal PC/ABS microstructure descriptors, namely the content of ABS and rubber, as well as the size and orientation of the ABS particles, that result in a blend with maximum toughness and strength at minimum cost and weight.

Keywords: Multi-scale modelling, Constitutive modelling, Polymer blends, PC/ABS, Material design, Reduced-order models, Derivative-free optimization

* Presenting author

References

[1] Seelig, T. and Giessen, E. 2007. Effects of microstructure on crack tip fields and fracture toughness in PC/ABS polymer blends. International Journal of Fracture. 145(3):205–222.

[2] Ferreira, B.P., Vila-Chã, J.V.C. and Andrade Pires, F.M. 2021. An adaptive multi-temperature isokinetic method for the RVE generation of particle reinforced heterogeneous materials, Part I: Theoretical formulation and computational framework. Mechanics of Materials. 163.

[3] A. F. Carvalho Alves, B. P. Ferreira, F. Andrade Pires. 2023. On the modeling of cavitation and yielding in rubber-toughened amorphous polymers: Fully implicit implementation and optimization-based calibration. International Journal of Solids and Structures. 283:112488.

[4] Rui Cardoso Coelho, A. Francisca Carvalho Alves, and F. M. Andrade Pires. 2023. Efficient constitutive parameter identification through optimisation-based techniques: A comparative analysis and novel composite bayesian optimisation strategy. Submitted to Computational Methods in Applied Mathematics. 289:107174.

[5] Bernardo P. Ferreira, F. M. Andrade Pires, and Miguel A. Bessa. 2023. Crate: A python package to perform fast material simulations. Journal of Open Source Software. 8(87):5594.

[6] Rui Cardoso Coelho, A. Francisca Carvalho Alves, T. M. Nogueira Pires and F. M. Andrade Pires. 2024. piglot: an Open-source Package for Derivative-free Optimisation. Submitted to Journal of Open Source Software.

Deep Learning-Based Longitudinal Analysis of Long-Term Gait Function Recovery in Post-Stroke Hemiplegic Patients

G. Kim [1], H. Kim [1] M.-T. CHoi [1, a]

[1] Sungkyunkwan University, E-mail: hn04008@skku.edu, gudxo1229@skku.edu, mtchoi@skku.edu

Long-term analysis of gait kinematic function recovery in post-stroke hemiplegic patients is important for personalized rehabilitation therapy. In this study, we present a long-term longitudinal clustering analysis to identify the type of gait recovery in post-stroke hemiplegic patients using kinematic time series data of lower limb joints directly. The analysis used data collected from 69 subacute patients aged 24-74 years, which consisted of eight joint (hip, knee, and ankle) gait cycles per patient (at 2, 3, 4, 6, 8, 10, 12 weeks, and 6 months after onset) using video motion capture. To process the time series data directly without human intervention for feature extraction, we created and optimized an end-to-end gait clustering model based on deep temporal clustering methods. Gait groups were extracted for different number of clusters, and kinematic characterization results were presented for the best performing clusters based on silhouette coefficients. This study can provide clinicians with an important tool for personalizing treatment plans for patients based on their gait recovery types in rehabilitation therapy.

Keywords: Post-stroke hemiplegia, Gait function recovery, Longitudinal analysis, Deep temporal clustering, Joint angle trajectories.

Acknowledgments: This study was supported by Translational Research Program for Rehabilitation Robots (NRCTR-EX23002), National Rehabilitation Center, Ministry of Health and Welfare, Korea.

[a] Presenting Author

Temporal Dynamics and Structural Relationships of Topics in Energy Security: An Integrated Approach Using Topic Modeling and Time-Series Analysis

Chankook Park [1], Yongwon Kim [2], Konghyun Kim [3, a]

[1] Korea Energy Economics Institute, E-mail: green@keei.re.kr

[2] Korea Energy Economics Institute, E-mail: yw.kim@keei.re.kr

[3] Korea Energy Economics Institute, E-mail: konghyun@keei.re.kr

Text mining and topic analysis have been key in identifying major themes and trends from vast text data, yet traditional topic modeling techniques fall short in fully capturing and interpreting the complex relationships and subtle meanings within text data. While traditional topic modeling methods like Latent Dirichlet Analysis (LDA) and Structural Topic Modeling (STM) analyze static relationships among topics, there's a need for advanced techniques that also consider dynamic relationships over time, especially for analyzing interrelations among multiple time-series topic data.

The aim is to understand the temporal relationships among key topics through the integration of topic modeling and time-series correlation analysis, tracking changes over time and deeply understanding their interrelationships. This includes analyzing which topics show similar patterns and which precede or follow in groups of topics with similar patterns.

Given the recent importance of energy security issues, heightened by events such as the Russia-Ukraine conflict and concerns around decarbonization, digitalization, and decentralization, this study focuses on energy security. The discussion around energy security is diversifying into various categories beyond the stability of fossil fuel supply and prices, including the supply of minerals for clean energy technologies and the security of power supply amid increasing intermittent renewable energy outputs.

The study utilizes academic papers related to energy security, employing abstracts from articles with "energy security" in their titles gathered from the SCOPUS database. The study aims to explore the long-term trends of issues related to energy security by collecting data spanning the last 20 years.

STM, advantageous for its ease in viewing topic proportion changes over time compared to LDA, will be used. STM allows for the application of time as a covariate, useful for examining the time-series changes of topic proportions. Furthermore, the Vector Auto Regressive (VAR) model will be utilized to understand the correlations among time-series data,

[a] Presenting Author

with the Akaike Information Criterion (AIC) or Bayesian Information Criterion (BIC) helping to examine the leading and lagging periods among topic time series.

The study expects to uncover how complex issues surrounding energy security evolve over time. By identifying correlations among various topics related to energy security, it aims to determine which topics exhibit similar patterns. Understanding the leading or lagging tendencies among topics will help design models for predicting the future direction of specific topics, combining topic modeling and time-series analysis to forecast the future landscape of latent topics hidden in text data.

Keywords: Energy security, Topic modeling, Time-series analysis

Decoding Artificial Intelligence's Impact on the Energy Sector through Structural Topic Modeling and Hierarchical Clustering

Chankook Park [1, a]

[1] Korea Energy Economics Institute, E-mail: green@keei.re.kr

The swift rise of Artificial Intelligence (AI) across various industries, particularly in the energy sector, offers notable benefits for efficiency, safety, and eco-friendliness, while introducing challenges including cybersecurity, data management, and the high cost and energy demands of AI integration. Issues also span from strategic operational integration within organizations to labor impacts and ethical considerations.

Research to date often examines AI's potential and challenges within specific sectors without a holistic overview, and there's a lack of objectivity in selecting which issues to address. For a meaningful, long-term application of AI in the energy sector, it's essential to comprehensively review related challenges and explore the interconnectedness of various topics.

Utilizing topic modeling for thematic analysis in literature is common, but it typically stops short of understanding the structural relationships between topics. Integrating hierarchical clustering with topic modeling can overcome this limitation, offering a deeper analysis that not only identifies but also understands how topics are interconnected. This combined approach facilitates a more detailed exploration of AI's role in the energy sector, supporting a nuanced analysis that captures the complexity of issues involved. This methodology not only prioritizes the breadth and depth of research topics but also enhances the strategic understanding necessary for addressing AI's multifaceted impacts on the energy sector.

The objectives of this study include the following:

- To develop an unbiased framework for identifying key issues related to AI integration in the energy sector, surpassing the constraints of prior research that lacked objectivity in selecting issues,
- To analyze how the identified issues structurally interrelate to grasp the overarching themes within the energy sector, thus guiding the strategic decisions of organizations and policymakers.
- To propose a methodology that compiles the vast array of knowledge from existing literature, employing a holistic research approach that values diversity and inclusivity over the selective examination of a few papers or reports.

Research abstracts containing the keywords "artificial intelligence" and "energy" were collected from SCOPUS, a leading academic research database. The selection criteria included

[a] Presenting Author

documents in English language, and the document types were articles, reviews, and conference papers. The timeframe focused on the recent trends, covering papers from the last ten years (2014 to 2023).

To systematically review the extensive knowledge discussed in the energy sector to date, we utilized Structural Topic Modeling (STM), a probabilistic topic modeling approach. Unlike Latent Dirichlet Analysis (LDA), which assumes independence between topics, STM offers the advantage of examining correlations among topics. By not only analyzing the correlations between topics through STM but also examining the hierarchical relationships among them, we can systematically understand the structural relationships between topics. Therefore, we plan to apply hierarchical clustering techniques in addition to STM to enhance our analysis.

This study may reveal how various issues related to AI in the energy sector are interconnected, providing insights into the complex web of technological, economic, environmental, organizational, labor, and ethical considerations. This could include identifying thematic clusters that capture overarching trends and challenges.

This study will uncover implications for future research, suggesting areas that need deeper investigation and offering strategic insights for academia and industry. This analysis will not only deepen our understanding of AI's current role in the energy sector but also guide future research towards addressing the sector's emerging challenges and opportunities, fostering a more holistic approach to AI integration.

Keywords: Artificial Intelligence, Energy Industry, Structural topic modeling, Hierarchical Clustering

Threshold Combinatorial Multicriteria Acceptability Analysis for Group Decisions with Subjective Interpretations of Objective Measurements

Jana Goers[1,*], **Graham Horton**[1]

[1]Otto-von-Guericke University Magdeburg, Universitaetsplatz 2, 39106 Magdeburg, Germany
E-mails: jana.goers@ovgu.de and graham.horton@ovgu.de

Abstract: Combinatorial Multicriteria Acceptability Analysis (CMAA) [1] is an algorithmic framework for supporting group decisions. It is designed for use with cooperative decisions such as are typically made by teams of Engineers, Physicians or Managers. CMAA can be used to convert any standard (i.e. single-user) decision method into a group method. The method uses Monte Carlo simulation to sample a combinatorial state space and the entropy of the preferredness of the alternatives as a consensus metric. It provides both facilitation guidance for a consensus-building process and analytical insights into the state of the decision at each discussion step.

Cooperative decisions are often based on objective values such as technical specifications or environmental measurements. Decision-makers have to convert this data into subjective estimates of its value contribution. For example, in the wind turbine selection problem [2], an Engineer might rate a 3MW wind turbine as 'Fair' and a 3.5MW turbine as 'Good' with respect to the criterion 'Power Output'. Such subjective estimates carry the risk of both intra-decision-maker and inter-decision-maker judgement inconsistencies, which can decrease the reliability of the recommendation. However, both types of inconsistency can be prevented by using threshold judgements, which define satisfaction levels that are applied to all alternatives. For example, in the wind turbine selection problem, threshold judgements might state that any power rating above 3.2MW and below 3.8MW is 'Good'.

In our presentation, we will introduce a new CMAA variant that is suitable for decisions that require threshold judgements. We show that the number of steps needed to reach consensus is typically small and is only weakly dependent on the size of the decision problem and the number of decision-makers. This makes the method suitable even for large group decisions. Furthermore, the computational space generated by the algorithm is much smaller than that of standard CMAA, and the cognitive load on the decision-makers is lighter.

The key advantage of CMAA over typical multi-criteria group methods is the efficiency of its consensus- building heuristic. At each step, the method computes the improvement in the degree of consensus that can be obtained by resolving each judgement conflict. The conflict with the greatest potential for improvement is presented to the decision-makers for resolution. For example, in the wind turbine selection problem, the algorithm might task the decision-makers with resolving their conflicting proposals for the threshold that separates a 'Fair' power output from a 'Good' one. By sharing their knowledge and experience, they create a shared understanding of the issue. The conflicting thresholds are replaced by a unanimous value which can be applied to all alternatives, resulting in an updated decision problem with significantly reduced complexity.

We illustrate the potential of the new method by applying it to two Engineering [2, 3] and two Forest Management [4, 5] group decisions from the literature. The initial analysis reproduced the most-preferred alternative in each case, and the consensus-building algorithm would have been able to guide the group to complete consensus in a small number of discussion steps. We conclude that the new method can provide

robust support and fast consensus-building for this class of Engineering and Management decisions and therefore represents a valuable extension to the range of applicability of the CMAA framework.

Keywords: group decision-making; consensus building; acceptability analysis, subjective judgements

* Presenting author

References

[1] J. Goers, G. Horton. 2023. Combinatorial multi-criteria acceptability analysis: A decision analysis and consensus-building approach for cooperative groups. European Journal of Operational Research, Vol. 308(1), pp. 243-254.

[2] V. Bagočius, E.K. Zavadskas and Z. Turskis (2014). Multi-person selection of the best wind turbine based on the multi-criteria integrated additive-multiplicative utility function. Journal of Civil Engineering and Management, Vol. 20(4), pp 590-599.

[3] R. Osmond, Z. Mollahoseini, J. Singh, A. Gautam, R. Seethaler, K. Golovin and A. Milani (2021). A Group Multicriteria Decision Making with ANOVA to Select Optimum Parameters of Drilling Flax Fibre Composites: A Case Study. Composites Part C: Open Access, Vol. 5(100156).

[4] A. Kangas, J. Kangas, R. Lahdelma and P. Salminen (2006). Using SMAA-2 method with dependent uncertainties for strategic forest planning. Forest Policy and Economics, Vol. 9(2), pp 113-125.

[5] S. Laukkanen, T. Palander, J. Kangas and A. Kangas (2005). Evaluation of the multicriteria approval method for timber-harvesting group decision support. Silva Fennica, Vol. 39(2), pp 249-264.

Rethinking materials simulations: blending numerical simulations with various machine-learning strategies

Rémi Dingreville[1,*]

[1]Center for Integrated Nanotechnologies, Sandia National Laboratories, E-mail: rdingre@sandia.gov

Abstract: Materials simulations are omnipresent across diverse scientific domains including physical, chemical, biological, and materials sciences. Existing state-of-the-art direct numerical solvers (DNS) used for these simulations are accurate but computationally expensive for predicting materials evolution across timescales, due to the complexity of the underlying evolution equations, the nature of multiscale spatio-temporal interactions, and the need to reach long-time integration. In this talk, I will discuss how we can rethink and accelerate such materials simulations by blending numerical solvers with various machine-learning strategies, notably phase-field simulations whose solutions involve high spatiotemporal gradients, an open challenge in this field of computational materials simulation. To that end, I will examine several points that need to be considered. First, I will discuss some of the trade-offs to account for in terms of solution reconstruction and stability when using a blending strategy [1]. Second, I will describe how to integrate a community (phase- field) numerical solver with various machine-learning strategies (recurrent neural networks, neural operators) to enable accurate extrapolation and efficient time-to-solution predictions of the dynamics [2, 3, 4, 5]. I will discuss the type of performance that can be expected, but also some of the remaining challenges in terms of efficient training and extrapolation of such an hybrid solver. SNL is managed and operated by NTESS under DOE NNSA contract DE-NA0003525.

Keywords:

* Presenting author

References

[1] Desai, S., Shrivastava, A., D'Elia, M., Najm, H. N., Dingreville, R. 2024. Trade-offs in the latent representation of microstructure evolution. *Acta Materialia*, 263, 119514.

[2] Montes de Oca Zapiain, D., Stewart, J. A., Dingreville, R. 2021. Accelerating phase-field-based microstructure evolution predictions via surrogate models trained by machine learning methods. *npj Computational Materials*, 7(1), 3.

[3] Hu, C., Martin, S., Dingreville, R. 2022. Accelerating phase-field predictions via recurrent neural networks learning the microstructure evolution in latent space. *Computer Methods in Applied Mechanics and Engineering*, 397, 115128..

[4] Oommen, V., Shukla, K., Goswami, S., Dingreville, R., Karniadakis, G. E. 2022. Learning two-phase microstructure evolution using neural operators and autoencoder architectures. *npj Computational Materials*, 8(1), 190.

[5] Oommen, V., Shukla, K., Desai, S., Dingreville, R., Karniadakis, G. E. 2023. Rethinking materials simulations: Blending direct numerical simulations with neural operators. *arXiv preprint* arXiv:2312.05410.

A Principled Robust Extreme Machine Learning (PRELM) with Minimax Optimization Scheme

Geng Deng[1,*], Han Wang[2], Guangning Xu[3], Xindong Wang[4], Qiang Fu[5]

[1]Wells Fargo Bank, E-mail: geng.deng@wellsfargo.com
[2]Wells Fargo Bank, E-mail: han.wang2@wellsfargo.com
[3]Wells Fargo Bank, E-mail: guangning.xu@wellsfargo.com
[4]Wells Fargo Bank, E-mail: xindong.wang@wellsfargo.com
[5]Wells Fargo Bank, E-mail: ken.fu@wellsfargo.com

Abstract:

Ensuring the robustness of machine learning models is essential, especially in real-world scenarios where data may be scarce, corrupted, or manipulated. The introduction of Extreme Learning Machine (ELM) [1] has offered efficient solutions for various machine learning tasks, thanks to its simplicity and computational efficiency. However, traditional ELMs may lack robustness when confronted with data noises and their inherent random mapping uncertainty.

ELM is essentially a single-hidden-layer feedforward neural network with untuned randomized weights in the hidden layer. Provided training data features X and responses Y , the ELM model is expressed as follows:

$$\min_{\beta} \text{Loss}(\text{H}(\text{X}^T\text{a} + \text{b})\beta, \text{Y}),$$

where a and b represent the randomized hidden layer weights, H denotes the activation function, and β is the output layer weights to be optimized. We consider the choice of loss function to be least square loss for regression and binary cross-entropy loss for binary classification problem.

In this paper, we introduce PRELM, a principled robust formulation of ELM inspired by the robust classification approach pioneered by Bertsimas et al. [2]. PRELM employs a minimax optimization strategy to bolster the resilience of ELM against l_p perturbations affecting training data, including features X and responses Y , and the model's random weights a and b. To elaborate, under the perturbation of input feature X, PRELM is expressed as follows:

$$\min_{\beta} \max_{||\Delta X||_p \le \rho} \text{Loss}(\text{g}((\text{X} + \Delta\text{X})^T\text{a} + \text{b})\beta, \text{Y}),$$

where the inner optimization problem quantifies the most adverse loss given the perturbation ΔX. We initially solve the inner maximum loss problem and subsequently minimize β over the most adverse loss within the perturbing region defined by the perturbation magnitude ρ under the l_p norm, thereby yielding our robust formulation. By doing so, PRELM effectively addresses worst-case scenarios arising from l_p perturbations in both data and randomized weights.

We conduct several simulation studies. For classification problems, we assume a true classification hyperplane alongside limited training data and add perturbing noise. Similarly, for regression problems, we assume true regression coefficients. PRELM consistently outperforms standard ELM, yielding improved out-of-sample accuracy. Experimental results for benchmark datasets are evaluated via 10-fold cross-validation, demonstrating that PRELM enhances baseline performance. Furthermore, more rigorous analyses are conducted to evaluate the impact of different norms and perturbation magnitudes for random weights, offering insights into the behavior of the ELM framework under various conditions.

Overall, this research contributes to the advancement of robust machine learning through a unified minimax optimization framework. The proposed approach holds promise for bolstering the reliability and efficiency of machine learning systems across diverse real-world scenarios.

Keywords: Extreme Machine Learning, Robust Learning, Minimax Optimization, l_p perturbation

* Presenting author

References

[1] Huang, G.B., Zhu, Q.Y. and Siew, C.K., 2006. Extreme learning machine: theory and applications. Neurocomputing, 70(1-3), pp.489-501.

[2] Bertsimas, D., Dunn, J., Pawlowski, C. and Zhuo, Y.D., 2019. Robust classification. INFORMS Journal on Optimization, 1(1), pp.2-34.

A principled distance-aware uncertainty quantification approach for enhancing the reliability of physics-informed neural network (PINN)

Jinwu Li [1, a], Xiaoge Zhang [2]

[1] Department of Industrial and Systems Engineering, The Hong Kong Polytechnic University, Kowloon, Hong Kong Special Administrative Region of China,
E-mail: jinwu.li@polyu.edu.hk

[2] Department of Industrial and Systems Engineering, The Hong Kong Polytechnic University, Kowloon, Hong Kong Special Administrative Region of China,
E-mail: xiaoge.zhang@polyu.edu.hk

Abstract: Physics-Informed Neural Network (PINN) is a special type of deep learning model that encodes physical laws in the form of partial differential equations as a regularization term in the loss function of neural network. Most existing methods add the collocation points in a uniform manner, while such a practice might lead PINN to produce large prediction errors in certain areas. To enhance the reliability of PINN, we develop a principled uncertainty quantification approach to characterize the model uncertainty of PINN, and the estimated uncertainty is then exploited as an informative indicator to identify collocation points where PINN produces a large prediction error. In the proposed approach, we seamlessly integrate spectral-normalized neural Gaussian process (SNGP) into PINN for principled and accurate uncertainty quantification. In the first step, we apply spectral normalization on the weight matrices of hidden layers in the PINN to make the data mapping from input space to the latent space distance-preserving. Next, the dense output layer of PINN is replaced with a random Fourier features (RFF)-approximated Gaussian process to make the quantified uncertainty distance-aware. To examine the performance of different UQ approaches, we define several performance metrics tailored to PINN for assessing distance awareness in the measured uncertainty and the uncertainty-informed error detection capability. Three representative physical problems are used to verify the effectiveness of the proposed method in uncertainty quantification of PINN and compare the proposed approach with Monte Carlo (MC) dropout using the developed performance metrics.

Keywords: Uncertainty quantification; PINN; Spectral normalization; Gaussian process; Model uncertainty

[a] Presenting Author

Inference of dynamic systems from noisy and sparse data via physics-informed Gaussian processes

Shihao Yang[1,*]
In collaboration with Yan Sun[1], **Zhaohui Li**[2], **Jeff C. F. Wu**[1], **S. C. Kou**[3], **Samuel Wong**[4]

[1]Georgia Institute of Technology, E-mail: shihao.yang@isye.gatech.edu
[2] Chinese Academy of Sciences
[3] Harvard University
[3] University of Waterloo

Abstract:

Parameter estimation for nonlinear dynamic system models, represented by ordinary differential equations (ODEs) or partial differential equations (PDEs), using noisy and sparse experimental data is a vital task in many fields. We propose a fast and accurate method, physics-informed Gaussian process Inference, for this task. Our method uses a Gaussian process model over system components, explicitly conditioned on the manifold constraint that gradients of the Gaussian process must satisfy the ODE/PDE system. By doing so, we completely bypass the need for numerical integration and achieve substantial savings in computational time. Our method is also suitable for inference with unobserved system components, which often occur in real experiments. Our method is distinct from existing approaches as we provide a principled statistical construction under a Bayesian framework, which rigorously incorporates the ODE/PDE system through conditioning, and provides statistical confidence with uncertainty quantification.

This talk summarizes a few key findings in the presenting author's recent work, which can be found in [1, 2, 3, 4, 5].

Keywords: ordinary differential equations, partial differential equations, physics-informed Gaussian processes, inverse problem, Bayesian statistics

* Presenting author

References

[1] S. Yang, S. W. K. Wong, and S. C. Kou, "Inference of dynamic systems from noisy and sparse data via manifold-constrained Gaussian processes", Proceedings of the National Academy of Sciences (2021)

[2] Y. Sun, S. Yang, "Manifold-constrained Gaussian process inference for time-varying parameters in dynamic systems", Statistics and Computing (2023)

[3] S. Wong, S. Yang, S. C. Kou, "MAGI: A Package for Inference of Dynamic Systems from Noisy and Sparse Data via Manifold-constrained Gaussian Processes", Journal of Statistical Software (2023)

[4] SWK Wong, S. Yang, SC Kou. "Estimating and Assessing Differential Equation Models with Time-Course Data". J Phys Chem B. 2023 Mar 23;127(11):2362-2374. doi: 10.1021/acs.jpcb.2c08932.

[5] Z. Li, S. Yang, C. F. Wu, "Parameter Inference via Nonlinear Partial Differential Equations Informed Gaussian Processes", SIAM ASA Journal on Uncertainty Quantification (JUQ), in press

Estimation of the Effect of Changing Resistance Parameters On Engine Efficiency in Electrical Vehicles With Convolutional Neural Network

Umut KİTİŞ[1, a], Övünç POLAT [2]

[1] Akdeniz University, E-mail: umutkitis@akdeniz.edu.tr

[2] Akdeniz University, E-mail: ovuncpolat@akdeniz.edu.tr

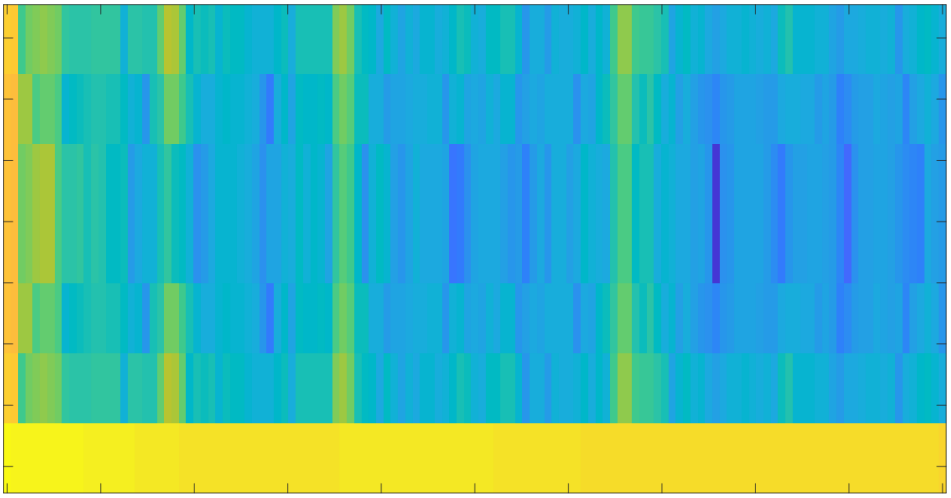
In asynchronous motors used in electric vehicles, the temperature of asynchronous motors changes due to coercive effects such as the slope or the friction coefficient of the road. As the temperature of asynchronous motors changes, the resistance values inside them also change, and this affects the efficiency of the asynchronous motor. In this study, the changing resistance parameters of the asynchronous motor were modeled, and the efficiency was estimated depending on the chance of stator resistance. The asynchronous motor was modeled in Simulink and Python programming language was used for Convolutional Neural Network via Spyder. Sequential model was used for CNN and Relu was chosen as the activation function. MaxPooling, Flatten and Dense layers were used in the intermediate layers.

In this study, the stator resistance of the induction motor was increased from 0.8 Ω to 4.75 Ω in 0.05 Ω intervals and the single-phase current values of the vehicle were measured at 80 different values. Then, image data generator was used to increase the dataset. The spectrogram of these values was taken and a dataset for CNN was created. %75 of the created data set was reserved for training, while %25 was used as test data. If the efficiency value obtained from measurement is below %80, the system is labeled as unsuccessful, and if it is above %80, the system is labeled as successful. The images of when the system is labeled as successful or unsuccessful are shown below.

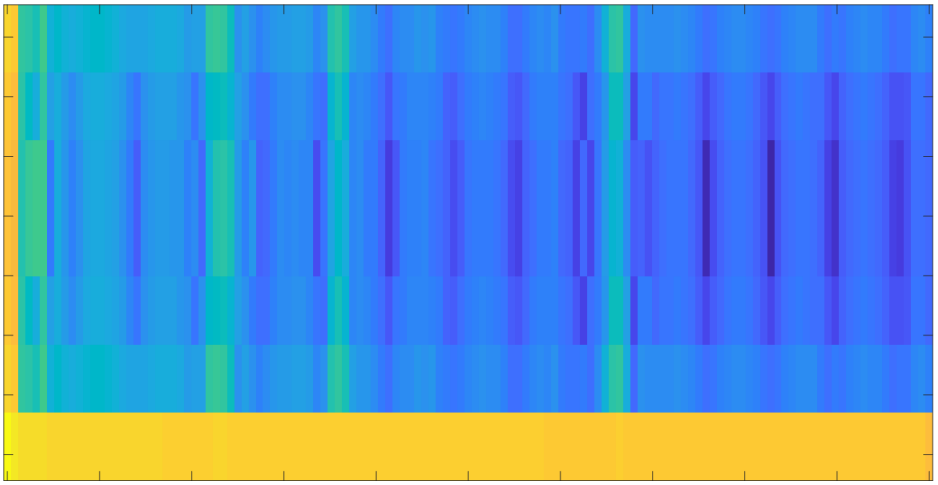
When the spectrogram window size is taken as 1024 and the epoch number is taken as 300, for the single-phase current values, train accuracy was found to be %100, and validation success was found to be %95.

Keywords: Electrical vehicles, CNN, Asynchronous motors, Python, Spectrogram

[a] Presenting Author



(a)



(b)

Figure 1 a) A Spectrogram image where the system is labeled as successful. b) A Spectrogram image where the system is labeled as unsuccessful.

Advancing Earthquake Prediction: An Evaluation of Deep Learning Approaches

MARAT NURTAS [1, 2, a], ZHUMABEK ZHANTAYEV[1], AIZHAN ALTAIBEK [1, 2], SERIK NURAKYNOV [1], BERIK ISKAKOV [1]

[1] Institute of Ionosphere, E-mail: maratnurtas@gmail.com

[2] International Information Technology University, E-mail: m.nurtas@iitu.edu.kz

This article emphasizes the significance of earthquake prediction in Kazakhstan and explores the application of deep learning to enhance prediction accuracy. Considering Kazakhstan's geographical position on the Eurasian plate—a hotspot for frequent seismic activity—the study adopts a Feed Forward Neural Network, a deep learning model tailored for regression problems, which demonstrates superior performance with the dataset used. The promising outcome, indicated by a mean square error of 0.22, underscores the potential of deep learning in improving earthquake prediction methodologies for the region.

Keywords: earthquake prediction, feed forward neural network, deep learning.

An earthquake is a natural phenomenon that occurs when the earth's crust suddenly moves. About 30% of the territory of Kazakhstan is under constant threat of destructive earthquakes, as there are more than 50 seismic active zones on the territory of the Republic, seismic potentials of some of them "provide" the formation of earthquakes with magnitudes up to 7-8. More than 6 million people live on this territory and 40% of the industrial potential of the Republic is concentrated. The territories of Almaty city, Almaty, East Kazakhstan, Zhambyl, Kyzyl-Orda, and South Kazakhstan regions are exposed to high potential seismic hazards. This means seismic impacts on settlements and other objects located near or within seismogenic zones can reach 9 or more points. In addition, earthquakes initiated by anthropogenic impact on the upper part of the Earth's crust due to the intensive development of oil, gas, and other fossil deposits, the creation of large water reservoirs, etc. may pose a potential danger.

Our work aims to revolutionize earthquake prediction using Deep Learning (DL) techniques [1]. Solving the problem of maximizing the accuracy of earthquake forecasting, it combines the computing power and capabilities of neural networks, offering a new solution to a long-standing geological problem [2].

The main scientific problem of this article is the unpredictability and complexity of earthquake phenomena. Currently, no recognized earthquake prediction method can determine the exact time, coordinates, and magnitude of earthquakes. But this problem can be solved by the growing potential of deep learning methods [3], as they are able to find patterns even in problems where at first glance one might conclude that there is no correlation. The deep learning network has many methods that need to be selected individually for each predicate task [4]. In our case, this is a feed-forward neural network. There are several layers hidden in

[a] Presenting Author

this model, each of which is fully connected to the next layer. Therefore, each layer has an activation function, an individual number of neurons, and an optimizer. This model is designed for a regression problem to predict the magnitude.

Our assembled dataset includes the following information: event timestamps, latitude and longitude coordinates, event depth, and magnitude values. The time, latitude, longitude, and depth columns were selected as input data. The output data is magnitude. For more convenient data training, we decided to divide the time column into year, month, and day [5]. As a result, we used 6 features to train the model: year, month, day, latitude, longitude, and depth. Pre-prepared training, validation, and test data were used for data training and outcome assessment. Train data comprise 0.7 part of the data, and the rest of the data in proportions of 0.5 were transferred to The output result of loss training and loss verification shows that there are no obvious deviations from the verification, we conclude that our data does not have overfitting.

References:

1. Yue Liu, Yuan Wang, Yuan Li, Bofeng Zhang & Gengfeng Wu, Earthquake Prediction by RBF Neural Network Ensemble,International Symposium on Neural Networks, Dalian, China, August 19-21, 2004, Proceedings, Part II, Advances in Neural Networks - ISNN 2004. doi:10.1007/978-3-540-28648-6_153.
2. W. Zhou, Y.W. Liang, Z. Ming, H.B. Dong, Earthquake prediction model based on danger theory in artificial immunity, Neural Network World 4/2020, pp. 231–247, doi: 10.14311/NNW.2020.30.016.
3. J. Reyes, A. Morales-Esteban, F. Martínez-Álvarez, Neural networks to predict earthquakes in Chile, Applied Soft Computing, Volume 13, Issue 2, February 2013, Pages 1314-1328. doi:10.1016/j.asoc.2012.10.014.
4. M.Nurtas, Zh. Zhantaev, A. Altaibek, S. Nurakynov, B. Iskakov and A. Ydyrys. Predicting the likelihood of an earthquake by leveraging volumetric statistical data through machine learning techniques. Engineered Scince Publisher. V. 26, Desember 2023, https://dx.doi.org/10.30919/es1031.
5. Marat Nurtas, Zhumabek Zhantaev, Aizhan Altaibek, Earthquake time-series forecast in Kazakhstan territory: Forecasting accuracy with SARIMAX, Procedia Computer Science, ISSN: 1877-0509, 231C (2024) pp. 353-358. https://doi.org/10.1016/j.procs.2023.12.216.

Acknowledgement: This thesis was conducted with the support of the Ministry of Education and Higher Sciences of the Republic of Kazakhstan, as part of the scientific project numbered-Grant No. BR20280979-OT-23.

Physics-Aware Recurrent CNNs for Extreme Physics Problems

Stephen S. Baek [1, a], H.S. Udaykumar [2]
[1] University of Virginia, E-mail: baek@virginia.edu
[2] University of Iowa, E-mail: hs-kumar@uiowa.edu

Physics-informed machine learning has increasingly been adopted for physics modeling and simulation. With the strong cognitive and predictive capabilities of modern ML algorithms, ML can now reduce the complexity of physical systems, learn the solution space of physics governing equations, bridge different physics across different length- and time-scales, discover the dynamics of unknown systems from observational data, etc. However, modeling unsteady, fast transient, and advection-dominated physics problems yet remains a pressing challenge for physics-aware machine learning. The physics of these extreme physical systems is governed by large systems of partial differential equations (PDEs) and ancillary constitutive models with nonlinear structures, as well as evolving state fields exhibiting sharp gradients and rapidly deforming material interfaces. Here, we investigate the efficacy of physics-aware recurrent convolutional neural networks (PARC) on field evolution problems with extreme dynamics characteristics. We first compare PARC with other physics-informed models on standard fluid dynamics benchmarks including Burgers' and Navier-Stokes equations. We then test PARC in more extreme dynamics settings including supersonic flow problems and shock-induced initiation of energetic materials, which exhibit unsteady fast transient behaviors with sharp gradients and discontinuous material interfaces evolving with the flow. On these problems, we examine the capabilities and limitations of PARC and discuss future research directions.

Keywords: Physics-informed machine learning; Physics-aware recurrent convolutional neural networks; Physics-aware deep learning; Data-driven modeling

[a] Presenting Author

Modelling of Unmanned Aerial Vehicle Behaviour Using Ground Effects

Jakub Djabin [1, a], Jakub Kochan [2], Krzysztof Falkowski [3]

[1] Military University of Technology in Warsaw, E-mail: jakub.djabin@wat.edu.pl

[2] Military University of Technology in Warsaw, E-mail: jakub.kochan@wat.edu.pl

[3] Military University of Technology in Warsaw, E-mail: krzysztof.falkowski@wat.edu.pl

The growing interest in unmanned aerial vehicles (UAVs) is prompting scientists to explore new rapid prototyping methods for developing such systems. While satisfactory results can be achieved through physical experimentation, new technologies enable a significant proportion of research to be conducted in the virtual realm. In this case, the UAVs are modeled, and their performance is simulated under given conditions.

The Wing-in-Ground-effect (WIG) is an aircraft designed to operate close to the surface of water or land. Such a solution allows a significant increase in flight efficiency while significantly reducing detectability. The ground effect is created by specially designed wings. The ground effect changes the pressure distribution around the wing, resulting in a different lift coefficient to that of an isolated wing. This means that the maximum lifting force occurs close to the water or land surface and decreases with altitude.

Modelling the mathematical dynamics of an unmanned aerial vehicle (UAV) utilizing the ground effect is a complex endeavor, involving a non-linear distribution of lift force intricately tied to the flight altitude. The quest for heightened precision leads to more elaborate formulations and calculations. The complexity is further heightened when the requirement involves sustaining a constant angle of attack. In such a situation, the multitude of variable factors significantly complicates the task of maintaining a constant desired altitude.

Modelling the mathematical dynamics of an unmanned aerial vehicle (UAV) using the ground effect is a complex endeavor, involving a non-linear distribution of lift force that is intricately linked to flight altitude. The quest for greater precision leads to more complex formulations and calculations. The complexity is further increased when the requirement is to maintain a constant angle of attack. In such a situation, the multitude of variable factors greatly complicates the task of maintaining a constant desired altitude.

This paper presents a method for investigating and analyzing the complex model of an unmanned aerial vehicle using the ground effect. The results obtained allow the precise determination of flight parameters under specific conditions. The presented model serves as a basis for the construction of a hardware-in-the-loop (HiL) research platform. The solutions

[a] Presenting Author

implemented allow the verification of the constructed structure without the risk of damaging or destroying its components.

Keywords: UAV, wing-in-ground-effect, ground effect, modeling, hardware-in-the-loop

Enhancing navigation systems on UAVs with image recognition

Jakub Kochan [1, a], Jakub Djabin [2], Krzysztof Falkowski [3]

[1] Military University of Technology in Warsaw, E-mail: jakub.kochan@wat.edu.pl

[2] Military University of Technology in Warsaw, E-mail: jakub.djabin@wat.edu.pl

[3] Military University of Technology in Warsaw, E-mail: krzysztof.falkowski@wat.edu.pl

The growing popularity of Unmanned Aerial Vehicles (UAVs) has led to increased research activity, particularly in navigation. UAVs are being used for a wide range of applications, including surveillance, mapping, delivery, and infrastructure inspection. As a result, there is a growing need to develop robust and reliable navigation systems specifically tailored to their unique requirements. As a result, researchers are exploring new methods to tackle the difficulties presented by GPS-denied or GPS-interfered environments, where conventional satellite-based navigation systems struggle. These environments can be found outside buildings, such as in military-occupied zones, where the GPS signal is often jammed, or inside buildings, such as hangars, where the GPS signal cannot penetrate. Additionally, counting systems suffer from localization errors that increase over time. Auxiliary systems can be used to reduce errors.

Image recognition-based navigation is a promising approach. It enables UAVs to navigate autonomously by interpreting visual cues from their environment. Advances in sensor fusion techniques, such as the integration of inertial sensors, rangefinders, and LiDAR, are paving the way for more accurate and robust navigation solutions. Research efforts are currently underway to improve the autonomy and adaptability of UAV navigation systems. This will enable them to dynamically respond to changing environmental conditions and unforeseen obstacles. In addition, new software approaches are also being developed. The increasing popularity of AI technology is also having an impact on new navigation methods, such as navigation by object detection or optical flow.

The identification and analysis of object features and edges using image processing algorithms is the core principle of the system. The system extracts valuable information based on spatial relationships and object motion by capturing and processing object positions in surrounding images. By tracking changes in object position over time, the system can accurately determine the real-time ground speed of moving objects such as UAVs. This information can be the basis for the calculation of a robot's motion during navigation.

The research aims to determine the motion of UAVs using Shi-Tomasi and Kanade-Lucas-Tomasi algorithms. The first of these algorithms identifies distinctive points that can be tracked over time in the subsequent frames taken by the camera. The camera must be mounted perpendicular to the ground and on a gimbal to keep its position. The second algorithm tracks

[a] Presenting Author

features in the image by searching for the same features in different frames. The system uses this information to calculate motion and ground speed.

This article presents a navigation system based on image recognition, designed for use on UAVs. The software is designed to be installed on common microcomputers such as Raspberry Pi 4 or Nvidia Jetson Xavier. The system can be an independent system that tracks the motion of UAVs or an auxiliary navigation system to compensate for errors in the counting system or in a GNSS-denied environment.

Keywords: UAV, GNSS, navigation, optical flow, features detection,

Data-driven Design and Optimisation of Mechanical Metamaterials

T. M. Nogueira Pires [1, a], R. P. Cardoso Coelho [2] and F. M. Andrade Pires [3]

[1] Faculty of Engineering, University of Porto, E-mail: up202200867@up.pt

[2] Faculty of Engineering, University of Porto, E-mail: ruicoelho@fe.up.pt

[3] Faculty of Engineering, University of Porto, E-mail: fpires@fe.up.pt

Keywords: *Mechanical metamaterials, Bayesian optimisation, Numerical response*

During the past decade, there has been a growing interest in the development of micro-architected materials that can offer tailored responses to mechanical, acoustic, thermal, chemical, or electromagnetic stimuli. These materials, known as metamaterials, exhibit exceptional specific stiffness or complex deformation modes such as bending under tension, torsion under tension and negative Poisson coefficient effects [1]. The geometry of the microstructure plays a significant role in their response, and choosing appropriate designs and optimising characteristic dimensions is crucial to achieving high-performing materials for a given application [2].

This work proposes a data-driven framework for designing and optimising mechanical metamaterials under various loading scenarios. We leverage multi-scale models incorporating computational homogenisation and Representative Volume Elements (RVEs) to analyse the material's behaviour. The framework employs a gradient-free optimisation approach using Gaussian Process (GP) regression and Bayesian optimisation. This strategy effectively addresses uncertainties inherent in the design process, enabling their quantification and usage throughout optimisation. Compared to traditional space-filling DoE methods, our framework efficiently explores the design space, with a fraction of function evaluations.

References:

[1] Dos Santos, W. F., Rodrigues Lopes, I. A., Andrade Pires, F. M., & Proença, S. P. B. (2024). Exploring novel mechanical metamaterials: Unraveling deformation mode coupling and size effects through second-order computational homogenisation. International Journal of Solids and Structures, 112724. https://doi.org/10.1016/j.ijsolstr.2024.112724

[2] Bessa, M. A., Glowacki, P., & Houlder, M. (2019). Bayesian Machine Learning in Metamaterial Design: Fragile Becomes Supercompressible. Advanced Materials, 31(48), 1904845. https://doi.org/10.1002/adma.201904845

[a] Presenting Author

Noise reduction study of structural monitoring data of in-service slab-on-girder bridge by means of topological data analysis method

Abstract: Road infrastructure in various countries, such as bridge projects, have now entered the stage of major maintenance and management, with various monitoring data and large amounts of data that urgently need to be analyzed and processed. Traditional data analysis techniques are challenged by the difficulty of extracting data features and the inaccuracy of removing noise from bridge monitoring data. Topological data analysis methods can help improve the noise reduction effectiveness of bridge monitoring data, as they can compute topological features at different scales in topological space and have advantages such as adaptive noise reduction. Specifically, the paper includes: (1) giving the basic algorithm of topological data analysis; (2) taking the displacement and strain sampled monitoring data of an in-service slab-on-girder bridge as the research object, and adopting the topological data analysis method to implement the noise reduction analysis on the sampled monitoring data; (3) In combination with wavelet transform, the topological data analysis method is further improved and reapplied to the noise reduction analysis of sample monitoring data, and the noise reduction effect under the topological data analysis method is compared with that under the improved topological data analysis method. The study shows that: bridge structural monitoring data belongs to typical time series data; topological data analysis method can be used to reduce the noise of bridge structure monitoring data; and the noise of bridge structure monitoring data can be further reduced by using the improved topological data analysis method. This study contributes to the scientific analysis and evaluation of the performance of in-service bridge structures by improving the accuracy of the analysis of bridge monitoring data.

Keywords: bridge monitoring data, topological data analysis method, noise reduction, wavelet transform, slab-on-girder bridge

Development of a Fast Wind Prediction Tool to Assess and Optimize Drone Flight Paths around Offshore Wind Turbines

G. Veiga-Piñeiro[1,*], P. Dominguez-Estevez[1], E. Aldao[1], G. Fontenla-Carrera, F. Veiga-López[1] E. Martin-Ortega[1] and H. González-Jorge[1]

[1]Instituto de F´ısica e Ciencias Aeroespaciais (IFCAE), Universidade de Vigo, Campus de As Lagoas, Ourense, 32004, Spain, E-mail: gonzalo.veiga@uvigo.gal

Abstract: Unmanned Aerial Vehicles (UAVs) are being considered as an effective solution for reducing maintenance costs of off-shore wind farms, owing to their versatility and ability to integrate payload for efficient and safe inspections. Although the use of these vehicles is considered one of the key elements for the profitability of offshore wind energy, the flight of these aircraft faces limitations as they are vulnerable to adverse weather phenomena such as wind shear, gusts, and wakes. Therefore, to ensure operational safety, high-resolution wind prediction models, such as those provided by Computational Fluid Dynamics (CFD), capable of adjusting to the local weather forecasting, are required in order to: (i) assess the safety of the future mission, and (ii) optimize the UAV path planning.

Nevertheless, the high computational cost of CFD simulations prevents a sufficiently fast prediction for the changing meteorological conditions. To address this challenge, this work presents a Reduced Order Model (ROM) based on High Order Singular Value Decomposition (HOSVD), a type of unsupervised Machine Learning technique based on dimensionality reduction [1], as a tool for a fast prediction of the wind flow around the off-shore turbine. The ROM model, which exploits efficiently a CFD database of Reynolds-Averaged-Navier-Stokes (RANS) simulations, provides a fast prediction of the flow variables (velocity, pressure, turbulent kinetic energy, ...) around the turbine and its platform in less than 1 min. The ROM model, in combination with a Dryden turbulence model to assess wind gusts, can be integrated in the response dynamic model of the UAV. To demonstrate the effectiveness of this model, a practical case study is presented here, where the simulation database, as well as the ROM model, are all built using open-source software (i.e, OpenFoam software for the CFD database and Python for the development of the ROM tool).

Keywords: Fast prediction models, High Order Singular Value Decomposition (HOSVD), Computational Fluid Dynamics (CFD)

* Presenting author

References

[1] S. L. Brunton,.B. R. Noack, P. Koumoutsakos. 2020. Machine Learning for Fluid Mechanics. Annual Review of Fluid Mechanics. Vol. 52, pp. 477-508.

Modelling energy consumption of vehicles serving people with special needs in the mountains

Grzegorz Sierpiński [1, a], Marcin Staniek [2]
[1] Silesian University of Technology, Poland, E-mail: grzegorz.sierpinski@polsl.pl
[2] Silesian University of Technology, Poland, E-mail: marcin.staniek@polsl.pl

Electricity, as a replacement for fossil fuels, is one of the options for powering vehicles in cities according to European Union guidelines. This is an environmentally friendly form, so it may also be allowed in protected areas, such as national parks or tourist trails in general (use of electric bicycles). The final decision rests with the manager of a given area and results from applicable regulations. The aim of the research project MOUNTAINS WITHOUT BARRIERS is to open the possibility of traveling and enjoying the charms of nature to people with special needs. For this purpose, a special vehicle is being built that will enable movement also on mountain trails, especially for people with limitations in independent physical functioning. This vehicle will be electrically assisted. The construction of such a vehicle also requires a decision to be made regarding the selection of the appropriate battery (which is related to distance limitation of the vehicle). Its rental will take place at a mobile rental base located close to the beginnings of the tourist trails. Manager and user should be sure that there will be enough energy for the entire route - leaving the base and returning along a specific route. The research problem is therefore to prepare an energy consumption model for an unusual vehicle and unusual traffic conditions.

In the case of electric cars, energy consumption in various conditions has been tested for many years, including by performing standardized driving tests (driving cycles) such as NEDC, FTP75, WLTC and others in laboratories equipped with chassis dynamometers. In the case of a special vehicle being built, a consumption model must be prepared from scratch. Two basic parameters were adopted, i.e. changes in terrain height and speed profile. Taking these parameters into account, it is possible to calculate the movement resistance forces and the demand for mechanical energy to carry out moving of the vehicle. The resistances occurring while driving are related to the vehicle parameters and variables describing the movement. The energy consumed in the vehicle is used to overcome resistance to movement, but also to power devices in the vehicle. In this situation, additional devices will include, among others: tablet and devices related to control and communication with the mobile rental base. To estimate the energy needed to overcome the resistance to motion, the value of the power needed to overcome it (multiplication result of the vehicle speed and the value of the resistance forces) can be used. Individual motion resistances (rolling resistance, hill resistance, aerodynamic resistance and inertia resistance) can be described by physical relationships. After summing them up, the value

[a] Presenting Author

of the demand for driving power at the wheels required for the vehicle to move is obtained. A particularly important variable for the energy consumption of traffic is the vehicle speed. Although it does not directly affect the value of each movement resistance force, it significantly affects the power of the movement resistance forces and thus also the energy required to overcome them. An additional problem is the need to take into account the use of energy also for other purposes - beyond engine. This applies to all electronic on-board equipment - from controlling the entire vehicle to lighting and multimedia. The electrical power consumed by devices other than the engine can be modelled as a constant power value averaging the variable demand during the test.

Building a model is possible by approaching the problem statistically. This means the need to collect statistical information from many trips in conventionally similar traffic conditions. For this purpose, a list of tourist routes has been designated. Then, those for which the maximum inclination is lower than the capabilities of the vehicle being built were identified. For such selected routes, using a digital terrain model, models were prepared divided into uniform sections containing information about the slope. The vehicle's on-board computer is capable of recording instantaneous energy consumption, and when combined with a route segment model, data on consumption, speed and inclination can be collected simultaneously (for a known segment length). A larger number of trips provides a larger statistical sample and at the same time increases the accuracy of the energy consumption model. This will help to decide on the number and total power of the batteries used.

The next stage of implementing the vehicle on tourist routes will be the preparation of an algorithm for selecting subsequent routes for the ready to use vehicle. In this case, after a numerical analysis of the terrain, a list of realistic routes to be travelled will be determined (part of the route is allowed if the entire route is not possible). The choice of the route will be possible by the fleet manager or the customer - depending on other factors, such as the degree of difficulty, windingness of the route, etc. (including tourist attractions), as well as depending on the state of current charge level of the vehicle batteries.

Keywords: GIS; spatial analysis; energy management, transport accessibility; disabled people; tourist routes

Acknowledgements.

The present research has been financed through the National Centre for Research and Development as a part of the competition within the scope of “Things are for people” in project with title: “Integrated platform for planning, organization, supervision and support for the availability of mountain tourism offer for people with difficulties in physical functioning and a specialized off-road vehicle for the implementation of the tourism offer - Mountains without barriers” realized by Silesian University of Technology.

Parameterisation of tourist trails for mountain travel safety with focus on people with disabilities

Marcin STANIEK [1, a], Grzegorz Sierpiński [2]

[1] Silesian University of Technology, Poland, E-mail: marcin.staniek@polsl.pl

[2] Silesian University of Technology, Poland, E-mail: grzegorz.sierpinski@polsl.pl

The aim of the research was to parameterize tourist trails, forest roads and bicycle routes located in mountainous areas of southern Poland. Using routing algorithms, parameterization of these roads allows you to identify safe routes for travel with a specialized off-road vehicle. The designed and manufactured vehicles will be used by people with special needs, in particular people with limitations in independent physical functioning. The vehicles created are one of the results of the ongoing MOUNTAINS WITHOUT BARRIERS project, which aims to improve the accessibility of the tourist offer in non-urbanized areas for people with special needs resulting from lack of full mobility. This is a change from the traditional approach to mountain tourism as a field of tourism intended only for people with full functionality, toward people who require additional support in its implementation.

One of the key assumptions of the project is to ensure the safety of mountain tourism for people, including people with disabilities, using new design solutions in manufactured specialized off-road vehicles. Mountain tourism requires the implementation of technical solutions that facilitate vehicle control, such as an uphill start assistant and a downhill descent assistant that prevents the vehicle from accelerating above the set downhill speed. It is also required to use additional modules to assess the position of the wheelchair and information for the driver or the reaction of the drive unit to a possible loss of stability in terms of movement on/down a hill.

Achieving an acceptable level of travel safety for people with special needs requires the implementation of routing algorithms in the travel planning system based on the criteria of minimising altitude gradients along the route. Using the open data source Open Street Map OSM and QGIS software, parameterisation of the inventoried routes was carried out. The DTM Digital Terrain Model was used to build the model, which is a discrete representation of the terrain height and, together with the interpolation algorithm, allows the calculation of the height at any point in the area for which the model was built. The algorithm developed in this way allowed for the parameterization of routes, among others: in longitudinal section. For the purposes of planning the routes of the routing algorithm, an elevation description was assumed with steps of 1 m along the route. As a result of using the QGIS tool, OSM and DTM data, a spatial record of routes was obtained.

As part of the database on tourist trails and forest roads, analyzes were carried out to characterize the potential of mountain areas in southern Poland as areas for mountain tourism

[a] Presenting Author

for people with special needs - moving using a specialized off-road vehicle. Of all the routes covered by the inventory, almost 70% are routes up to 10 km long and 87% are routes up to 20 km long; however, routes less than 1 km long were excluded from the analysis. The distribution of altitude differences of the routes for the following intervals: 100-200 m, 200-300 m, 300-400 m is similar and concerns approximately 18% of the routes for each interval. Further analyzes concerned the route and the possibility of traveling by disabled people using a specialized off-road vehicle. The analysis of the results shows that there are over 30% of routes with an even distribution in terms of uphill and downhill traffic. There are also routes in which at least 0.8 of the route length is uphill, and this applies to 7% of the inventoried routes. Similarly, routes with a slope are available (at least 0.8 of the entire route), constituting 11% of the routes covered by the analyses. Furthermore, the analyses carried out show that almost 3/4 of the routes are characterised by at least 80% of the route length within the assumed slope of 20% per 1 m for both uphill and downhill movement.

The analysis of data regarding tourist trails, forest roads and bicycle routes allows for the preliminary identification of roads with an acceptable level of travel safety for people with special needs, however, it is required to check the proposed routes in real conditions before completing the journey.

Keywords: GIS; spatial analysis; transport accessibility; disabled people; tourist routes

Acknowledgements.

The present research has been financed through the National Centre for Research and Development as a part of the competition within the scope of “Things are for people” in project with title: “Integrated platform for planning, organization, supervision and support for the availability of mountain tourism offer for people with difficulties in physical functioning and a specialized off-road vehicle for the implementation of the tourism offer - Mountains without barriers” realized by Silesian University of Technology.

Modelling transient flow in porous media under pumping conditions with physics-informed neural networks

Adhish Guli Virupaksha [1,2,a], François Lehmann[2], Marwan Fahs[3,4], Hussein Hoteit[4], Thomas Nagel[5]

[1]Université de Strasbourg, TU Bergakademie Freiberg, E-mail : agvirupaksha@unistra.fr

[2]Université de Strasbourg, E-mail : lehmann@unistra.fr

[3]Université de Strasbourg, [4]King Abdullah University of Science and Technology, E-mail : fahs@unistra.fr

[4]King Abdullah University of Science and Technology, E-mail : hussein.hoteit@kaust.edu.sa

[5]TU Bergakademie Freiberg, E-mail : thomas.nagel@ifgt.tu-freiberg.de

[a] Presenting Author

Physics-informed neural networks (PINNs) are a category of neural networks that combine the governing physical laws and the neural network architecture [1]. These models intend to take advantage of the power of data-driven approaches, like neural networks, by constraining them with the governing equations of physical processes to improve accuracy and generalization, particularly in scenarios with limited or noisy data.

PINNs are beginning to be utilized for modelling flow in porous media [2, 3]. However, they are often limited to steady state problems. In this work, we show how PINNs can be used in transient cases with pumping involved. As transient simulations are required, we suggest a time scaling approach to normalize the space and time domains.

The flow processes in saturated porous media are governed by Darcy's law and the continuity equation, given as follows:

$$S\frac{\partial H}{\partial t} - \frac{\partial}{\partial x}(k\frac{\partial H}{\partial x}) - \frac{\partial}{\partial y}(k\frac{\partial H}{\partial y}) = Q \qquad (1)$$

where $S[L^{-1}]$ represents the storativity, $H[L]$ represents the pressure head, $k[L \cdot T^{-1}]$ represents the hydraulic conductivity, and $Q[T^{-1}]$ is the source/sink term.

H is assumed to be the output of the deep neural network. The derivatives are approximated using automatic differentiators with respect to the inputs of the neural network (time and space). The approximated terms are used to satisfy the governing partial differential equation (PDE) on a given number of collocation points. Since PINNs do not utilize any predefined datasets, the neural network is trained by creating data points in line with the initial and boundary conditions. The loss function is defined by the mean square error, as follows:

$$\text{MSE} = \text{MSE}_{\text{PDE}} + \text{MSE}_{\text{BC}} + \text{MSE}_{\text{IC}} \qquad (2)$$

Where MSE_{PDE}, MSE_{BC}, and MSE_{IC} represent the errors related to the PDE, the boundary conditions and the initial conditions, respectively.

The three components of the loss function are defined as follows:

$$\text{MSE}_{\text{PDE}} = \frac{1}{N_f}\sum^{N_f} f(t_i, x_i, y_i)^2 \qquad (3)$$

$$\text{MSE}_{BC} = \frac{1}{N_b}\sum^{Nb}(H^b(t_i, x_i, y_i) - H^b_i)^2 \quad (4)$$

$$\text{MSE}_{IC} = \frac{1}{N_I}\sum^{NI}(H^I(t_i, x_i, y_i) - H^I_i)^2 \quad (5)$$

Here $H^I(t_i, x_i)$ and $H^b(t_i, x_i)$ represent the initial and boundary conditions, N_f, N_b and N_I are the number of collocation points used to impose the physical equations, the boundary and initial conditions, respectively. The temporal domain is scaled by a factor of 10^{-3} such that $t^* = t \times 10^{-3}$.

The function f used in MSE_{PDE} is defined as the residual form of Eq. (1):

$$f = 10^{-3}S\frac{\partial H}{\partial t^*} - \frac{\partial}{\partial x}(k\frac{\partial H}{\partial x}) - \frac{\partial}{\partial y}(k\frac{\partial H}{\partial y}) - Q \quad (6)$$

As a first step, the PINN-based method has been applied to a 1D case. The application to 2D problems is under development. A sample of the results obtained with PINNs in a 1D scenario is presented in Figure 1. The scenario involves a 1D confined aquifer of length 3 m, with a pressure head on left being 5 m and the right-hand side pressure head being 4.5 m. The initial condition is the steady state condition of the aquifer. A constant pump discharge is then introduced at the middle of the aquifer at the rate of 1 kg $m^{-3}s^{-1}$. The transient solution every 2 s is then obtained and compared to the equivalent result from COMSOL Multiphysics. The results show good agreement with each other.

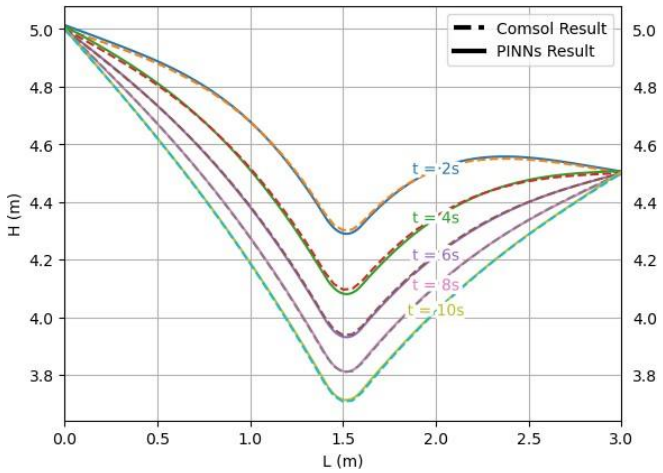


Figure 1: Pressure head distribution at different time steps in aquifer: Comparison of PINNs and COMSOL

Keywords: PINNs, Porous Media, Aquifer with pumping, Darcy's law

References:

[1] M. Raissi et. Al., Physics-informed neural networks: A deep learning framework for solving forward and inverse problems involving nonlinear partial differential equations, Journal of Computational Physics, Volume 378, Pages 686-707 (2019).

[2] Lal Dangi et al. Predicting flow in porous media: a comparison of physics-driven neural network approaches," Mathematical Models in Engineering, Vol. 9, No. 2 (2023).

[3] Lehmann et al. A mixed pressure-velocity formulation to model flow in heterogeneous porous media with physics-informed neural networks, Advances in Water Resources, Vol 181 (2023) 104564.

Leveraging Enhanced Dimensionality Reduction Techniques for Biometric Profiling and Verification: Subspace-Adaptive Autoencoder Vector (SAAV) Systems

Alvaro Paricio-Garcia[1,*], Miguel A. Lopez-Carmona[1], Sergio Sierra-Arquero[1]

[1]Universidad de Alcalá, E-mail: alvaro.paricio@uah.es, miguelangel.lopez@uah.es, sergio.sierra@edu.uah.es

Abstract:

Physical asset authentication and authorization have been classical challenges in security frameworks. This challenge increases its complexity when the assets require association with specific persons (for property, usage, permissions, and others) using biometric capabilities. Concerns like connectivity, smartphones, personal data protection, legal, and traceability arise. One of the most significant issues still open is storing large amounts of biometric features, typically high-dimensional, in a small space such as an RFID card or a QR code. Dimensionality reduction enables data suitable for a wide range of real-world applications. In biometric profiling and verification, most systems rely on a given metric measuring the similarity between features to determine whether two samples belong to the same person. For this reason, the dimensionality reduction method must be measure-preserving, meaning that it should retain the underlying structure of the data, as any loss of information may lead to a decrease in accuracy. Existing methods such as Principal Component Analysis (PCA) or Linear Discriminant Analysis (LDA) are only sometimes practical for this purpose, as they assume that the data is linearly separable, which is not always the case. AI-based autoencoders enable the catching of non-linear structures in the data, reducing biometrics dimensionality. In this paper, we propose a novel biometric profiling and verification method, Subspace-Adaptive Autoencoder Vectors (SAAV), which provides efficient and accurate dimensionality reduction properties. The effectiveness of SAAV is demonstrated through extensive experiments on public benchmark datasets for facial recogni- tion, showing that it outperforms existing methods in accuracy and efficiency. It reduces the facial footprint payload dramatically (up to 80%, depending on the encoding structure) while preserving the recognition rates.

Keywords: Biometrics, Computer vision, Face recognition, Artificial Intelligence, Autoencoders

* Presenting and correspondence author

Bibliography

[1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15, 16]

References

[1] A. Jain, A. Ross, and S. Pankanti, “Biometrics: A tool for information security,” *IEEE Transactions on Information Forensics and Security*, vol. 1, no. 2, pp. 125–143, Jun. 2006.

[2] W. Qian and N. Jian-wei, “Encryption Algorithm Based on RSA,” *Journal of Chongqing University*, 2005.

[3] Z. J. Luo, R. Liu, and A. Mehta, “Understanding the RSA algorithm,” Aug. 2023.

[4] M. Nofer, P. Gomber, O. Hinz, and D. Schiereck, “Blockchain,” *Business & Information Systems Engineering*, vol. 59, no. 3, pp. 183–187, Jun. 2017.

[5] M. Di Pierro, "What Is the Blockchain?" *Computing in Science & Engineering*, vol. 19, no. 5, pp. 92–95, 2017.

[6] "General Data Protection Regulation (GDPR) – Official Legal Text," https://gdpr-info.eu/.

[7] R. Want, "An introduction to RFID technology," *IEEE Pervasive Computing*, vol. 5, no. 1, pp. 25–33, Jan. 2006.

[8] 14:00-17:00, "ISO/IEC 18004:2015," https://www.iso.org/standard/62021.html.

[9] S. Lancaster, D. Yen, S. Lancaster, and D. Yen, "Biometric Controls and Privacy," https://www.igi-global.com/gateway/chapter/www.igi-global.com/gateway/chapter/60966, Jan. 1.

[10] F. Schroff, D. Kalenichenko, and J. Philbin, "FaceNet: A Unified Embedding for Face Recognition and Clustering," in *2015 IEEE Conference on Computer Vision and Pattern Recognition (CVPR)*, Jun. 2015, pp. 815–823.

[11] S. Z. Li, A. K. Jain, and J. Deng, Eds., *Handbook of Face Recognition*. Cham: Springer International Publishing, 2024.

[12] H. Abdi and L. J. Williams, "Principal component analysis," *WIREs Computational Statistics*, vol. 2, no. 4, pp. 433–459, 2010.

[13] A. Tharwat, T. Gaber, A. Ibrahim, and A. E. Hassanien, "Linear discriminant analysis: A detailed tutorial," *AI Communications*, vol. 30, no. 2, pp. 169–190, Jan. 2017.

[14] D. Bank, N. Koenigstein, and R. Giryes, "Autoencoders," Apr. 2021.

[15] U. Michelucci, "An Introduction to Autoencoders," Jan. 2022.

[16] M. Refinetti and S. Goldt, "The dynamics of representation learning in shallow, non-linear autoencoders*," *Journal of Statistical Mechanics: Theory and Experiment*, vol. 2023, no. 11, p. 114010, Nov. 2023.

Dynamic SpatioTemporal Graph Attention Network for Enhanced Urban Traffic Demand Prediction

Alvaro Paricio-Garcia[1]*, Miguel A. Lopez-Carmona[1], Pablo Manglano-Redondo[1]

[1]Universidad de Alcala, Alcala de Henares, 28805, Madrid, Spain
E-mail: alvario.paricio@uah.es, miguelangel.lopez@uah.es, pablo.manglano@edu.uah.es

Abstract:

In urban mobility, accurately forecasting traffic demand is paramount for the efficacy of traffic management systems. We introduce a traffic flow calibration methodology employing the Dynamic SpatioTemporal Graph Attention Network (DSTGAT) neuronal networks mechanism. It is acclaimed for its proficiency in deciphering the spatiotemporal patterns prevalent in urban traffic flows. DSTGAT stands out by dynamically appraising the relevance of distinct segments within the road network and their temporal correlations through advanced graph attention mechanisms. This capability allows DSTGAT to dissect the multifaceted nature of traffic demand, distinguishing between periodic trends and stochastic variations, thereby refining the understanding of traffic behaviors. Crucially, this approach reduces the impact of data noise, elevating the precision of traffic predictions. To enhance DSTGAT's efficacy, we apply some optimization techniques to finetune essential model parameters, including the configuration of hidden layers, the learning rate, and the iteration count during training. This bespoke optimization ensures the model's alignment with the unique characteristics of the traffic data, optimizing its predictive performance for dynamic traffic scenarios. Our validation, conducted with real-world data from densely populated urban settings, illustrates notable advancements in predictive accuracy over conventional models and contemporary deep learning techniques. The empirical evidence showcases a marked diminishment in prediction errors, such as the mean absolute and root mean square errors, affirming DSTGAT's transformative potential in advancing traffic demand prediction for dynamic traffic management.

Keywords: Artificial Intelligence, Traffic Flow Calibration, DSTGAT, Urban Mobility, Machine Learning.

* Alvaro Paricio-Garcia

Bibliography

[1, 2, 3]

References

[1] H. Rakha, B. Hellinga, M. V. Aerde, & W. Perez, "Systematic Verification, Validation and Calibration of Traffic Simulation Models."

[2] C. Tang, J. Sun, & Y. Sun, "Dynamic Spatial-Temporal Graph Attention Graph Convolutional Network for Short-Term Traffic Flow Forecasting," in *Proceedings of the 2020 IEEE International Symposium on Circuits and Systems (ISCAS)*, Oct. 2020, pp. 1-5. doi: 10.1109/ISCAS45731.2020.9181234.

[3] T. Chai & R. R. Draxler, "Root mean square error (RMSE) or mean absolute error (MAE)?," *Numerical Methods*, preprint, Feb. 2014. doi: 10.5194/gmdd-7-1525-2014.

Prediction of the Combustion Process for a Hydrogen-Air Mixture Based on Neural Network Modeling

Karandashev I.M.[1,2, a], Mikhalchenko E.V.[1], Malsagov M.Yu.[1], Stamov L.I.[1]
[1] SRISA RAS, Moscow, E-mail: karandashev@niisi.ras.ru
[2] RUDN University

Direct integration of detailed chemical mechanisms with many components and reactions into three-dimensional gas-dynamic problems is currently limited by available computational resources. With the continuous development of computing power, numerical modeling of complex phenomena such as combustion is becoming cheaper and more efficient. Currently, the approach using neural networks is promising for accelerating the solution of problems of gas dynamics of chemically reacting media. The advantages are obvious: the number of chemical components involved in the process is not critical for a neural network and the same architecture can be used for different kinetic mechanisms.

In this paper, the problem of combustion of a hydrogen-air mixture is considered. The initial state of the system is given by pressure, temperature, and molar densities of hydrogen, oxygen, and other compounds formed in the combustion process, including possible radicals: H_2, O_2, H_2O, OH, HO_2, H_2O_2, H, O, OH*. Also involved in the process are N_2 and Ar, which remain chemically neutral and whose amount does not change over time. During the combustion process, the temperature of the medium rises. The mathematical formulation of the problem is as follows. The system of differential equations is solved:

$$\frac{dX_k}{dt} = \omega_k(X_1,...,X_{N_C};T),$$

where X_k is the molar density of the component k, $\dot{\omega}_k$ is the intensity of production of a mole of the component in a unit volume, $k = N_C$, N_C is the number of components. The functions $\dot{\omega}_k$ are calculated based on a given kinetic mechanism like that of GriMech 3.0 (1999).

Using this numerical approach, 10,000 numerical experiments were performed, each with 500 time steps for various time step dt chosen randomly from 1ns to 10mks, which formed a dataset for training and testing the neural network.

Figure 1 shows the architecture of the neural network. To make such a compact architecture able to describe our system of differential equations, we needed to change the training algorithm. We included the prediction of several steps in recurrent mode in the training process. The network was trained for several steps at once, i.e., the network output was fed to the input some number of times n_{step}, and the loss function was calculated from the accumulated data:

$$Loss = \sum_{t=1}^{n_{step}} MSE\left(Y_t, Y_t^{pred}\right)/t,$$

[a] Presenting Author

where Y_t and Y_t^{pred} are the reference and the prediction by the network at step t, respectively.

By summing the prediction errors several steps ahead, the network automatically learns to account for recurrent error accumulation and minimize it. This approach avoided the problem of error accumulation when using a neural network recurrently, and it was able to predict the development of a chemical process over hundreds of steps. In the experiments, we used $n_{step} = 50$.

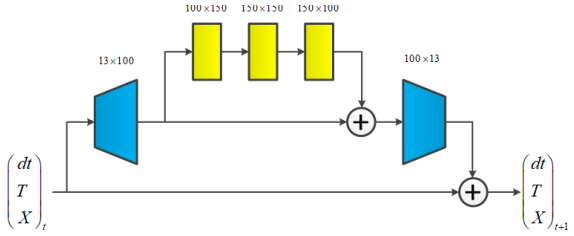


Figure 1. The neural network architecture. The network takes as input the modeling time step dt, initial temperature T and molar densities of the components X.

The main difficulty in solving this problem is that the processes strongly depend on environmental conditions (pressure, temperature, density) and observation parameters (time step, number of steps). For example, during the observation interval, no fire may occur (the time step is too small), or, due to the time step being too large, the system will jump directly from the initial state to the final state. As a result, most of the training data are almost constants. This is clearly visible in Figure 2, where an example of one process at three different steps (1ns, 300ns and 10mks) is shown in different colors. All three processes are derived from the same starting state. The graphs at the bottom were obtained by a trained neural network in recurrent mode for 500 steps. With a small time step, the process proceeds smoothly, but with an increase in the step, we get a sharp jump to an equilibrium state. Despite this, the neural network managed to learn and predict quite well.

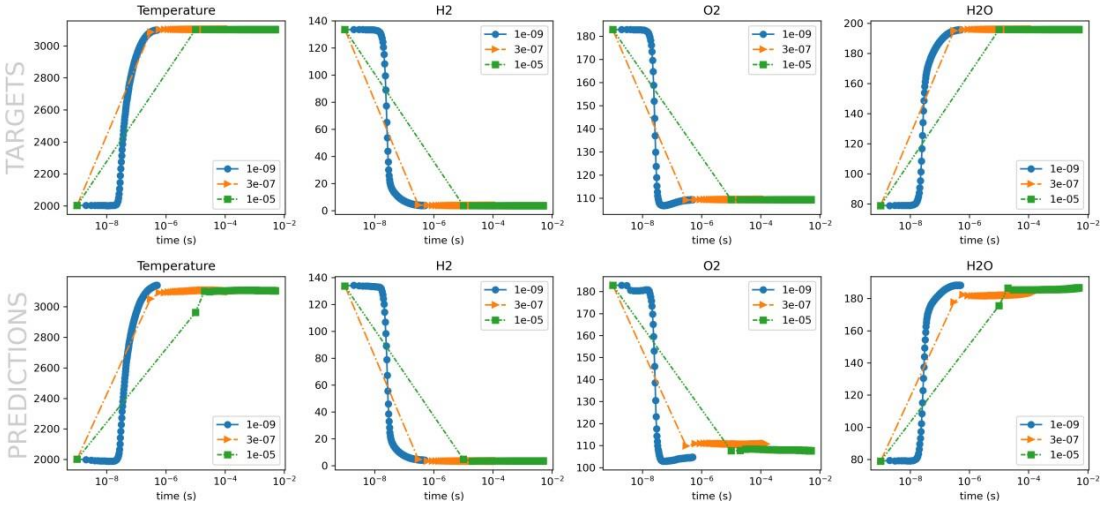


Figure 2. Results: exact numerical calculation (top); neural net approximation (bottom).

Keywords: numerical modeling of chemical processes, combustion, neural networks, deep learning, hydrogen-air mixture.

Bayesian Optimisation for Data-Driven Design of Polycrystalline Materials

R. P. Cardoso Coelho[1,*], **F. M. Andrade Pires**[2]

[1]Faculty of Engineering, University of Porto, E-mail: ruicoelho@fe.up.pt
[2]Faculty of Engineering, University of Porto, E-mail: fpires@fe.up.pt

Abstract: In recent decades, there has been a significant exploration into modelling intricate material systems, particularly in the automotive, aeronautical, and aerospace industries. This exploration has yielded accurate models for the material response under various conditions. Simultaneously, advancements in computational power have enabled the rapid execution of simulations, crucial for meeting industrial demands. These developments have paved the way for tackling inverse problems, wherein numerical techniques are employed to address real-world optimisation challenges such as parameter identification and material design.

This study delves into a data-driven framework for designing polycrystalline materials, inspired by previ- ous research [1]. Crystal plasticity models are used to obtain the constitutive response in a multi-scale framework. The problem is framed as a gradient-free optimisation task, using Gaussian Process regression and Bayesian optimisation for its numerical solution. Furthermore, this framework facilitates optimisation under uncertainty and outperforms classical space-filling techniques in the exploration of the design space. The optimisation problem is solved with the in-house optimisation toolbox piglot, which has been recently open-sourced.

Moreover, inspired by recent advances in parameter identification through composite Bayesian optimisation strategies [2], similar approaches are explored to enhance the quality of surrogate models in material design problems. This endeavour aims to refine the design process further and reduce the computational cost of the inverse problem.

Keywords: material design, Bayesian optimisation, inverse problems

* Presenting author

References

[1] Bessa MA, Glowacki P, Houlder M. Bayesian Machine Learning in Metamaterial Design: Fragile Becomes Supercompressible. Advanced Materials. 2019;31(48):1904845.

[2] Cardoso Coelho R, Alves AFC, Pires F. Efficient Constitutive Parameter Identification Through Optimisation-Based Techniques: A Comparative Analysis and Novel Composite Bayesian Optimisation Strategy. SSRN; 2023.

Informed Machine Learning-Driven Optimization of BVP Solvers for Enhanced Melt Spinning Process

Viny Saajan Victor [1, 2, a], Manuel Ettmüller [1], Andre Schmeißer[1], Heike Leitte[2], Simone Gramsch[1, 3]

[1] Fraunhofer ITWM, Kaiserslautern, E-mail: viny.saajan.victor@itwm.fraunhofer.de

[2] RPTU Kaiserslautern University, Kaiserslautern, E-mail: leitte@cs.uni-kl.de

[3] Frankfurt UAS, Frankfurt, E-mail: simone.gramsch@fb2.fra-uas.de

The melt spinning process constitutes the initial step in the production of technical textiles, which form the basis for nonwoven fibers with distinct characteristics such as strength, durability, wrinkle resistance, and moisture-wicking capabilities. These textiles have widespread applications in sectors like manufacturing, healthcare, sanitation, transportation, etc. The primary objective of the textile industry concerning the melt spinning process is to enhance textile quality while ensuring economical and sustainable production. Achieving this requires the efficient adjustment of complex production lines through a systematic analysis of various production parameters and material properties. Data-driven analysis within an industrial setting is challenging due to several constraints. Line operators often lack the necessary domain knowledge, and continuous manufacturing, coupled with limited types of measuring equipment, makes data collection impractical. Consequently, the process is typically modeled as a system of ordinary differential equations, facilitating systematic optimization and analysis in an ideal machine. Additionally, due to the process conditions, certain fiber properties are predetermined at the start and end positions of their production, resulting in differential equations with boundary values. Typically, classical boundary value problem (BVP) solvers are used to solve these equations, which provide state-of-the-art accuracy suitable for engineering applications. However, their computational demand makes them unsuitable for real-time applications. Additionally, these solvers use iterative techniques that require an initial guess for the solution. The choice of this guess affects the solvability and performance of the solver. Currently, determining the initial guesses either involves trial-and-error methods or relies on domain expertise.

In this study, our goal is to address challenges faced by BVP solvers through the integration of machine learning. We present a workflow designed to reduce the time and domain expertise required for optimizing and analyzing the melt spinning process. This comprehensive approach entails three primary contributions. Firstly, we enhance optimization by training a machine-learning model (neural network) to solve the differential equations that provide accurate predictions for effective initial guesses. This accelerates the convergence of numerical BVP solvers, reducing both time and domain expertise requirements. Secondly, we enhance analysis by introducing a real-time visualization tool. This tool, utilizing the trained machine-learning model, assists various stakeholders involved in the analysis process. Thirdly, we integrate domain knowledge into our machine-learning pipeline in the form of differential

[a] Presenting Author

equations. This ensures that the machine-learning model is informed by the underlying physics of the melt spinning process, in conjunction with training data from numerical BVP solvers. This integration enhances the overall efficacy and reliability of our workflow. In our previous work, we introduced this workflow for the isothermal melt spinning process. We demonstrated the notable acceleration achieved in both the optimization and analysis phases **[1]**. Additionally, we visually illustrated how integrating physics knowledge into the machine-learning algorithm could enhance its accuracy and reliability **[2]**. Building on this foundation, our current work extends to encompass melt spinning processes with varying temperatures, incorporating the influence of another critical process property—crystallization **[3]**. We also consider the interaction between the surrounding airflow and the fibers in production. With this expanded scope, our objective is to capture the nonlinearities inherent in a more complex production setting, thereby achieving a higher degree of acceleration. In the context of integrating domain knowledge, we explore the inclusion of process-specific physical laws in both the learning and design phases of the machine-learning pipeline for improved accuracy and reliability.

In summary, our objective is to leverage the potential of machine learning to improve traditional numerical models within the realm of scientific machine learning. While we illustrate our workflow specifically for the BVP solver in the context of melt spinning processes **[4]**, this approach has the potential for generalization to other numerical solvers that use an iterative approach to solve differential equations requiring an initial guess.

Keywords: Melt Spinning, Textile Industry, Manufacturing, Optimization, Sustainable Production, Numerical Solvers, Ordinary Differential Equations, Boundary Value Problems, Informed Machine Learning, Scientific Machine Learning

References

[1] V.S. Victor, M. Ettmüller, A. Schmeißer, H. Leitte, S. Gramsch. 2024. Informed Machine Learning for Optimizing Melt Spinning Processes. Submitted to IEEE Conference on Artificial Intelligence.

[2] V.S. Victor, M. Ettmüller, A. Schmeißer, H. Leitte, S. Gramsch. 2023. VisForPINNs: Visualization for Understanding Physics Informed Neural Networks. IEEE 6th Workshop on Visualization for AI Explainability. IEEE VIS.

[3] M. Ettmüller, W. Arne, N. Marheineke, and R. Wegener. 2023. Product integration method for the simulation of radial effects in fiber melt spinning of semi-crystalline polymers. PAMM, Wiley Online Library, vol. 22, no. 1, p. e202200210.

[4] J. Kierzenka, and L. F. Shampine. 2001. A BVP solver based on residual control and the Maltab PSE. ACM Transactions on Mathematical Software (TOMS), ACM New York, NY, USA, vol. 27, no. 3, pp. 299–316.

Harnessing Color: Predicting Copper Recovery in Bioleaching Processes with RGB Measurement

[1] Jordi Vives Pons, [2]Teresa Escobet, [3]Albert Comerma, [4]Antonio D. Dorado, [5]*Marta I. Tarrés-Puertas , E-mail: marta.isabel.tarres@upc.edu

[1] Department of Mining, Industrial and ICT Engineering, Informatics Engineering Section, Universitat Politècnica de Catalunya—BarcelonaTech (UPC), 08242 Manresa, Spain
[2] Department of Mining, Industrial and ICT Engineering, Electronics Engineering Section, Universitat Politècnica de Catalunya—BarcelonaTech (UPC), 08242 Manresa, Spain
[3] Serra Húnter Fellow, Department of Mining, Industrial and ICT Engineering, Electronics Engineering Section, Universitat Politècnica de Catalunya—BarcelonaTech (UPC), 08242 Manresa, Spain
[4] Department of Mining, Industrial and ICT Engineering, Chemical Engineering Section, Universitat Politècnica de Catalunya—BarcelonaTech (UPC), 08242 Manresa, Spain
[5] Department of Mining, Industrial and ICT Engineering, Informatics Engineering Section, Universitat Politècnica de Catalunya—BarcelonaTech (UPC), 08242 Manresa, Spain
* Author to whom correspondence should be addressed.

Electronic waste, commonly referred to as e-waste, is known to contain valuable metals, particularly copper. Bioleaching, an established method for metal recovery, exploits the capabilities of microorganisms to extract metals in an environmentally sustainable manner. This study presents a novel approach for predicting copper recovery by leveraging RGB values captured using a color sensor. Through the application of machine learning techniques, a predictive model is developed to forecast copper recovery based on color data collected throughout the solution of the bioleaching process. The model is trained and validated using a dataset of RGB values and pH. The investigation explores various regression methodologies to predict copper values, ultimately identifying Random Forest Regressor and Multivariate Polynomial Regressor algorithms as the most effective techniques. This significant finding, combined with real-time data acquisition, paves the way for the future development of a digital twin for the bioleaching industry, enabling precise control actions and corrective measures without disrupting the involved biomass. In conclusion, this research underscores RGB data analysis as a practical and efficient approach for assessing copper content in bioleaching processes and making decisions in case of deviation from optimal behavior.

Keywords: industrial IoT; real-time systems; open-source; copper recovery; real-time monitoring system; color sensing; metal recovery; bioleaching; machine learning; Random Forest Regression

INTRODUCTION

This paper presents an innovative and cost-effective monitoring approach aimed at tracking chemical reactions crucial for copper recovery from electronic waste (e-waste).

Building upon our prior research, notably detailed in [1], which elucidated the hardware model, and [2], introducing an open-source software tool for monitoring key parameters in a real bioleaching station prototype.

The bioleaching plant is divided into five distinct stations, each with its own purpose: Bioreactor, Tank 1, Leaching, Tank 2, and the Copper Recovery System, as documented in [2]. Our current study is centered on an advanced monitoring station equipped with a digital RGB sensor. This sensor at the Bioreactor station is particularly adept at detecting subtle color changes within the solution, facilitating real-time observation and analysis of metal dissolution and recovery processes. The hardware, comprising a color sensor and a rugged ESP32 based Programmable Logic Controller (PLC) compatible with Arduino tools, processes and transmits data for analysis, enabling real-time monitoring, improving process efficiency, and sustainability compared to traditional methods. It is beneficial for researching bioprocesses for metal recovery from e-waste and applicable to other hydrometallurgical processes involving direct contact with leaching agents. Previous literature, as evidenced by works such as those cited in [3], indicates that Random Forest Regression stands out as the preferred algorithm for estimating recovery rates in bioleaching studies, utilizing a variety of input variables such as initial pH or atomic number. In our approach, we introduce a novel application of Random Forest Regression, employing RGB values as input variables to predict copper recovery.

METHODOLOGY

This research aims to forecast the copper volume recovered using data from a smart color sensor. This data guides the bioleaching plant to halt the process upon reaching an optimal threshold, thereby conserving energy. Currently, plant operators determine process cessation based on sensor readings, experience, and occasional material analysis. Subsequently, a performance indicator, typically Root Mean Square Error (RMSE), is chosen for regression problems. RMSE quantifies prediction errors, with larger errors carrying more weight. The Pearson correlation coefficient and the coefficient of determination are also used in our research. To obtain a dataset, four trials of the bioleaching process were conducted to establish a relationship between the color of Fe2+/Fe3+ and concentration. Each trial involved filling the prototype plant column with 16g of shredded cables and 10g of filler (created using a 3D printer) and using 1.3L of Fe3+ solution produced by microorganisms.

During the trial, multiple samples were gathered to track the Fe2+/Fe3+ values and establish a connection between the concentration of these ions and the color of the solution identified by the smart color sensor installed in the plant, along with a pH sensor employed on-site.

RESULTS

The proposed method can well-estimate the concentrations of Cu(II) and Fe(III) ions from the color of the solution and pH on the training set, both when working with PCBs, with determination coefficient equal to 0.97 for Cu(II) and equal to 0.98 for Fe (III), respectively. Therefore, it was determined that the model predicts the concentration of Fe(III) more accurately than that of Cu(II). In summary, the results indicate a promising research direction concerning the correlation between the color sensor and the recovered material's value.

CONCLUSIONS

It is advisable to augment the dataset used for model training and explore alternative independent variables. For instance, one could explore excluding the blue value from the sensor data. Subsequent to this adjustment, conducting a comparative analysis of the resulting values is essential for refining the experiment. Furthermore, optimizing all facets of the real-time bioleaching monitoring system and control infrastructure, including color sensors, harbors the potential for substantial advancements in large-scale bioleaching plants.

ACKNOWLEDGEMENTS

This work was supported by the Spanish Agencia Estatal de Investigación Project Ref PID2020-117520RA-I00/AEI/10.13039/501100011033 and the UPC Research group RIIS under AGAUR SGR-CAT 2021 Grant.

REFERENCES

Morell J, Escobet A, Dorado AD, Escobet T. Design of a RGB-Arduino Device for Monitoring Copper Recovery from PCBs. Processes. 2023; 11(5):1319. https://doi.org/10.3390/pr11051319

Tarrés-Puertas MI, Brosa L, Comerma A, Rossell JM, Dorado AD. Architecting an Open-Source IIoT Framework for Real-Time Control and Monitoring in the Bioleaching Industry. Applied Sciences. 2024; 14(1):350. https://doi.org/10.3390/app14010350

Parastou Mokarian and Ivan Bakhshayeshi and Firouzeh Taghikhah and Yasaman Boroumand and Eila Erfani and Amir Razmjou, The advanced design of bioleaching process for metal recovery: A machine learning approach, Separation and Purification Technology, Volume 291, 2022, 120919, ISSN 1383-5866, https://doi.org/10.1016/j.seppur.2022.120919

The effectiveness of deep learning algorithms in solving sign road recognition problems

MARAT NURTAS [1,2] [a], MOHAMMAD ALI SHEIKH SOLTANI[2], AIZHAN YDYRYS [2], AIZHAN ALTAIBEK[1,2]

[1] International Information Technology University, Email: a.ydyrys@iitu.edu.kz

[2] Institute of Ionosphere, Email: maratnurtas@gmail.com

This research investigates road sign recognition using deep learning methods, comparing them to traditional approaches and emphasizing the potential of simplified convolutional neural networks. Evaluations were conducted on a diverse dataset, encompassing images from different cameras and varying weather conditions. The study aimed to assess the effectiveness of various neural network architectures in road sign recognition. Results demonstrate that, in specific scenarios, simplified convolutional neural networks surpass conventional methods, providing more efficient solutions. This study highlights the practicality of such networks, particularly when addressing diverse data sources and conditions. These results can be applied to solving the problem of recognizing road signs in practice in systems related to the movement of vehicles. The article also provides a comparative analysis of some of the main methods used to classify objects with a created convolutional neural network, which allows researchers to choose algorithms more suitable for their purposes in the future. Future research could explore the optimization and fine-tuning of these architectures for enhanced practical performance.

Keywords: convolutional Neural Network, VGG16, Residual Neural Network, MobileNet, Traffic-sign recognition.

[a] Presenting Author

Improving Vegetation Dynamics Analysis in Kazakhstan with Deep Learning: Insights from Satellite Imagery

AIZHAN ALTAIBEK [1, 2, a], DAUREN AMANGELDI[2], MARAT NURTAS [1,2], SERIK NURAKYNOV[1], BERIK ISKAKOV[1], SALIKHOV NAZIF[1]

[1] Institute of Ionosphere, E-mail: aizhan.altaibek@yandex.ru

[2] International Information Technology University, maratnurtas@gmail.com

Abstract — This study pioneers the application of deep learning methodologies to satellite imagery analysis for enhancing vegetation mapping in Kazakhstan. Employing a convolutional neural network (CNN) model, we aim to refine the accuracy of vegetation identification and classification across diverse Kazakh landscapes. Performance evaluation through the Intersection over Union (IoU) metric demonstrates significant advancement over traditional image processing methods. Our findings suggest deep learning as a robust alternative for agricultural management and environmental surveillance in Kazakhstan, fostering conservation and sustainable land use practices.

Key words: drought impact, vegetation health, remote sensing, machine learning, climate change, vegetation indices.

Vegetation mapping, critical for understanding global ecosystem dynamics, benefits from satellite imagery by enabling worldwide vegetation monitoring, offering insights into climate change, agricultural development, and conservation efforts. NASA's Worldview application is instrumental in this research, providing extensive satellite data, including Earth observation imagery, to analyze Kazakhstan's vegetation patterns. This study enhances vegetation mapping accuracy using high-resolution Worldview satellite images, advanced image processing, and deep learning models. Technological progress, especially in satellite imagery, has markedly influenced vegetation mapping evolution, introducing various sources and methodologies that contribute uniquely to the field:

- Satellite imagery stands as the modern cornerstone of vegetation mapping, offering detailed Earth surface coverage.
- Drones supplement satellite data with high-resolution, localized insights, filling gaps and adding detail in inaccessible areas.
- Ground surveys, though labor-intensive, provide crucial ground-truth data for remote sensing model calibration.
- Digital tools facilitate the integration of diverse data sources and the application of complex analytical models.
- CNN application to satellite data revolutionizes vegetation mapping by automating and enhancing the analysis process.

[a] Presenting Author

Deep learning, specifically CNNs, has proven effective in processing complex image data, including satellite and aerial photos used in vegetation analysis. This research introduces an advanced CNN model tailored to address vegetation analysis challenges, featuring additional layers, batch normalization, dropout, and sophisticated activation functions for enhanced learning and generalization. Evaluated using high-resolution satellite images, our advanced CNN model achieved an IoU score of approximately 82-83% on training data and 73-74% on test data, demonstrating superior generalization capabilities and setting a new standard in vegetation analysis accuracy.

Comparatively, our advanced CNN model outperforms traditional and other machine learning techniques in vegetation analysis. Its capacity for autonomous pattern learning from image data without extensive preprocessing or manual feature extraction establishes a new benchmark in the field.

The IoU metric confirmed our advanced CNN model's accuracy in vegetation classification and segmentation. Incorporating Mean Squared Error Loss (MSELoss) in our approach further refined accuracy by quantifying the discrepancy between predicted and actual values, enhancing model optimization.

Our findings highlight the importance of hyperparameter tuning, particularly the learning rate, for optimal model performance. The advanced CNN model exemplifies the state-of-the-art in leveraging deep learning for vegetation analysis via satellite imagery. It represents a sophisticated approach to environmental data analysis and prediction, enhancing our understanding of vegetation dynamics in Kazakhstan's diverse ecosystems.

References:

[1] NASA Worldview. (n.d.). *Worldview: Explore Your Dynamic Planet*. Retrieved from https://worldview.earthdata.nasa.gov/

[2] Li, J.; Pei, Y.; Zhao, S.; Xiao, R.; Sang, X.; Zhang, C. A Review of Remote Sensing for Environmental Monitoring in China. *Remote Sens.* **2020**, *12*, 1130. https://doi.org/10.3390/rs12071130

[3] W. S. Lee, V. Alchanatis, C. Yang, M. Hirafuji, D. Moshou, and C. Li. 2010. Review: Sensing technologies for precision specialty crop production. Comput. Electron. Agric. 74, 1 (October, 2010), 2–33. https://doi.org/10.1016/j.compag.2010.08.005

[4] Ma, Yue & Hu, Yingjie & Moncrieff, Glenn & Slingsby, Jasper & Wilson, Adam & Maitner, Brian & Zhou, Ryan. (2022). Forecasting vegetation dynamics in an open ecosystem by integrating deep learning and environmental variables. International Journal of Applied Earth Observation and Geoinformation. 114. 103060. 10.1016/j.jag.2022.103060.

[5] Bochenek, B.; Ustrnul, Z. Machine Learning in Weather Prediction and Climate Analyses—Applications and Perspectives. Atmosphere 2022, 13, 180. https://doi.org/10.3390/atmos13020180

Acknowledgement: This thesis was conducted with the support of the Ministry of Education and Higher Sciences of the Republic of Kazakhstan, as part of the scientific project numbered-Grant No. BR18574092

Evolutionary Optimization of Laser Beam Path in Additive Manufacturing

Primož Potočnik [1, a], Andrej Jeromen [1], Edvard Govekar [1]
[1] University of Ljubljana, Faculty of Mechanical Engineering,
Aškerčeva 6, SI-1000 Ljubljana, Slovenia,
E-mail: primoz.potocnik@fs.uni-lj.si

Additive manufacturing (AM) has revolutionized the production landscape, and laser-based additive manufacturing (LBAM) stands out as one of the key technologies in this field. Despite its advantages, LBAM faces challenges in achieving the desired quality and accuracy due to complex interplay of material characteristics, process parameters, and part geometry, which can lead to issues such as porosity, microstructural inconsistency, and dimensional inaccuracies. Residual stresses and deformation result from suboptimal heat management during the metal powder melting and solidification process. Controlling temperature distribution in the fabricated part is identified as a key challenge in laser-based additive manufacturing, as non-uniform temperature distribution can lead to undesirable effects.

This study introduces an innovative evolutionary approach based on a genetic algorithm (GA) for optimizing laser beam paths in LBAM processes. The optimization of the laser beam (LB) path is a critical factor influencing the efficiency and quality of the additive manufacturing process. This study approaches the problem by formulating the LB path optimization as a quest for the optimal sequence of laser beam irradiation into cells on a thin metal substrate. The optimization objective is guided by a fitness function which is composed of two components: thermal fitness and process fitness. Thermal fitness is expressed through the average thermal gradient, employing a simple yet effective thermal model to simulate the intricate effects of laser-induced heat on the temperature distribution within the substrate. Meanwhile, process fitness evaluates the suitability of the proposed LB path for LBAM implementation from the technological perspective.

The GA framework developed for LBAM includes custom initialization, crossover, and mutation operators which are customized and adapted to address the challenges of laser beam path optimization. For the initialization of the initial populations of LB path solutions, various path generators are applied in this study. In addition to the conventional standardized tool paths such as raster and spiral, novel LB path generators are proposed, including the stochastic-based "rand-worm" generator. These generators contribute to defining the initial LB path population, thereby diversifying the genetic material upon which the algorithm operates.

The crossover operation involves selecting two parent solutions (LB paths) and combining their genetic information to generate offspring. This process, mirroring biological recombination, includes defining a crossover point within the effective length of the path strings, splitting the parent path strings at this point, and matching substrings to create an initial

[a] Presenting Author

offspring. Duplicate elements are progressively removed, leading to a successful crossover operation if no duplicates remain. Missing elements are then filled by a randomly chosen LB path generator. The resulting child undergoes further evaluation, potentially undergoing mutation, and is assessed using the fitness function to determine its viability for propagation in the genetic algorithm evolution.

The mutation operation introduces additional diversity into the population by randomly altering the genetic material of a selected individual (parent) to generate a new offspring. The mutation process involves selecting a parent path, randomly determining a mutation startpoint and endpoint, and then deleting the path within the selected interval. The resulting gaps are filled by one of the available and randomly chosen LB path generators, creating new offspring. This mutation strategy facilitates the exploration of the solution space by making small, random changes to a solution, aiming to discover potentially improved solutions.

The efficacy of the proposed approach is demonstrated through simulation case studies. These simulations aim to identify LB paths that represent optimized solutions concerning the defined fitness criteria. This GA-based optimization approach exhibits superiority over traditional trial-and-error LB path formulations, offering an automated and improved methodology for the efficient selection of laser beam paths in LBAM.

The initial research presented in this study will be sustained through future research endeavors which will include more elaborated thermo-mechanical modeling and extensive experimental validation of the proposed GA-based optimization approach. The validation will span across different LBAM processes, encompassing variations such as selective laser melting (SLM) and direct laser deposition (DLD). By bridging the gap between simulation and practical implementation, this research aims to foster continued advancements in LBAM technology and its applications across diverse industrial sectors.

Keywords: additive manufacturing; laser beam path; genetic algorithm; optimization.

Ensemble of Deep Learning Networks More Suitable for Electric Current Analysis of Rotating Machinery

G. G. B. Ferri [1], R. N. Tominaga[2], S. L. Avila[1,2,a], R. M. Monaro[2], M. B. C. Salles[2] , B. S. Carmo[2]

[1] Laboratory of Applied Scientific Computing, Federal Institute of Santa Catarina, Brazil

[2] Advanced Electrical Networks Laboratory, University of São Paulo, Brazil

Keywords: rotating machinery, electrical current, deep learning, ensemble

Improvements in the operational monitoring of rotating machinery like wind turbines are mandatory due to catastrophic accidents that have been occurring. Furthermore, inadequate monitoring can accelerate the degradation of components, leading to reduced economic viability of the equipment, as it may result in costly repairs, increased downtime, and compromised safety. The monitoring methodology most used by the industry is mechanical vibration analysis. Another approach is to use the machine current signature analysis (MCSA). MCSA typically uses frequency domain analysis of the current signal through steady-state machine operation. MCSA highlights are non-invasive technology, simple infrastructure compared to mechanical sensing (phase sensor (B in Fig. 1); 2 accelerometer sensors (C), at 45°; 4 displacement sensors (D), at 0° and 90°), early detection of faults before they become catastrophic, reduce lost production, and increase plant readiness, detect faults in new assets or recently repaired failed assets because of, for example, manufacturing defects, improper installation, etc., and possible to be integrated into a SCADA supervision system. MCSA drawbacks are driver system produces many harmonics, noise from anywhere, power quality concerns, quality of measuring instrumentation, and sample size and cost to store the dataset.

Study case and dataset acquisition.

Fig. 1 shows a test bench designed to investigate unbalance in rotating machinery. There are three prevalent unbalance types of according to ISO 1940-1: static, coupled, and dynamic. This classification considers the relative position between the axis of rotation and mass. The 1HP 3-phase induction motor is powered by a conventional industrial drive system directly connected to the grid without any power quality concerns. Data were gathered at 300 RPM, corresponding to a frequency of 10Hz from the inverter, and sampled at 50 kHz. The task entails classifying three distinct types of unbalances and discerning three severity levels for each category alongside a class representing a healthy condition. We choose to work with 3 severity fault levels (A). This leads to a total of 10 possible classifications. Each class consists of 60 series and each series contains 200,000 data points, equivalent to a duration of 4 seconds at a sampling rate of 50kHz.

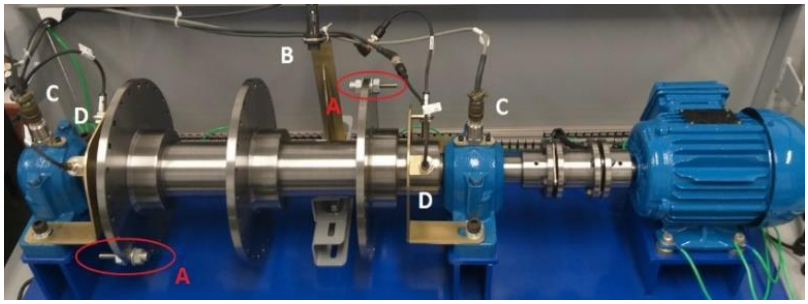


Fig. 1. Mechanical Unbalance test bench.

It is a nonlinear multi-class classification problem.

[a] Presenting Author – Sergio.Avila@ifsc.edu.br

This research is supported by Total Energy Inc. under grant ANP: 23683-6.

Each series was resampled into 80 series, each containing 20,000 points, with overlap. It was split into training, validation, and test sets with proportions of 80%, 10%, and 10%, respectively. Table 1 shows the results for several different machine learning topologies.

Table 1 – Machine Learning algorithms accuracy results and parameters.

Machine Learning Algorithm	Accuracy	Model Parameters
Support Vector Machine	89.58 %	kernel = 'rbf'
Logistic Regression	87.04 %	solver = 'lbfgs'
Random Forests	86.20 %	n_estimators=100
XGBoost	83.66 %	booster='gbtree', n_estimators=500
KNN	81.39 %	neighbors: 18, metric: manhattan

Ensemble of Deep Learning Networks more suitable for MCSA

This work proposes an ensemble of deep learning networks to explore the features of an electrical current signal: time, frequency, and frequency over time. The time feature is analyzed by a temporal series data study using a Long Short-Term Memory (LSTM), a recurrent neural network (RNN) architecture for long-time dependencies. The LSTM network utilizes recurrent layers to model temporal sequences, culminating in a softmax output layer. The frequency feature is analyzed by a Fast Fourier Transform (FFT) data study using a Multilayer Perceptron (MLP). The MLP network comprises dense layers with ReLU activation and dropout for regularization. The frequency over time feature is analyzed by a spectrogram data study using a Convolutional Neural Network (CNN). The CNN employs convolutional and max-pooling layers to extract features from the spectrogram matrix, followed by dense layers for classification. The final model concatenates the outputs of the three networks, with fusion layers and a final classification layer. Notably, the individual networks have their softmax layers removed before concatenation. Thus, the concatenation of models occurs before the individual softmax layers. Table 2 shows the results of our proposal. Fig. 2 presents the framework. Our proposal has better accuracy than that obtained by traditional machine learning techniques.

Table 2 – Ensemble of deep learning networks accuracy results and model layers description.

Method	Accuracy	Model Layers Description
LSTM	88.15 %	Reshape, LSTM tanh, LSTM tanh, Dense Softmax
CNN	80.08 %	Conv relu, MaxPooling, Conv relu, MaxPooling, Flatten, Dropout, Dense Softmax
MLP	90.79 %	Dense relu, Dropout, Dense relu. Dropout, Dense Softmax
Ensemble	98.23 %	Concatenate, Dense relu, Dense relu, Dense softmax

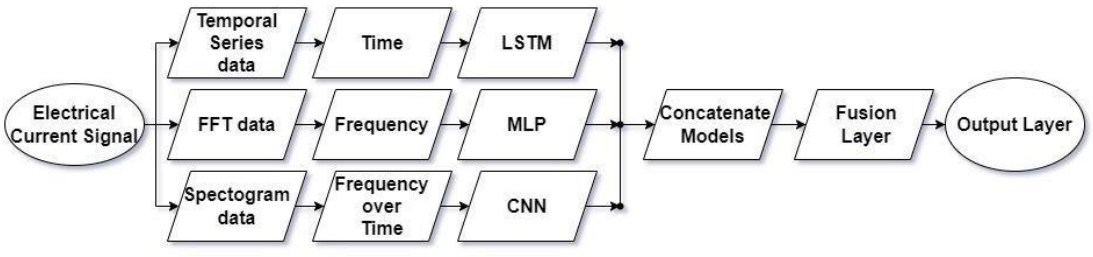


Fig. 2 Ensemble of deep learning networks more suitable for MCSA.

MVJSN-HiTS: Enhancing Real Estate Forecasting Accuracy with Entropy-based Behavioural Pattern Analysis and Economic Sentiment Integration

Dat Le[1], Sutharshan Rajasegarar [2], Maia Angelova[3,*]

[1]Deakin University, E-mail: d.le@deakin.edu.au
[2]Deakin University, E-mail: sutharshan.rajasegarar@deakin.edu.au
[3]Aston University, E-mail: m.angelova@aston.ac.uk

Abstract: Forecasting in the real estate market presents challenges due to factors such as data quality, market evolution, and the intricate behavioral dynamics of variables. Accurately modeling these patterns is crucial for improving forecasting accuracy [1]. However, existing methodologies often overlook the explicit incorporation of multivariate patterns of behavior [2]. To address this gap, we propose a novel framework named Multivariate Jensen-Shannon Divergence-based clustering with Neural Hierarchical Interpolation for Time Series (MVJSN-HiTS). This framework utilizes a Jensen-Shannon Divergence-based entropy cluster- ing approach to efficiently capture multivariate behavior patterns, coupled with a deep neural hierarchical interpolation method for time series forecasting.

The main contributions of this work are:

- Creation of a new real dataset from the Australian real estate market, comprising over a million records, utilized for modeling and evaluation. The evaluation highlights the significant improvement in MVJSN-HiTS performance in forecasting facilitated by the proposed entropy-aided clustering.
- Introduction of a novel framework, MVJSN-HiTS, featuring an interpolation component, a Jensen-Shannon divergence-based multivariate clustering module, and a deep neural-based forecasting mod- ule.
- Proposal of a novel Jensen-Shannon divergence-based clustering method for multivariate time series, effectively assimilating distribution patterns and associations in multiple variables over time, thereby revealing distinct collective behavior patterns.
- Integration of a deep neural hierarchical interpolation model with each cluster of multivariate time series data to conduct forecasts. Comprehensive evaluation on the new dataset, along with compar- ison with other closely related models, demonstrates the superior performance of MVJSN-HiTS in achieving highly accurate multivariate time series forecasts.

Additionally, we assembled a comprehensive dataset spanning twenty years (2003-2023) from 2075 Australian suburbs, incorporating price, volume, sentiment analysis of headline news, and consumer price index (CPI). Our evaluation reveals that integrating CPI into the forecasting process significantly improves accuracy, suggesting that economic indices have a stronger impact than news sentiment. Surprisingly, we found that incorporating breaking news sentiment did not lead to improved forecasting results

The findings demonstrate the effectiveness of our entropy-based behavioural pattern detection mechanism in enhancing forecasting accuracy across multivariate scenarios. Comparative analysis with alternative methodologies, complemented by an ablation study, underscores the superiority of MVJSN-HiTS for multivariate real estate time series forecasting.

Keywords: Entropy, Multivariate clustering, Neural networks, Real estate, Sentiment analytics, Inflation

* Presenting author

References

[1] Balemi, N., Fuss, R., Weigand. 2021. Covid-19's impact on real estate markets: review and outlook. Financ Mark Portf Manag. Vol 35, pp.495–513.

[2] Anundsen, A.K., Kivedal, B.K., Larsen, E.R. 2023. Thorsrud, L.A.: Behavioral changes in the housing market before and after the COVID-19 lockdown. Jnl. of Housing Econ. Vol 59, 101907.

Integrating modeling and machine learning for lithium-ion batteries design and state of health prediction

Mahshid Nejati Amiri [1, a], Jacob Joseph Lamb [2]

[1] Norwegian University of Science and Technology (NTNU), E-mail: mahshid.n.amiri@ntnu.no

[2] Norwegian University of Science and Technology (NTNU), E-mail: jacob.j.lamb@ntnu.no

Lithium-ion batteries (LIBs) are promising energy storage devices that are widely being used as the prime mover of electric vehicles. This is mainly due to their high volumetric and gravimetric energy density and long cyclic life compared to other types of rechargeable batteries. The vast application and high demand for these batteries requires continuous improvements in both their design and lifetime prediction.

Physics-based models have been employed in the study of LIB behavior, providing valuable information regarding the complex multi-physics nature of the battery. However, the challenge regarding these models is that there is always a tradeoff between the accuracy and computational time. While simplified models can provide real-time predictions, they fail to correctly predict the variables at extreme conditions such as high current rates. On the other hand, more sophisticated models are suitable for design applications, but in case of a requirement for optimization, the computational time can be prohibitive.

Machine learning models can make quick predictions of the behavior of a physical system without having an exact knowledge of the underlying equations. Different machine learning models are being used for battery capacity and temperature predictions based on early life experimental data of batteries. Nonetheless, a significant challenge in case of an extreme change in battery performance, which is not seen in the training data, leading to inaccurate trend predictions.

Given the inherent advantages and challenges of both methods, a hybrid approach harnesses the strength of each. For design applications, an intricate model of the battery can provide a training dataset in a defined design space. The machine learning can then learn the model behavior and act as a surrogate for the original model, facilitating the fast optimization by interpolating into the design space. In case of battery lifetime monitoring, a simplified model can be used to guide the machine learning, which is trained based on the early life experimental data of the battery to make more accurate predictions of the late life capacity of the battery.

[a] Presenting Author

Concluding, this abstract highlights the significance of integrating physics-based models and machine learning techniques for enhancing lithium-ion battery design and lifetime prediction. The upcoming presentation will delve deeper into the details of these methods, providing a comprehensive discussion on their application in addressing the challenges of battery technology. Additionally, preliminary findings from our ongoing research will be presented, providing valuable insights into the advancements made in this field.

Ensuring Compliance with the EU's Monitoring, Reporting, and Verification and Emissions Trading System through Data-Driven Verification

Qin Liang[1,2,a] Erik Vanem[1] , Knut Erik Knutsen[1], Houxiang Zhang[2]

[1] DNV Group Research and Development, E-mail: qin.liang@dnv.com

[2] Norwegian University of Science and Technology, E-mail: qinlia @ntnu.no

The European Union's Monitoring, Reporting, and Verification (MRV) Regulation, in conjunction with the Emissions Trading System (ETS), is a foundational element of the EU's policy framework aimed at combating climate change through the reduction of greenhouse gas emissions. Ensuring adherence to these regulatory mechanisms is essential for meeting the EU's ambitious environmental goals. This paper aims to offer a comprehensive analysis of how data-driven verification strategies can improve the effectiveness and integrity of compliance with the EU MRV and ETS. It proposes exploring the integration of advanced data analytics, artificial intelligence (including machine learning and deep learning techniques), and blockchain technology to enhance the monitoring, reporting, and verification process. The methodology is anticipated to include a comparative analysis of traditional versus data-driven verification methods, assessing their impact on compliance rates and administrative efficiency. Preliminary findings suggest that adopting data-driven verification strategies might substantially minimize errors in emissions reporting, more effectively detect non-compliance, and encourage participants to adopt cleaner technologies. Furthermore, the paper will discuss the challenges and opportunities associated with implementing these technologies, including concerns over data privacy, cybersecurity risks, and the necessity for regulatory adjustments in response to technological advancements. This work intends to contribute to the discussion on improving environmental policy compliance through technology and proposes a collaborative pathway for regulators, market participants, and technology providers towards a more sustainable and low-carbon economy.

Keywords:
MRV, ETS, data-driven, machine learning, blockchain, deep learning

[a] Presenting Author

A hybrid solution to consider the stochastic nature of safety incidents on project delays in construction planning methods

Cristiano Saad Travassos do Carmo [1, a], Elisa Dominguez Sotelino [2]
[1] Pontifical Catholic University of Rio de Janeiro, E-mail: csaad@puc-rio.br
[2] Pontifical Catholic University of Rio de Janeiro, E-mail: sotelino@puc-rio.br

The construction sector, marked by inherent uncertainties like political and social concerns, becomes even more complex in infrastructure projects due to their scale. Despite these challenges, construction safety hazards are often overlooked in construction planning methods. A systematic literature review revealed the need for practical research linking technical applications with industry practices in the scope of infrastructure construction projects. Thus, this study addresses these gaps by proposing a novel construction planning method that integrates safety events and their impact on project delays. Leveraging the stochastic quasi birth and death process, we employ neural network models – specifically, Convolutional Neural Network (CNN) and Long Short-Term Memory (LSTM) frameworks. This work focuses on filling partially research gaps by utilizing a real-life database tailored to energy infrastructure construction projects. Results highlight that neglecting safety variables may lead to unjustified assumptions about safety occurrences. The stochastic solution enables construction planners to comprehend the ramifications of safety events on delays and vice versa. For real-time planning, we advocate the use of statistical and neural network algorithms capable of forecasting bivariate time series. Validation scores demonstrate the superior performance of neural networks, with the LSTM model outperforming statistical methods and the CNN model – particularly evident in cases with limited dataset size. As data volume increases, both statistical and AI techniques exhibit satisfactory performance. In conclusion, this study posits that a substantial number of project delay days are unlikely without a corresponding increase in accidents. Future investigations can delve into the integration of other random variables in multivariate time-series analysis, such as cost and productivity, further enriching our understanding of project delays.

Keywords: neural networks, LSTM, CNN, construction projects, safety management

[a] Presenting Author

Deep Adaptive Experiment Design for Quantum Engineering

Anurag Saha Roy [1], Shai Machnes [2]
[1] Qruise GmbH, E-mail: anurag@qruise.com
[2] Qruise GmbH, E-mail: shai.machnes@qruise.com

Existing quantum computers suffer from the lack of high-fidelity operations and challenges in reliable and scalable manufacturing. Detailed device characterization is often necessary for both obtaining the optimized set of operations (gates) on a given quantum device as well as identifying imperfections, deviations from specifications and error sources to help improve the next design iteration. Textbook characterization techniques consist of experiments designed assuming simplified models and point statistics for quantum computers which not only fail to capture all the imperfections of these devices but also do not scale efficiently to large multi-qubit systems. Additionally, for certain system parameters, there also do not exist standard simplified models making characterization non-trivial. This necessitates the development of characterization techniques based on statistical and information theoretic foundations.

We present the application of Deep Learning based Bayesian characterization techniques that adaptively recommends optimal experiments at every step to maximize the expected information gain about the system, while considering the entire history of past experiments. The cost of calculating expensive Bayesian posteriors is amortized using a Reinforcement Learning system which simultaneously learns both the design policy and lower bounds on the otherwise computationally intractable Expected Information Gain. Once trained, the network efficiently predicts experiment designs and approximate posterior distributions. A physics accurate fully differentiable digital twin that models the open quantum dynamics of the quantum computer, the control electronics and the noise & transfer functions for the whole stack lies at the heart of this closed loop adaptive calibration and characterization process. We demonstrate the application of these Bayesian adaptive experiments on multi-qubit superconducting QPU systems.

References:

1. Tom Rainforth, Adam Foster, Desi R Ivanova, & Freddie Bickford Smith. (2023). Modern Bayesian Experimental Design.
2. Wittler, N. et al. (2021). Integrated Tool Set for Control, Calibration, and Characterization of Quantum Devices Applied to Superconducting Qubits. Physical Review Applied, 15(3).

Keywords: Optimal Experiment Design, Bayesian Inference, Reinforcement Learning, Quantum Computing, Quantum Engineering

Morphology Ambiguity Resolution with Pre-trained Language Models

Gulmira Tolegen[1,2]*, Alymzhan Toleu[1,2], Rustam Mussabayev[1,2], Bagashar Zhumazhanov[1]

[1]Institute of Information and Computational Technologies, Almaty, Kazakhstan
[2]Satbayev University, Almaty, Kazakhstan
E-mail: gtolegen@.iict.kz, atoleu@iict.kz

Abstract: Morphology ambiguity resolution, a.k.a., morphological disambiguation (MD) is a long-standing problem in processing morphologically complex languages (MCL). It is akin to part-of-speech (POS) tagging, however for MD, not only the POS tag but the lemma/root along with its corresponding morphological tags should be predicted. For example, depending on the context, a Turkish word *adam* can be analyzed as [1]:

i) a man – adam+Noun+A3sg+Pnon+Nom;

ii) my island – ada+Noun+A3sg+P1sg+Nom

Given the fact that analysis contains a variety of tags, considering it as a tagging problem complicates the task, resulting in an extremely large tagset with sparsities. To solve this issue, a number of approaches are proposed, the general idea behind those approaches is breaking down the morpheme sequence into smaller parts. For instance, in an HMM-based approach [1], the author attempted to decompose the analysis into smaller pieces, like inflectional groups, and under a strong assumption that the tags of the current analysis are only dependent on the preceding one, to perform the disambiguation. One of the drawbacks of this approach is that the assumption prevents the model from capturing the long-term dependencies that exist in the nature of the task. Second, this approach still results in a large set of tagsets.

To alleviate this issue, a voted perception approach as proposed [2], instead of using a certain part of the analysis, the author proposed a set of features and tried to represent a sequence analysis with feature vectors. It utilized a tri-gram decoding, which loosens the previous assumption a little, compared with the HMM-based approach may be able to capture longer dependencies between tags. The underlying hypothesis of this approach is that the model will maximize the objective function, which ensures the feature vectors from the correct path of analyses obtain larger values than those in the non-correct path of analyses. This is a discrete feature-based approach, requires manual feature engineering and it still cannot capture long-term dependencies.

To avoid this problem, a deep learning-based approach is proposed [3], which is considered the current best for this task. The authors segment an analysis into ii) the root, ii) its POS and iii) the morpheme chain (MC), then uses a non-linear layer to calculate a dense representation for an analysis. In order to capture the long-term dependencies, a bi-directional long short-term memory (LSTM) was applied for context learning from sentences. Another character-level LSTM is utilized for capturing word internal features. Combing that fine-grained information from characters, the contextualized representation obtained for each word, and guided by the intuition that the correct analysis should be most similar to the context's representation, they use a dot product of two representations to perform disambiguation. One of the disadvantages of this approach is that it utilizes a binary vector for calculating analysis embeddings, it is not in the continuous space. One of the limitations of this approach is that it utilizes a biLSTM to compute the contextual representation which fails to capture the nuances of language use in complex syntactic and semantic contexts compared with the embeddings generated from large language models.

With the advent of large language models (LLMs), many results for downstream tasks of natural language processing (NLP) have improved significantly. However, the impact of pre-trained large language models on the performance of MD remains unclear.

This article proposes a language-independent deep learning approach designed to leverage the contextualized embedding from pre-trained language models (PLMs) trained on large multilingual corpora, to enhance the performance of the disambiguation model. One of the aims of this work is to analyze the impact of the effectiveness of PLMs on MD and how the knowledge can be transferred from high-resource language to low-resource language. The proposed approach integrates pre-trained contextual embeddings with dense morphological representations to perform ambiguity resolution. The architecture of the model can be briefly described as follows:

1. **Subword-aware context representation**: with a transformer-based neural network, we calculate contextual embeddings for input tokens by transferring knowledge from a PLM, capturing the fine-grained usage of words across various contexts and as well as the long-term dependencies captured by multi-headed attentions. Sub-word tokenizer captures word-internal features, then a transformer layer calculates subword-aware representation for the input sequence, ranging from fine to coarse. In addition to the surface word context representation, we introduce a morphological context embedding to improve the model performance. it calculates analysis embedding, from previous tokens, and goes through layers which able to extract morphological-aware context representation.
2. **Analysis embeddings**: for each tag in an analysis, instead of using a binary vector, we use a dense representation for each tag and sum up the dense embedding of each tag in an analysis and calculate with a non-linear to generate its embedding.
3. **Ambiguity Resolution**: combining morphological-aware and subword-aware context embeddings, two different ways of the ambiguity resolution are proposed: i) calculating the similarity between context and analysis embeddings with dot product; ii) combining those embeddings to calculate similarity score with a neural network layer.

The proposed approach improves the performance of morphology ambiguity resolution by effectively leverag- ing the rich contextual information encoded in pre-trained language models and morphology-aware context. The approach evaluated the different datasets with different languages (Kazakh and Turkish, two morphologically complex languages) to demonstrate their language independence. Experimental results show that the approach outperforms the state-of-the-art methods for MD in languages with complex morphological structures. In the case of Kazakh, as a low-resource language, experiments related to knowledge transfer learning (from high-resource to low-resource language) from the different PLMs such as monolingual and multilingual are carried out.

Keywords: Morphologically Complex Languages, PLMs, Morphological Disambiguation, Knowledge Transfer

* Presenting author

Acknowledgement

The work was funded by the Committee of Science of Ministry of Science and Higher Education of the Republic of Kazakhstan under the grant AP19676744.

References

[1] *Dilek Z. Hakkani-Tür, Kemal Oflazer, and Gökhan Tür* Statistical Morphological Disambiguation for Agglutinative Languages.// In COLING 2000 Volume 1: The 18th International Conference on Computational Linguistics.

[2] *Gulmira Tolegen, Alymzhan Toleu, and Rustam Mussabayev.* 2020. Voted-Perceptron Approach for Kazakh Morphological Disambiguation. In Proceedings of the 1st Joint Workshop on Spoken Language Technologies for Under-resourced languages (SLTU) and Collaboration and Computing for Under-Resourced Languages (CCURL), pages 258–264, Marseille, France. European Language Resources association.

[3] *Alymzhan Toleu, Gulmira Tolegen, and Aibek Makazhanov.* 2017. Character-Aware Neural Morphological Disambiguation. In Proceedings of the 55th Annual Meeting of the Association for Computational Linguistics (Volume 2: Short Papers), pages 666–671, Vancouver, Canada. Association for Computational Linguistics.

Concurrent Geospatial Data for Supervising Invasive Species in Small and Dispersed Areas

Alba Closa Tarres [1, a], Fernando Rojano [2]

[1] Computer Science, West Virginia State University, E-mail: aclosatarres@wvstateu.edu

[2] AERS, West Virginia State University, E-mail: fernando.rojano@wvstateu.edu

Geospatial data from multiple disciplines are strategic for identifying small and dispersed areas of interest (AOI) that aim to determine habitat suitability for specific vegetation types across large-scale aerial images. Although valuable, integrating multiple geospatial datasets can substantially increase computational time. To address this challenge, we propose a preprocessing stage using a limited set of geospatial data to efficiently define the AOI.

This study focuses on developing an approach utilizing geospatial data to define the AOI of the kudzu plant (Pueraria montana), an invasive species found in many regions of the globe. Characterized by its prevalence in small, dispersed areas, the kudzu plant is commonly found in environments that underwent human modification, including roadsides, and areas favorable to soil moisture retention.

We employed geospatial datasets obtained from the United States Geological Survey (USGS) containing habitat suitability information and kudzu plant locations. To verify the presence of kudzu along roadsides, we employed a set of Google Street View images obtained from a virtual field campaign. Furthermore, to quicken the confirmation procedures and enhance the efficiency of our analysis, we implemented image recognition and classification techniques, alongside object detection algorithms.

Habitat suitability analysis was conducted associating global human modification (GHM) and the topographic wetness index (TWI) as primary proxies for outlining potential areas for kudzu plant propagation. Through interrelated geospatial information, we successfully assessed field conditions where this invasive species is likely to thrive, thereby minimizing the need for extensive field trips as well as computational time during analysis. Moreover, our innovative approach signifies a pivotal shift in invasive species monitoring and management and to reducing the proliferation of invasive flora within our ecosystems.

Keywords: geographic information systems, google street view, ecology, kudzu, workflow, image classification, object detection, convolutional neural networks

[a] Presenting Author

Big Data analysis and dimensionality reduction to predict price trends in the Brazilian electricity market considering interdisciplinary phenomena

L. F. R. Barboza, J. V. R. Benedet, K. V. P. Lima, L. Y. Imamura, E. T. Sica, S. L. Avila
Federal Institute of Santa Catarina, E-mail: sergio.avila@ifsc.edu.br

B. E. Pizani, E. Santos, E. Calogeras
Urca Trading Ltd

Economic studies of energy planning show that microeconomic phenomena, such as supply and demand, and environmental factors, such as the utilization of natural capital, influence the behavior of the electricity market. Thus, the modeling and simulation strategy for long-term decision-making support in the future electricity market should be integrated and multivariate, correlating market trends and simulating multiple scenarios. Market simulation models prospect scenarios of conditional evolution. Decision-makers should have access to the largest possible number of relevant variables, and the modeling must have the capacity to measure the differences of future scenarios. Electricity is a non-storable commodity, and its spot price in the future markets exhibits pronounced seasonal patterns and is highly sensitive to real-time demand and supply in trading. Therefore, it presents more volatile price developments compared to other energy sources, such as crude oil and natural gas. Multivariate long-term price trend forecasting models require data input organization to ensure precise and correct forecasting. To achieve this, it is suggested to model a variable tree for decision support, with well-defined categories and layers, encompassing both qualitative and quantitative phenomena. With the chosen variables, it is necessary to consider the characteristics of the energy system, of the electricity market and of the mutuality of decision variables to evaluate the mathematical and economic relevance to the model proposed. The great difficulty of long-term multivariate forecasting is the significant number of specificities and their variables, categorizing it as a Big Data problem. Therefore, this prediction model (Fig. 1a) is highly complex and requires high computational performance. This work is a multidisciplinary exploration challenge (Fig. 1b) involving integrated resource planning engineering, statistical mathematics, data science, and High-performance computing (HPC). In this way, machine learning techniques are implemented to assist in the modeling of forecasting the spot price trend and selecting which data and variables of the modeled phenomena will be excluded or reduced from the systemic modeling proposed.

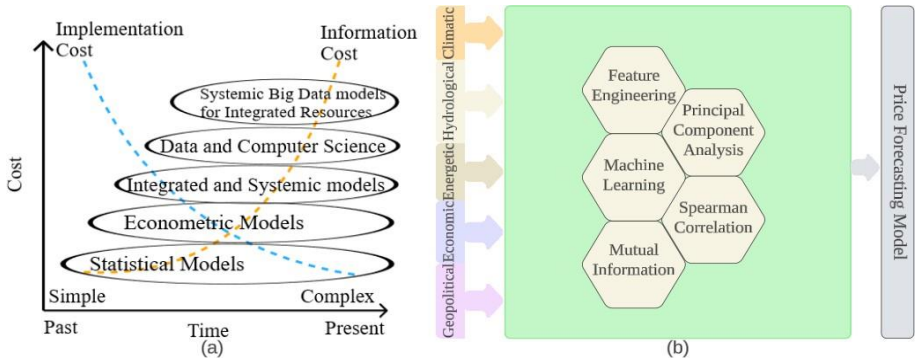


Fig. 1a. Complexity and cost of information and implementation.
Fig. 1b. Multidisciplinary exploration for the systemic model

Thus, this paper's objective is to explore, integrate, and analyze the number of relevant and related phenomena to modeling the problem of forecasting spot price trends in the Brazilian electricity futures market. The analyzed phenomena are measured in interdisciplinary variables through mutual information, feature engineering, component analysis, and statistical correlation to reduce the problem's dimensionality, without losing crucial information. The main intention of this paper is to treat the number of phenomena and their attributed variables so that the systemic pricing trend model is parsimonious and reliable. To evaluate which variables will be resized or excluded in the model, the feature engineering process will be used, selecting, and transforming the phenomena attributed to the modeling problem.

To this end, Spearman Correlation (SC) techniques were applied, to measure the relationship between two chosen variables, and Mutual Information (MI) to verify the existence of similar attributes between variables. The systemic model database consists of more than 15 phenomena that resulted in more than 4000 different variables (time series). Due to the size of the database, analysis using SC and MI alone is not effective. In this way, a linear technique for dimensionality reduction was implemented. This linear technique uses vector orthogonalization to transform correlated variables into a set of linearly uncorrelated values, to improve computational performance without compromising the accuracy and reliability of the results. In this paper, the study was conducted on the Brazilian electricity market and various variables such as seasonality and hydrological phenomena must be considered, as the Brazilian grid is predominantly hydro-thermal-wind. Several relevant phenomena for long-term forecasting can be modeled, such as Affluent Natural Energy (ANE), Stored Hydro Energy (EAR), Turbined Spillable Hydro Energy (EVT), Spot Price, Gross Domestic Product (GDP), Marginal Cost of Operation (MCO), Economic Activity Index (IBC-Br), Load Projections, Available and Projected Power, Transmission Constraints, Oceanic Niño Index (ONI), Geopolitical Risk Index (GPR), Tropical Northern Atlantic Index (TNA), Hydraulic Constraints, and other economic and regulatory factors. Fig. 2. describes an integrated resource planning model, indicating the multidisciplinary and complexity of the problem.

The exploration of the attributed phenomena to the problem of future electricity pricing trends presents significant results for reducing the complexity of the problem and helps long-term forecasting to be more accurate and agile. The analysis of both correlation techniques and computational results can generate better and parsimonious results. This paper is part of a research and development project between Urca Trading, Embrapii, and the Federal Institute of Santa Catarina.

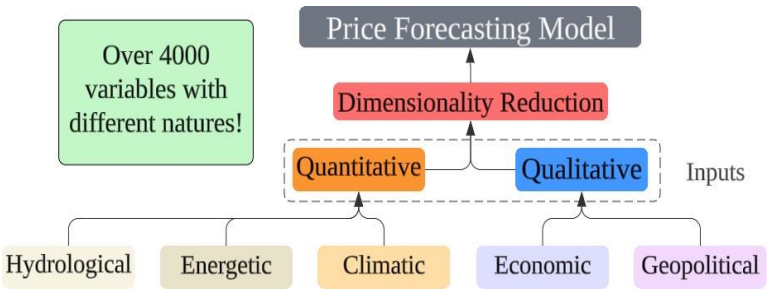


Fig.2. Integrated Resource Planning Model

Machine Learning Models to Predict the Static Failure of Double-Lap Shear Bolted Connections

Hasan Almuhanna [1, a], Giacomo Torelli [2], Luca Susmel [3]

[1] The Univerisity of Sheffield, E-mail: haealmuhanna1@sheffield.ac.uk

[2] The Univerisity of Sheffield, E-mail: g.torelli@sheffield.ac.uk

[3] The Univerisity of Sheffield, E-mail: l.susmel@sheffield.ac.uk

The design estimations of the codes tend to be conservative in estimating the failure loads of bolted connections. This is because the final design failure load is determined using simplistic equations to calculate the failure corresponding to several specific modes and then taking the lowest of the obtained values. This can lead to inaccurate estimation of the failure mechanism and make the codes unreliable. To overcome this limitation, this paper explores the potential of machine learning models as a tool to predict the failure loads and modes of double-lap shear bolted connections. Specifically, four machine learning algorithms are explored: adaptive boosting, decision tree, support vector machine with radial basis function kernel, and K-nearest neighbours. A database of experimental tests representing 221 combinations of input variables was collected to build the models.

In contrast to previously published machine learning studies, the input data included bolted connections with different materials, such as various grades of stainless steel and carbon steel, resulting in a more comprehensive dataset and, thus, a trained model with more capabilities. The correlation between input variables was evaluated by assembling a correlation matrix. To make the most of the limited available experimental data, reduce biases associated with data split, and minimise overfitting, k-fold cross-validation is implemented to replace the classical 0.8 split ratio.

The results revealed that both regression and classification models exhibit a high coefficient of determination for all used algorithms, with the adaptive boosting producing the most accurate estimations for failure loads, and both this model and support vector machine stands out for their accuracy for failure modes. This study's outcomes demonstrate the potential advantages offered by adequately trained machine learning models over codified methods.

Keywords:
Bolted connections, Machine learning, Support vector machine, Decision tree, Adaptive boosting, K-nearest neighbours, cross-validation

[a] Presenting Author

Physics Informed Neural Networks for Two-Phase Flows with Phase Change: Forward and Inverse Problems

Logan M. Pirnstill[1,*], Thanh-Hoang Phan[2,*], Chirag Kharangate[3]

[1]Case Western Reserve University, E-mail: logan.pirnstill@case.edu
[2]Case Western Reserve University, E-mail: thanhhoang.phan@case.edu,
[3]Case Western Reserve University, E-mail: chirag.kharangate@case.edu

Abstract: Convective thermal transport with phase change is an incredibly effective and efficient means for thermal load management. These systems combine sensible heat transfer through convection with latent heat transfer through material phase change, and as a result offer themselves as a viable alternative to single phase thermal management systems. However, the physics of these types of flow regimes is complicated and often difficult to model. Effective and accurate CFD has been achieved for simple systems however high fidelity simulation of complex flow regimes in the two-phase region is still a far cry from what is required for academic and industrial research. This study offers physics informed neural networks (PINNs) as a viable alternative to traditional simulation methods. We propose PINNs not only as a methodology for doing inverse problems such as continuous time identification problems for two-phase flows with phase change, but also as a means to compute forward problems directly from a sampled computational domain.

Keywords: Two-Phase Flow, Phase Change, Machine Learning, Physics Informed Machine Learning

* Presenting author

Two-phase flows with phase change consist of flows for boiling and flows for condensation, and this transfer of mass, momentum, and energy at the two-phase interface is a multi- physics problem that significantly complicates the simulation process. This transfer of mass, momentum, and energy can be modelled using the volume of fluid method, where a volume fraction parameter α denotes the amount of volume occupied by one phase relative to the total volume. This phase may be advected and thus a single set of momentum and energy equations may be solved to describe the system.

$$\frac{\partial \alpha_g}{\partial t} + \vec{u} \cdot \nabla \alpha_g = \frac{\dot{m}}{\rho_g} \tag{1}$$

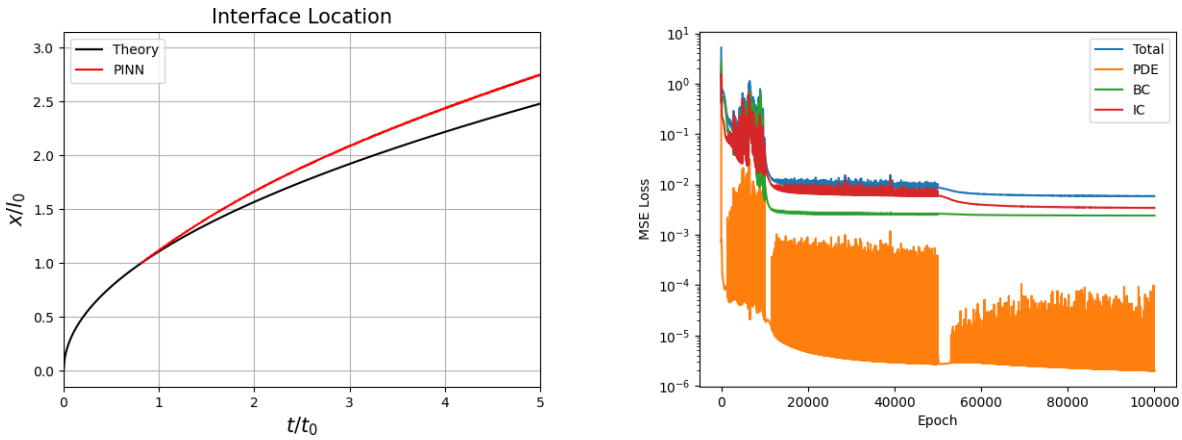
$$\nabla \cdot \vec{u} = \left(\frac{1}{\rho_g} - \frac{1}{\rho_f} \right) \dot{m} \tag{2}$$

$$\rho \left(\frac{\partial \vec{u}}{\partial t} + \vec{u} \cdot \nabla \vec{u} \right) = -\nabla P + \nabla \cdot \left[\mu \left(\nabla \vec{u} + \nabla \vec{u}^T \right) \right] + \vec{f_\sigma} + \rho \vec{g} \tag{3}$$

$$\frac{\partial}{\partial t}(\rho h) + \nabla \cdot (\rho h \vec{u}) = \nabla \cdot (\lambda \nabla T) + \dot{m} h_{fg} \tag{4}$$

Here ρ, μ, λ, and h are mixture properties described as $\phi = \alpha_g \phi_g + \alpha_f \phi_f$. We also must model the mass transfer term $\dot{m}$ and the surface tension forces f_σ. In general two phase PINN

models, such as those developed by Qiu et. al. [1] only look at adiabatic systems that do not involve energy transfer and phase change. Using the standard PINN methodology as first established by Raissi et. al. [2] we show preliminary results of the Stefan problem where interface motion is driven exclusively by phase change and all advection terms are ignored tracking only the volume fraction equation (1) and the energy equation (4). We demonstrate that PINNs is capable of capturing the phase change phenomenon and explore its uses for two-phase thermal management.



(a) Interface location (b) Loss Profile

Figure 1: 1D Stefan problem for liquid-vapor phase change of water

We initialize the interface at location $x/l_0 = 1$ and show that the general shape and trend of the interface is captured as compared to the theoretical solution. The PINN learns the initial and boundary conditions well and sufficiently minimizes the PDEs.

References

[1] R. Qiu, R. Huang, Y. Xiao, J. Wang, Z. Zhang, J. Yue, Z. Zeng, and Y. Wang, "Physics-informed neural networks for phase-field method in two-phase flow," *Physics of Fluids*, vol. 34, no. 5, 2022.

[2] M. Raissi, P. Perdikaris, and G. E. Karniadakis, "Physics-informed neural networks: A deep learning framework for solving forward and inverse problems involving nonlinear partial differential equations," *Journal of Computational physics*, vol. 378, pp. 686–707, 2019.

GADEM: a geometry-aware energy-based method for structural mechanics problems

Thi Nguyen Khoa Nguyen[1,2,3]*, Thibault Dairay[1,2], Raphael Meunier[2], Christophe Millet[1,3], Mathilde Mougeot[1,4]

[1]Universite Paris-Saclay, ENS Paris-Saclay, CNRS, Centre Borelli, Gif-sur-Yvette, 91190 France
[2]Michelin, Centre de Recherche de Ladoux, C´ebazat, 63118 France
[3]CEA, DAM, DIF, F-91297 Arpajon, France
[4]ENSIIE, Évry-Courcouronnes, 91000 France

Abstract: Physics-Informed Neural Networks (PINNs) have gained significant attention in various engineering domains thanks to their capacity to incorporate physical laws into models. Recently, geometry-aware models have been proposed to integrate geometric information into the model using the strong formulation of the physical systems underlying equations. However, the assessment of PINNs in problems involving different geometries remains an ongoing area of research [2,3]. In this study, we introduce a novel physics-informed deep learning framework called the Geometry-Aware Deep Energy Method (GADEM). GADEM employs a weak form of the physical system equations to infer solutions across different geometric shapes. We explore various methods for representing geometric information, including spatial coordinates of boundaries and image-based approaches. Additionally, we investigate different techniques for encoding geometric latent vectors, such as explicit parametric encoding, linear dimensionality reduction (PCA), and non-linear algorithms (VAE). The loss function minimizes the potential energy across all considered geometries. To enhance the performance of GADEM, we employ an adaptive learning method [1] for the sampling of collocation points. Applications of GADEM include solving solid mechanics problems involving elastic or hyperelastic materials. We also successfully apply GADEM to an industrial scenario for toy tire loading simulation. The numerical results highlight the capability of GADEM to infer solutions on different geometries using a single trained model.

Keywords: Physics-informed neural networks, deep energy method, geometry-aware, solid mechanics

* Presenting author

References

[1] T.N.K. Nguyen, T. Dairay, R. Meunier, C. Millet, and M. Mougeot. Fixed-budget online adaptive learning for physics-informed neural networks. towards parameterized problem inference. In International Conference on Computational Science, pages 453–468. Springer, 2023.

[2] A. Kashefi and T. Mukerji. Physics-informed pointnet: A deep learning solver for steady-state incompressible flows and thermal fields on multiple sets of irregular geometries. Journal of Computational Physics, 468:111510, 2022.

[3] J. Oldenburg, F. Borowski, A. Öner, K. Schmitz, and M. Stiehm. Geometry-aware physics informed neural network surrogate for solving navier–stokes equation (gapinn).

Advanced Modeling and Simulation in Engineering Sciences, 9(1):8, 2022

Fusion of Transformer Based Deep Learning and Monte-Carlo Fish Growth Simulation for Aquaculture Smart Transformation

Hsun-Yu Lan [2, a], Naomi A. Ubina[1, b], Kai-Xiang Zhang[1], Shyi-Chyi Cheng [1,c]

[1] Department of Computer Science and Engineering, National Taiwan Ocean University, Taiwan, E-mail: {20857002,11057001,csc}@mail.ntou.edu.tw

[2]Department of Aquaculture, National Taiwan Ocean University, Taiwan, E-mail: sherry72727@gmail.com

The deep learning based fish growth prediction model aims at precision aquaculture to achieve the goal of smart transformation. Although deep learning has been widely used to perform simulations and predictive functions, its dependence on learning from high quality big data is a major challenge. Collecting continuous, complete and big data even with the presence of sensors is a challenge for open sea aquaculture cages because of the access to location and connectivity limitation. To deal with these difficulties, we employed a technique utilizing Monte Carlo approach to generate the required big data for training the proposed deep learning based fish growth models. Our data augmentation process starts by modeling each key factor of the physical fish growth model with a Gaussian distribution which is further parameterized by the fish growth dataset captured from the real-world fish ponds using our Internet of Things based monitoring system or open weather datasets. The transformer based deep learning model follows to be trained to predict the fish growth. To combine with Q-learning, the optimal feeding strategy is obtained to control our remotely controlled smart feeding machine which automates the feeding process. The results show that our fish growth prediction model performs well in predicting fish growth during the cultivation period. The accuracy of the fish growth prediction results when compared to the actual values has an error range from 2-8%. Additionally, Q-Learning as an optimization technique provides viable information to improve feeding strategies by reducing feed consumption up to at most 28.5% which helps eliminate excessive feed waste and reduce production cost. It can also reduce the breeding duration by at least 5% of the culture days. Based on the results, our proposed approaches can be an effective strategy as the result of this aquaculture smart transformation.

Keywords: aquaculture smart transformation, fish growth model, Monte-Carlo simulation, reinforcement learning, fish growth prediction, fish feeding optimization.

[a] Presenting Author

[b] Presenting Author

[c] Corresponding Author

A Physics-Informed Machine Learning Framework for Time-domain Modeling of Vortex-Induced Vibrations

Martin Andersen[1,*], Benjamin Tapley[2], Sølve Eidnes[3], Svein Sævik[4], Jie Wu[5], Bernt Leira[6]

[1]Norwegian University of Science and Technology, E-mail: martin.andersen@ntnu.no
[2]SINTEF Digital, E-mail: ben.tapley@sintef.no
[3]SINTEF Digital, E-mail: solve.eidnes@sintef.no
[4]Norwegian University of Science and Technology, E-mail: svein.savik@ntnu.no
[5]SINTEF Ocean, E-mail: jie.wu@sintef.no
[6]Norwegian University of Science and Technology, E-mail: bernt.leira@ntnu.no

Abstract: In fluid mechanics, vortex-induced vibration (VIV) is a phenomenon that poses substantial challenges in the design and operation of slender marine structures. VIV is a response type known to contribute significantly to fatigue damage in structures, thereby posing a considerable risk to safe operations of marine risers in oil and gas exploration and power cables for offshore renewable energy development [1]. VIV is often a stochastic and nonlinear response, where the local vortex shedding frequencies try to synchronize with the eigenfrequencies of the structure. The resulting VIV responses are non-stationary, especially at high mode orders.

A recent state-of-the-art model for VIV applies a time-domain formulation where external loads are based on the physical drag and excitation related to vortex shedding [2]. However, the model relies on empirical hydrodynamic force coefficients and does not explain all the physics of the phenomenon. The VIV load model relies on the strip theory assumption and the hydrodynamic force coefficients can be obtained from laboratory tests with a rigid cylinder section simulating VIV responses at various defined motions [3]. However, such motions are typically simplified and different from the true motions of an elastic structure. For installed offshore cables and marine risers, it is not possible to directly measure the external hydrodynamic loads along the structure, and the response measurements are only acquired at sparse locations where sensors are installed. Therefore, the true hydrodynamic force coefficients are difficult to model using the existing data, which leads to high uncertainties related to the simulations of VIV.

In this paper, a hybrid VIV model is presented. It applies physics-informed machine learning methods [4] to train an artificial neural network (ANN) for describing the unknown physics in the VIV time-domain load model [5, 6]. The physical system is based on the same principles as the pseudo-Hamiltonian Neural Networks (PHNN) explained in [7], but is instead formulated to conserve the equilibrium equation. The external load vector can be fully or partially data-driven, by informing it with physical terms from the time-domain VIV model. To explain the unknown physics, a corrective term may be added to the load term and learned from the data. The riser structure is modeled as a flexible, tensioned beam using the finite element method (FEM), where the stationary current speed can vary along the length of the structure (Figure 1). Data are acquired only at sensor locations, but a higher resolution is required in the FEM formulation to capture detailed responses. Therefore, another surrogate model is trained to interpolate response time series between the sensor locations. The interpolation model and the load model are trained simultaneously using the same loss function. An overview of the hybrid model framework is presented in Figure 2.

Keywords: Vortex-Induced Vibrations, Physics-Informed Neural Networks, Hybrid model, Marine risers

* Presenting author

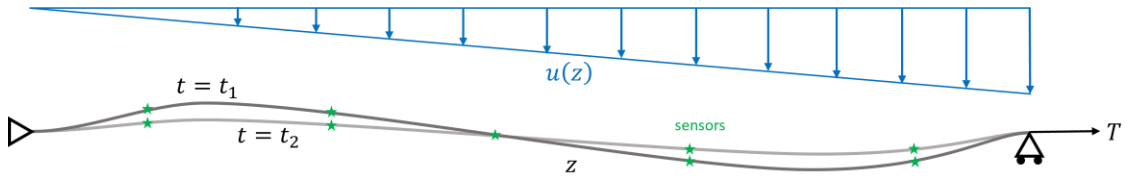


Figure 1: VIV sketch of a beam with tension, T, under a sheared current, u(z), at time steps t = t_1 and t = t_2. Sensors locations are marked with green stars.

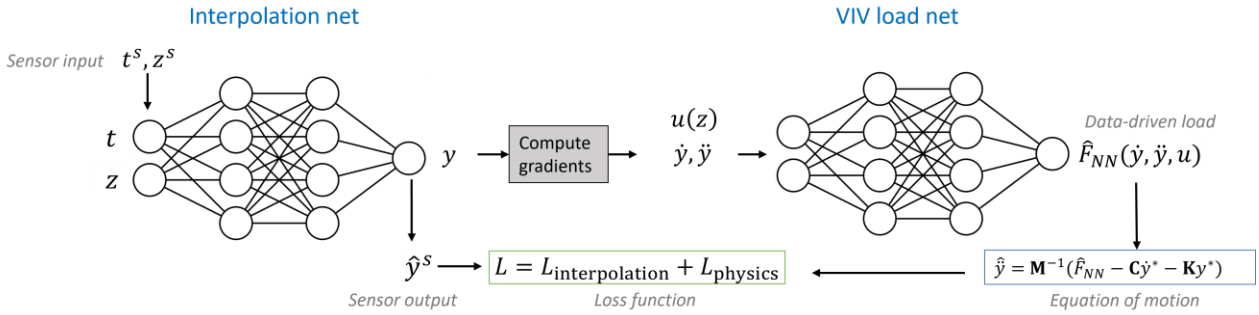


Figure 2: Outline of the hybrid model framework. The displacement response, y^s, at sensor location z^s and time, t^s, are used to train the Interpolation net. A dense sample (t, z) is used to estimate y between sensors. Using automatic differentiation, the derivatives, $y^{\cdot}$ and $y^{\cdot\cdot}$ are computed. The derivatives and the measured current velocity, u(z), are used to train the VIV load net. The predicted load, $\hat{F}_{NN}$, is applied to compute a predicted structural acceleration using the equation of motion, where **M**, **C**, **K** are the mass, damping and stiffness matrices, which are all assumed deterministic. The loss function applies a mean squared error (MSE) between the estimated and measured response at sensor locations ($L_{\text{interpolation}}$) and a MSE between the acceleration from the equation of motion and the predicted acceleration from the interpolation net (L_{physics}).

References

[1] Guijie Liu, Haiyang Li, Zhaozun Qiu, Dingxin Leng, Zhixiong Li, and Weihua Li. A mini review of recent progress on vortex-induced vibrations of marine risers. *Ocean Engineering*, 195:106704, 2020.

[2] M.J. Thorsen, S. Sævik, and C.M. Larsen. A simplified method for time domain simulation of cross-flow vortex-induced vibrations. *Journal of Fluids and Structures*, 49:135–148, 2014.

[3] Ramnarayan Gopalkrishnan. Vortex-induced forces on oscillating bluff cylinders. Technical report, Woods Hole Oceanographic Institution MA, 1993.

[4] Maziar Raissi, Paris Perdikaris, and George E Karniadakis. Physics-informed neural networks: A deep learning framework for solving forward and inverse problems involving nonlinear partial differential equations. *Journal of Computational Physics*, 378:686–707, 2019.

[5] Maziar Raissi, Zhicheng Wang, Michael S Triantafyllou, and George Em Karniadakis. Deep learning of vortex-induced vibrations. *Journal of Fluid Mechanics*, 861:119–137, 2019.

[6] Ehsan Kharazmi, Dixia Fan, Zhicheng Wang, and Michael S Triantafyllou. Inferring vortex induced vibrations of flexible cylinders using physics-informed neural networks. *Journal of Fluids and Structures*, 107:103367, 2021.

[7] Sølve Eidnes and Kjetil Olsen Lye. Pseudo-hamiltonian neural networks for learning partial differential equations. *Journal of Computational Physics*, 500:112738, 2024.

From Data to Insights: Leveraging Informed Machine Learning for Fiber Laydown Quality Optimization in Spunbond Processes

Paulami Banerjee [1, 2, a], Simone Gramsch [1, 2]

[1] Frankfurt University of Applied Sciences, Frankfurt am Main, E-mail: paulami.banerjee@fb2.fra-uas.de, simone.gramsch@fb2.fra-uas.de

[2] Fraunhofer ITWM, Kaiserslautern, E-mail: paulami.banerjee@itwm.fraunhofer.de, simone.gramsch@itwm.fraunhofer.de

Abstract: The global nonwoven market, valued at USD 13.18 billion in 2022 **[1]**, is projected to sustain a steady annual growth rate of 6.1% over the next decade **[2]**. This showcases the extensive applications of spunbond nonwovens across hygiene to automotive sectors. Despite the high demand, current process and product design practices rely on trial-and-error methods implemented directly on production lines, which are time-consuming and costly. Additionally, optimization results obtained from pilot lines can't always be scaled up to full-scale production plants due to the nonlinear nature of influencing factors. This was highlighted during 2020-2021, when FFP2 mask manufacturers faced heightened demand resulting from COVID-19 **[3]**, surpassing production capacities. However, enhancing production speed proved challenging as operators heavily relied on their inherent understanding of manufacturing equipment. Given these challenges, numerical solvers emerge as pivotal tools for designing spunbond processes tailored to meet customer-specific needs. Simulations enable enterprises to digitally optimize their processes without halting production. However, running extensive simulations requires considerable computation time. Under such circumstances, gathering large amounts of data for fast analysis and optimization can be challenging.

In this study, we aim to deal with such challenges with the help of informed machine learning (ML)**[4]** strategies. We develop and train an ML model using simulation data generated using Fraunhofer ITWM's Fiber Dynamics Simulation Tool (FIDYST) **[5]** that encapsulates the complex dynamics of nonwoven fibers during spunbond processes. Our model aims to predict fiber laydown quality based on input parameters such as process conditions and material properties. Due to our reliance on the time-intensive nature of generating simulation data, we employ an active learning **[6]** strategy in both the data generation and the training phase, in conjunction with ensemble decision tree-based regression algorithms to maximize the utility of our limited dataset. By integrating active learning techniques, our aim is twofold: efficient traversal of the sample space to generate the data from, and make our model iteratively select the most informative samples from the simulation data, allowing for efficient model training and optimization. Ensemble decision trees provide a flexible framework for capturing nonlinear relationships between input parameters and fiber laydown quality, enabling us to uncover intricate patterns and insights that traditional statistical methods may overlook. This is supported by a preliminary analysis that we conducted by training a simple decision tree model on an initial dataset of 200 test cases within our sample space, which gave us promising insights. We now aim to further improve the model behavior by involving a larger dataset and integrating

[a] Presenting Author

active learning strategies with ensemble tree-based regression models. To summarize, through this research, we seek to bridge the gap between simulation-driven insights and practical process optimization in spunbond manufacturing with the help of informed machine learning strategies. This approach aims to optimize process design, cut costs, and elevate the quality and sustainability of spunbond materials across various industries, promising improved efficiency and performance in the global nonwoven market.

Keywords: Spunbond Processes, Nonwoven, Informed Machine Learning, Active Learning, Decision Tree, Regression, Manufacturing, Optimization, Simulations

References

[1] Reports & Data Spunbond Nonwovens Market, By Material Type, By Function, By Method, By Application By End-use, and By Region Forecast to 2032. (2023), https://www.reportsanddata.com/report-detail/spunbond-nonwovens-market

[2] Research, P. Nonwovens Market - Global Industry Analysis, Size, Share, Growth, Trends, and Forecast, 2022-2032. (https://www.persistencemarketresearch.com/market-research/non-wovensmarket.asp,2022), Accessed on March 5, 2024

[3] Statista FFP2 grade protective masks market worldwide between 2016 and 2027, by application (in million U.S. dollars). (https://www.statista.com/statistics/1284924/fff2-masks-market-worldwide-by-application/), Retrieved March 07, 2024

[4] Von Rueden, L., Mayer, S., Beckh, K., Georgiev, B., Giesselbach, S., Heese, R., Kirsch, B., Pfrommer, J., Pick, A., Ramamurthy, R. & Others Informed machine learning–a taxonomy and survey of integrating prior knowledge into learning systems. IEEE Transactions On Knowledge And Data Engineering. 35, 614-633 (2021)

[5] Gramsch, S., Hietel, D. & Wegener, R. Optimizing spun bond, melt blown and air lay processes with FIDYST,Mit FIDYST Spunbond-, Meltblown- und Airlay-Prozesse optimieren. Melliand Textilberichte. 96, 96-98 (2015)

[6] Settles, B. Active learning literature survey. (University of Wisconsin-Madison Department of Computer Sciences,2009)

Enhancing NMR Analysis: Deep Neural Network Inversion of NMRD Profiles with Quadrupolar Dips

Davide Evangelista[1], Liwei Hu[2], Giovanni Vito Spinelli[2,*], Fabiana Zama[2]

[1]Department of Computer Science and Engineering, University of Bologna, Bologna, Italy
[2]Department of Mathematics, University of Bologna, Bologna, Italy, email: giovanni.spinelli4@unibo.it

Abstract: Fast Field-Cycling (FFC) Nuclear Magnetic Resonance (NMR) relaxometry is a powerful non-destructive magnetic resonance technique to investigate molecular dynamics [1]. This technique can play a key role in many areas, e.g., food industry research [2], and environmental research [3]. Moreover, FFC-NMR represents an important tool to analyze the structure of porous media and their interactions with hydrogenous fluids, ranging from biological systems to hydrocarbon-bearing sedimentary rocks [4]. Nevertheless, interpreting Nuclear Magnetic Resonance Dispersion (NMRD) profiles, especially when quadrupolar dips are present [5], can pose challenges due to their intricate nature [6].

The NMRD profile measures the variation of the longitudinal relaxation rate, R_1 with the angular frequency ω of the applied magnetic field [7]:

$$R_1(\omega) = R_0 + R^{HH}(\omega) + R^{NH}(\omega), \qquad \omega = 2\pi\nu$$

where R_0 is an offset accounting for fast correlation times; $R^{HH}(\omega) = {}_1(f(\tau))$ is a linear term depending on $f(\tau)$, the correlation time distribution, and it describes the ^1H ^1H relaxation. The τ's represent the correlation times, i.e., the average times required by a molecule to rotate one radiant or to move for a distance as large as its radius of gyration, and f is the distribution to be recovered. Finally, $R^{NH}(\omega) = F_2(\psi)$ describes the *quadrupolar enhancement relaxation term* and it depends on 6 physical parameters we want to extract (i.e., $\psi = [C^{NH}, \theta, \phi, \tau_Q, \nu_-, \nu_+] \in R^6$) [5].

To solve the parameter identification problem, software tools based on optimization methods have been investigated and presented in literature [6, 8].

However, the large-scale diffusion of FFC – NMR could be limited both by the complexity of analytical tools and the need for deep expertise in NMR and materials physics. These reasons lead to finding different strategies employing deep learning techniques to rapidly process big datasets to characterize material properties. Some attempts applied to NMR spectroscopy and low-field relaxometry have been developed [9, 10].

Recent advancements in artificial intelligence present encouraging solutions to this difficulty. In particular, Deep Neural Networks (DNNs) have demonstrated significant potential in efficiently inverting NMRD profiles, even when complicated by quadrupolar interactions.

We present a novel computational approach based on DNNs for identifying the model parameters in the presence of quadrupolar dips.

The mathematical method is implemented by combining a numerical method and the *Plug and Play* (P-n-P) approach [11]. Specifically, the estimation of the parameters of interest is carried out by a coordinate descent method, where an iterative algorithm solves the problem divided into two parts: the linear part (i.e., to extract R_0, $\boldsymbol{f}$) is formulated as a constrained least-squares problem with an L_1 penalty term, and it is solved by the *Truncated Newton Interior-Point* method [12]. The quadrupolar dips parameters estimation is solved by applying a trained feed-forward neural network (*NMRNet*), following the P-n-P approach:

Two-Blocks Plug and Play Algorithm

1. Initialize j = 0, choose starting $(R_0, \boldsymbol{f})^{(0)}, \boldsymbol{\psi}^{(0)}$.
2. **Repeat:**
   - Update $(R_0, \boldsymbol{f})^{(j+1)}$ solving $\min_{R_0, \boldsymbol{f} \geq 0} \{ \|R_1 - (R_0 + F_1(\boldsymbol{f}))\|_2^2 + \lambda \|\boldsymbol{f}\|_1$

     using the *Truncated Newton Interior-Point method.*
     $\lambda > 0$ is the regularization parameter updated following the balancing principle [13].
   - Update $\boldsymbol{\psi}^{(j+1)}$ with *NMRNet.*
   - Increment j
3. **Until** exit condition is met.

NMRNet is a feed-forward neural network with 5 hidden layers. The input layer has the dimension of the NMRD profile, and the output layer has dimension 6, i.e., the number of parameters we want to extract. The last activation function is tailored using the constraints coming from the physical a priori information.

Moreover, we formulated a novel loss function that combines L_1 loss from output predictions and predicted R_1 signal, essential for training on predictions and NMRD profile fitting:

$$\text{loss}_{\text{NMRNet}} = (1 - \alpha) \sum_{i=1}^{6} |\psi_i^{(\text{pred})} - \psi_i| + \alpha \sum_j |R_{1_j}^{(\text{pred})} - R_{1_j}|$$

The present contribution aims to illustrate the outcomes of utilizing DNNs for NMRD profile inversion, comparing them with the results obtained by the robust optimization method previously developed [6]. These results indicate a good agreement between the two strategies, showing that DNNs-based approaches could play a crucial role in this analysis, speeding up the analysis of a large amount of data.

Keywords: Deep Neural Network, Parameter Estimation, Plug-and-Play, Fast Field Cycling NMR relaxation

* Presenting author

References

[1] R. Kimmich, Field-cycling NMR relaxometry, in: NMR, Springer, 1997, pp. 138–148.

[2] M. Marcone et Al. Diverse food-based applications of nuclear magnetic resonance (NMR) technology. Food Research International 51, 2013.

[3] A.J. Simpson et Al. Nuclear Magnetic Resonance Spectroscopy and Its Key Role in Environmental Research. Environ. Sci. Technol. 46, 21, 2012.

[4] V. Bortolotti et Al. Uniform Penalty inversion of two-dimensional NMR Relaxation data. Inverse Problems, 2016.

[5] D. Kruk et Al. Dynamics of Solid Proteins by Means of Nuclear Magnetic Resonance Relaxometry. Biomolecules, 9 (11): 652, 2019.

[6] F. Zama et Al. An Automatic L1-based regularization method for the analysis of FFC dispersion profiles with quadrupolar peaks. Applied Mathematics and Computation, 444, 2023.

[7] P. Lo Meo et Al. Heuristic Algorithm for the Analysis of Fast Field Cycling (FFC) NMR Dispersion Curve. Analytical Chemistry, 93 (24): 8553-8558, 2021.

[8] P. Sebasti¯ao. The Art of Model Fitting to Experimental Results. European Journal of Physics, 35, 2014.

[9] D. Hansen. Using deep neural networks to reconstruct non-uniformly sampled NMR spectra. Journal of Biomolecular NMR, 73, 11 2019.

[10] T. Osheter et Al. Semi-autonomic AI LF-NMR sensor for industrial prediction of edible oil oxidation status. Sensors, 23(4), 2023.

[11] S. V. Venkatakrishnan et Al. Plug-and-Play priors for model based reconstruction. 2013 IEEE Global Conference on Signal and Information Processing, 2013.

[12] L. Grippo et Al. Introduction to Methods for Nonlinear Optimization. Springer, 2023.

[13] K. Ito et Al. A Regularization Parameter for Nonsmooth Tikhonov Regularization. SIAM Journal on Scientific Computing, 33, 3, 2011.

Optimising the operation of district heating networks by combining forecasting and decision-making tools

José L. Hernández [1, a], Pablo Marcos [2], Javier Martín [2], Ignacio de Miguel [3]

[1] CARTIF technology centre, E-mail: josher@cartif.es

[2] VEOLIA Servicios LECAM, E-mail: pablo.marcos-celestino@veolia.com, javier.martin@veolia.com

[3] Universidad de Valladolid, E-mail: ignacio.miguel@tel.uva.es

District heating networks play a crucial role in providing efficient and sustainable heating solutions for urban areas. Effective management and optimization of these networks are essential to maximize energy efficiency, reduce environmental impact, and ensure reliable heat supply to end-users. To enhance management, advanced monitoring and control systems are implemented to continuously collect data on temperature, flow rates, and pressure throughout the network. This real-time data enables operators to identify potential issues, such as heat losses or system inefficiencies, and respond promptly.

Optimization of district heating networks involves fine-tuning various parameters to achieve the most efficient energy distribution. Smart technologies, like weather forecasting and demand response systems, contribute to dynamic load balancing, ensuring that the network adapts to changing conditions and minimizes energy waste. By continually assessing and improving the system, district heating networks can become integral components of environmentally friendly and economically viable urban heating solutions.

Several researches have been conducted in this line. The use of machine learning models, including neural networks, support vector machines, and ensemble methods, for accurate prediction of heat demand have been explored. The focus is on developing models that can adapt to changing conditions and provide more reliable forecasts. Advanced optimization algorithms, such as genetic algorithms, particle swarm optimization, and simulated annealing, have been applied to optimize various aspects of district heating networks. These algorithms aim to find the best configuration of parameters to maximize energy efficiency and minimize costs. Thanks to the integration of smart sensors and the Internet of Things enables artificial intelligence algorithms to analyze operation data to make informed decisions about system operation. Finally, some research has delved into dynamic pricing models and demand response strategies. These approaches aim to encourage consumers to modify their heating patterns in response to real-time energy availability and pricing.

This work proposes a hybrid approach between simulation, machine learning and decision-making tools to optimize the operation of a district heating network located in

[a] Presenting Author

Valladolid, Spain. A grey-box methodology (combination of physics and data-driven models) is followed, where the simulation part is in charge of modelling the physical assets of the district heating network to determine the heat and pressure losses within the distribution circuit. The data-driven models are split into two main aspects. Firstly, forecasting relies on machine learning to predict the buildings' energy demand and renewable energy production. Secondly, decision-making algorithms calculate recommended parameters to operate the boilers both providing supply temperatures and load balancing results to cover the total demand (the aggregation of the simulation and machine learning results).

This optimization approach is being applied in one of the VEOLIA's district heating networks. In particular, FASA case, which is located in Valladolid, Spain. It is composed of twenty buildings, with same number of substations (one-by-one relationship), and three boilers (two biomass and one gas-fired as support for demand peaks). Initial results show the possibility to reduce the supply temperature between 3ºC and 5ºC of the generation systems to minimize the waste energy. This reduction is obtained to maintain 21ºC comfort set-point in the buildings, while energy savings represent approximately the 5% of the total district heating energy.

Keywords: Optimization, district heating network, grey-box approach, district heating operation.

Spatiotemporal Analysis of In-Game Team Performance Consistency in Association Football

Ishara Bandara[1,*], Sergiy Shelyag[2], Sutharshan Rajasegarar[3], Daniel B. Dwyer[4], Eun-jin Kim[5], Maia Angelova[6]

[1]Deakin University, E-mail: isharabnd@gmail.com
[2]Flinders University, E-mail: sergiy.shelyag@flinders.edu.au
[3]Deakin University, E-mail: sutharshan.rajasegarar@deakin.edu.au
[4]Deakin University, E-mail: dan.dwyer@deakin.edu.au
[5]Coventry University, E-mail: ad3116@coventry.ac.uk
[5]Aston University, E-mail: m.angelova@aston.ac.uk

Abstract: Unpredictable ball movements while utilizing space are critical in association football (commonly known as football or soccer) for outsmarting opponents. Ensuring consistent dominance of this tactical advantage throughout all phases of a game is equally crucial. Any inconsistencies in team performance will present opportunities for opponents to take control of the game. Given the low-scoring and unpredictable nature of association football, maintaining dominance and delivering consistent performances throughout the match is vital. A single goal often proves decisive, proving the significance of consistency in team performance.

In this study, the relationship between consistency in team performance across different phases of a game (in-game consistency) and match-winning performances was investigated. Team performance was evaluated using spatial event distribution analysis which evaluates the team's ball movement distribution. Prior work, identified the importance of higher spatial event distribution randomness in team performances for match-winning performances[1]. This analysis aimed to capture changes or patterns in the spatial event distribution randomness over time, providing valuable insights into consistency in team performance across different time intervals. A publicly available event-log dataset containing spatiotemporal information of named events was used[2]. The dataset contained events from top-tier club competitions and international tournaments.

The proposed approach involved generating region-based spatial event distribution matrices at defined equal duration time periods (t_i, $0 \leq i < 10$) of the game for temporal feature extraction. For each time period and each team, the spatial event distribution randomness of a particular team was compared with its spatial event distribution randomness of the previous time period or spatial event distribution randomness up to the considered time period using relative entropy measures. Relative entropy measures of the two teams were compared next to evaluate relative consistency in spatial event distribution randomness between the two teams. These quantified comparison measures, representing the relative consistency in ball movement of teams across defined time periods, were used as temporal features for the development of a match- winner prediction model with generalized linear models (GLM). GLM feature coefficients and p-values were evaluated to identify the feature importance and correlation directions. Additionally, correlation matrices were generated and evaluated to identify relationships between temporal features.

The developed GLM model exhibited a notable accuracy of 70% in predicting the winner of the match. Existing studies have considered multiple performance evaluation metrics for the development of match-winner prediction models. However, the proposed approach only took into account spatial event distribution, which was extracted through the event locations of the ball-carrier and their duration. Nevertheless, the primary objective of this research was not to develop a match-winner prediction model but rather to assess the significance and correlation of in-game consistency in team performance on match-winning performances. Yet, the high accuracy in predicting the match winner highlights the relationship between temporal features reflecting in-game consistency and match-winning performances.

The analysis of temporal feature patterns has provided valuable insights into the consistency of team performances across different phases of a game. Winning teams demonstrated a higher spatial event distribution[1] and maintained consistency in higher spatial event distribution in the early stages of the game. During these stages, in order to gain an advantage with scores, winning teams were observed to maintain higher randomness in ball movements consistently than their opponents which will eventually help them to create more chances by outsmarting opponents. But as the game progressed, a notable decline in this consistency was observed, reflecting a shift towards defensive, cautious, and compact strategies commonly adopted by leading teams in the latter part of matches[1, 3]. This behavior leads to inconsistencies in spatial event distribution of the leading teams towards the end of the game.

In summary, the proposed method has assessed the in-game consistency of team performance concerning ball movement and its impact on match outcomes. It has also analyzed the time-series aspect of team performance

by extracting temporal features. The higher accuracy reported in classifying match winners underscores the significance of in-game consistency on match-winning performances. Furthermore, this research adds value to the football community by uncovering hidden insights into in-game consistency in team performance.

Keywords: Association Football, Entropy, Soccer, Time-Series, Consistency, Performance Evaluation, Team Performance

* Presenting author

References

[1] I. Bandara, S. Shelyag, S. Rajasegarar, D. Dwyer, E.Kim, M. Angelova. 2019. Winning with Chaos in Soccer: Spatiotemporal Event Distribution Randomness Metric for Team Performance Evaluation. Abstract presented at the ANZIAM 2024.

[2] Statsbomb. 2021. “Statsbomb open data”. [Online]. Available: https://github.com/statsbomb/open-data.git.

[3] T. Guan, J. Cao, T. Swartz. 2021. “Should you park the bus?” [Online]. Available: https://www.sfu.ca/ tswartz/papers/bus.pdf.

Digital Twins for Treatment Recommendation

Sam Nallaperuma-Herzberg*, Kevin Monteiro

University of Cambridge, Email*: snn26@cam.ac.uk

Abstract: Digital twins have become a disruptive technology that drive industrial applications across numerous engineering sectors, including construction, energy, transportation and bio-engineering etc. This work presents a digital twin framework that can transform bio-engineering sector in the context of diagnosis and treatment recommendation. As a proof of concept this has been applied to sleep disorders and has potential to be applied to wider healthcare sector.

Keywords: digital health, digital twins, bio-engineering, artificial intelligence, insomnia

* Presenting author

1 Introduction

Insomnia is a common sleeping disorder that affects 1 and 3 adults on a weekly basis [1]. The underlying causes for insomnia vary widely from case to case including mental health disorders such as anxiety and depression, physical illnesses such as migraine or cancer, medications, hormonal changes occurring in menstrual cycle, pregnancy and menopause and neurological problems etc [2]. Thus personalisation is essential in insomnia treatments. Recently, the national health service (NHS), UK recommended [3] two digital therapy apps: Pzizz [4] based on music therapy and Sleepio [5] based on cognitive behavioural therapy for insomnia (CBT-I). However, these products lack in the personalised feedback aspect.

By integrating digital therapy, artificial intelligence (AI), electroencephalography (EEG), BrainTwin system generates adaptive treatments based on music therapy, CBT-I, and hypnotherapy, depending on the patient's brain function. The BrainTwin core model is based on a digital twin of the patient's brain, adapted to the state of the patient, evolving with age. This technology will revolutionise healthcare and well-being by providing digital treatments that are accessible to patients globally, reducing the burden on healthcare. Moreover, the BrainTwin's brain simulation approach has great potential to contribute to the wider healthcare research in early diagnosis and treatment recommendations for other difficult to treat brain related issues such as neuro-degeneration, mental health illnesses and brain tumours.

2 Proposed Approach

The proposed BrainTwin system consists of three modules: a Treatment recommendation module, a Brain simulator (digital twin) module, and a Sleep scoring module. The system generates an objective score based on the quality of the patient's sleep after a particular treatment which is used to adapt the treatment recommendation process, thereby providing a highly personalised approach to insomnia treatment (see Figure 1). Eventually, these per-

sonalisation data will be embedded in the digital twin simulator mimicking the particular

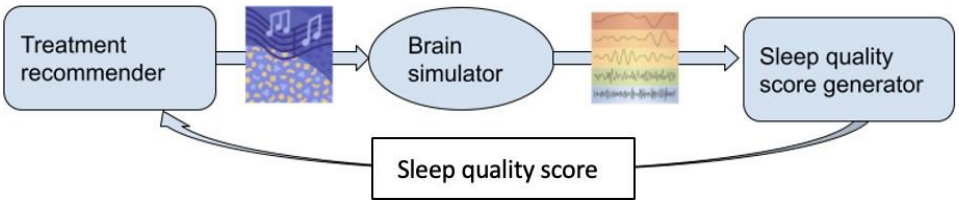


Figure 1: BrainTwin system overview

patient's brain allowing the BrainTwin system to operate without the need of an integrated device. For the initial brain simulator model, we develop a graph-based functional brain model using EEG sensor data. In this model, each EEG sensor aligns with a specific brain region, represented as a node in the graph, whilst the connections between these regions are depicted by the edges. We employ spatio-temporal graph neural networks (ST-GNN) [6] to construct this preliminary model, aiming to encapsulate these spatial and temporal relationships. Once trained, the model can ingest therapy data inputs, for instance, sequence data from a music therapy generator, and yield EEG sequences as node-based outputs, with each node representing an individual EEG sensor.

3 Conclusion and Further Work

This paper presents BrainTwin, a digital twin framework for diagnosis and treatment recommendation. As a proof of concept this has been applied to insomnia, a common sleep disorder. BrainTwin system integration and testing will be carried out and its expected to perform clinical trials to evaluate the efficacy of the system in a clinical setting.

Acknowledgements: Authors thank Prof. Pietro Lio and Prof. George Malliaras at University of Cambridge, Prof. Steve Neiderer at Alan Turing Institute and Dr. Martina Mason at Royal Papworth Hospital for their valuable insights.

References

[1] Wilson S. et al., British Association for Psychopharmacology consensus statement on evidence-based treatment of insomnia, parasomnias and circadian rhythm disorders: An update., J Psychopharmacol 2019.

[2] The American Academy of Sleep Medicine, Insomnia, 2008, https://aasm.org/resources/factsheets/insomnia.pdf.

[3] National Institute of Health and Care Excellence, 2022, https://www.nice.org.uk/news/article/nice-recommends-offering-app-based-treatment-for-people-with-insomnia-instead-of-sleeping-pills.

[4] Ananth S. Sleep apps: current limitations and challenges. Sleep Sci. 2021.

[5] Michael Darden and others, Cost-effectiveness of digital cognitive behavioural therapy (Sleepio) for insomnia: a Markov simulation model in the United States, Sleep, 2021.

[6] Jianghong Zhao et al., Advances in spatiotemporal graph neural network prediction research, International Journal of Digital Earth, 2023.

Rigorous Model Comparison for Semi-Crystalline Polymers: A Bayesian Approach

José L. P. Vila-Chã[1,*], Bernardo P. Ferreira[2], and F. M. Andrade Pires[1]

[1]DeMec, Faculty of Engineering, University of Porto, s/n, R. Dr. Roberto Frias, 4200-465 Porto, Portugal
[2]Brown University, 184 Hope St., Providence, RI 02912, USA

Abstract: Semi-crystalline polymer morphology is heterogeneous, hierarchical, and complex. These features contribute to a richly featured mechanical response that may include double yield, strain rate dependence, and rubber-like hardening [1]. Given the variety of behaviors that semi-crystalline polymers display, alterna- tive constitutive descriptions abound. In fact, given its rich micro and mesostructure features, models range from homogenized to mean- or even full-field descriptions of the material [2]. When employing the last two approaches, an appropriate description of the behavior and interactions of the crystalline and amorphous phases is also required.

It is thus clear that a rigorous and systematic model selection approach is needed when facing this complex modeling scenario. On the one hand, complex models with a high number of degrees of freedom may be able to fit the experimental results but often fail to generalize to yet unobserved deformation history paths (overfitting). On the other hand, simple models with fewer degrees of freedom may not be able to explain the experimental results (underfitting).

In this contribution, we adopt a Bayesian framework for model selection and comparison in semi-crystalline polymer modeling. We explore the use of prior regularization and metrics such as the Watanabe-Akaike information criterion (WAIC) and Pareto-smoothed importance sampling (PSIS) to estimate out-of-sample accuracy [3]. This approach aims to provide a more comprehensive and reliable means of comparing models, considering both their complexity and predictive performance.

Keywords: semi-crystalline polymers, model selection, Bayesian statistics, regularization, WAIC, PSIS.

* Presenting author

References

[1] Argon, Ali. The Physics of Deformation and Fracture of Polymers. Cambridge University Press, 2013.

[2] Mirkhalaf, Mohsen, and Rahele Vadizadeh. “Micro-Mechanical Modeling of Semi-Crystalline Polymers: A Review.” International Journal of Solids and Structures 290 (March 15, 2024)

[3] McElreath, Richard. Statistical Rethinking: A Bayesian Course with Examples in R and Stan. 2nd Edition. CRC Press, 2020.

Enhancing Oxygen Safety in Engineering Applications: Data-Driven Insights into Oxygen Pressure Surge Testing

P. Karthick Selvam [1, a], Thomas Andreas [2], Stephan Leyer[1]

[1] University of Luxembourg, E-mail: karthick.selvam@uni.lu; stephan.leyer@uni.lu
[2] Rotarex S. A., Luxembourg, E-mail: andreas.thomas@rotarex.com

This abstract presents a comprehensive study on oxygen pressure surge testing (OPST) in Mechanical Engineering, focusing on the critical role of data analytics and computational fluid dynamics (CFD) in enhancing safety and reliability. OPST, a vital procedure governed by the ISO 10297 standard, evaluates the performance of oxygen systems under high-pressure conditions.

In our research, we employ advanced data analytics techniques to analyze test data collected during OPST experiments up to 100 bar. Leveraging large volumes of test data, we extract valuable insights into flow behavior and system dynamics. This data-driven approach enables us to identify patterns, anomalies, and critical parameters that influence system safety.

Furthermore, we utilize computational fluid dynamics (CFD) simulations, conducted using Ansys Fluent on a supercomputer cluster, to complement experimental findings. By integrating CFD with test data analytics, we gain a deeper understanding of flow behavior during OPST, particularly focusing on adiabatic compression effects and their implications for system safety.

Through meticulous analysis of CFD results and test data, we uncover nuanced insights into pressure-temperature surges, supersonic flow characteristics, and pressure profile variations. These insights play a pivotal role in informing engineers during the design phase, enabling them to develop safer and more reliable products.

Overall, our research underscores the importance of data-driven approaches in Mechanical Engineering, demonstrating how the fusion of test data analytics and CFD simulations enhances our understanding of complex phenomena like OPST. By leveraging these insights, engineers can make informed decisions and design oxygen systems that meet stringent safety standards and regulatory requirements.

Keywords: OPST, ISO 10297, 300 bar test, 750 mm geometry, ANSYS FLUENT, supersonic flow, pressure-temperature surge

[a] Presenting Author

Physiology-Informed Neural Network for prediction of post-harvest firmness of avocados

R.G.M. van der Sman[1,*], M. Vollebregt[1], R. Schouten[1]
[1] Wageningen Food & Biobased Research, the Netherlands
E-mail: ruud.vandersman@wur.nl

We present Physiology-Informed Neural Networks (PhINNs), applied to describe the firmness of avocados. PhINNs are derived from Physics-Informed-Neural-Networks, where mathematical models describing postharvest physiology are included in the loss function. As a start we have taken the physiological model an earlier model of Hertog, using only two state variables, namely firmness and a cell-wall degrading enzyme. We assumed that the kinetic factors are controlled by the metabolic rate, which was described by Michaelis-Menten kinetics with uncompetitive inhibition by CO2. PhINNs learned us that experimental data from several different sources can be collapsed after proper rescaling of the time at different temperature/gas conditions using the expressions for metabolic rate. However, they can be clustered in two groups: one cluster representing fruits in the preclimacteric state, and the second cluster representing fruits in the post-climacteric state. These clusters have two different ripening rates, that can not be explained by the simple model of Hertog. Better explanation can be delivered by the biological switch model, we have developed earlier for firmness of apples. Using the biological switch model PhINNs can cope with experiments, where shifts in storage conditions have been made from low-temperature controlled-atmosphere conditions, to ripening conditions at atmospheric conditions and room temperature.

Keywords: Postharvest-physiology ; Physics-Informed-Neural Networks ; Metabolism ; Fruit

Geometry-aware Physics-informed Machine Learning

Zack Xuereb Conti[1,*], Nick Pepper[2], Sharana Shivanand[3]

[1]The Alan Turing Institute, E-mail: zxuerebconti@turing.ac.uk
[2]The Alan Turing Institute, E-mail: sshivanand@turing.ac.uk
[3]The Alan Turing Institute, E-mail: npepper@turing.ac.uk

Abstract: Machine learning (ML) methods that seek to emulate dynamical systems frequently struggle with generalisation to unseen domains and initial conditions, limiting their trustworthiness. It is often necessary for the full breadth of behaviour of the dynamical system to be present in the training data in order for the ML model to learn a global enough representation to generalise for unseen scenarios and conditions.

Physics-informed biasing strategies have been proposed that combine laws of physics within the machine learning architectures as a means of addressing this limitation. One of the more popular approaches involves embedding differential equations into the training loss function of an artificial neural network, commonly referred to as Physics-informed Neural Networks (PINNs) [1]. However, it has been shown that this biasing strategy tends to not generalise robustly when varying the initial conditions [2, 4, 5].

We suggest that generalising robustly for varying initial conditions implies a model that successfully captures the fundamental structure governing the global phenomena. In dynamical systems theory, the structure underlying a differential equation can be defined by the geometry of the phase space, whose underling vector field governs the system's state trajectories for any initial condition. The geometric structure of the phase space is closely related to the stability of the dynamical system. When emulating stable dynamical systems, it is therefore desirable for this structure to be incorporated within the loss function of the ML model.

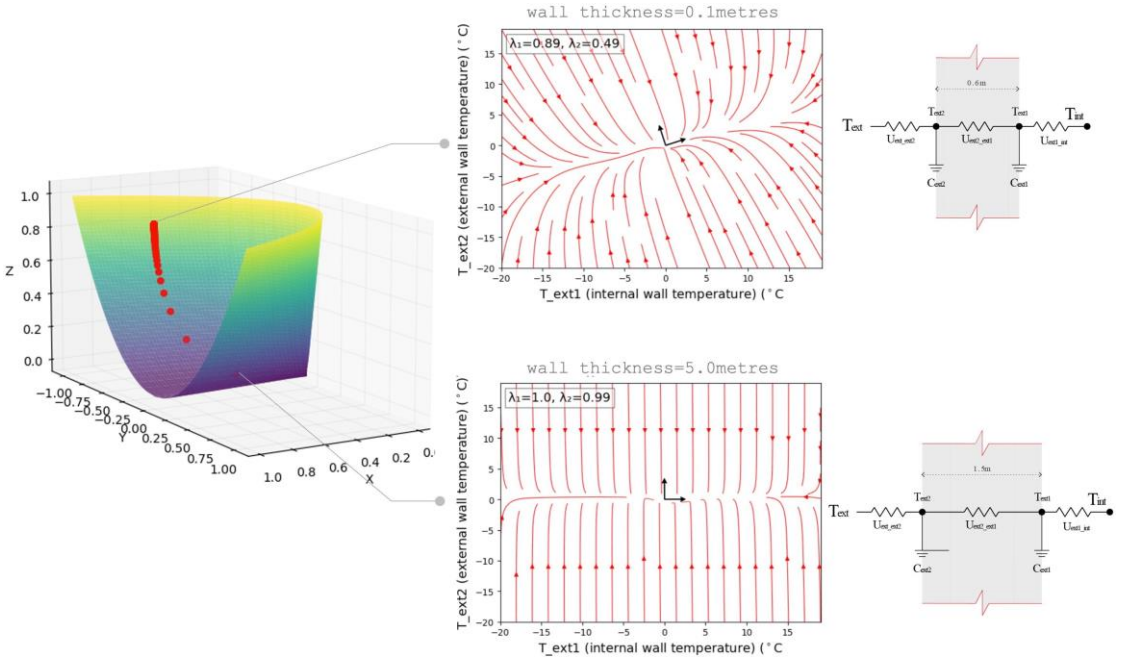


Figure 1: A family of heat balance ordinary differential equations on the symmetric positive definite manifold.

In this context, this paper suggest a methodology for improving the generalisation of ML models of dynamical systems by embedding constraints based on geometry within the training loss function. In particular, we focus on linear time-invariant (LTI) state space models whose state-transition operators belong to the Symmetric Positive Definite (SPD) manifold. State space models are widely used for control engineering

across applications including transportation systems, power generation and distribution, robotics, military and defense, and building and home automation. Given data from a measured system, the proposed method aims to learn a state transition operator that preserves the structural properties, defined by the positive definiteness of the manifold. More specifically, we aim to train an ML model that learns the state space operator, using non-Euclidean metrics that are specific to the manifold to measure accuracy. Additionally, a penalty term is imposed in the loss function that penalises the ML model if it generates operators that do not lie within the SPD manifold, preserving the structure.

We demonstrate the improved generalisation features of the method by means of a benchmark study across a number of test case scenarios, including heat transfer through a building facade wall. Figure 1 illustrates the SPD manifold for this family of heat balance equations and the phase plane at two locations on the manifold. For each test case, ML models were trained using three constraining approaches: no constraints, PDE-informed constraints, and geometry-informed constraints. The ML models were validated by their ability to generalise accurately in time for a set of unseen initial conditions. Lastly, for each test case scenario, we visualise and discuss the geometry of the learned state space through phase plane analysis.

Keywords: dynamical systems, manifold learning, physics-informed machine learning

---

* Presenting author

References

[1] Raissi, M., Perdikaris, P. & Karniadakis, G. Physics-informed neural networks: A deep learning framework for solving forward and inverse problems involving nonlinear partial differential equations. *Journal Of Computational Physics*. **378** pp. 686-707 (2019), https://www.sciencedirect.com/science/article/pii/S0021999118307125

[2] Cuomo, S., Di Cola, V., Giampaolo, F., Rozza, G., Raissi, M. & Piccialli, F. Scientific machine learning through physics–informed neural networks: Where we are and what's next. *Journal Of Scientific Computing*. **92**, 88 (2022)

[3] North, J. The "Structure" of Physics: A Case Study. *The Journal Of Philosophy*. **106**, 57-88 (2009), http://www.jstor.org/stable/20620153

[4] Dwivedi, V. & Srinivasan, B. Physics Informed Extreme Learn- ing Machine (PIELM)–A rapid method for the numerical solution of partial differential equations. *Neurocomputing*. **391** pp. 96-118 (2020), https://www.sciencedirect.com/science/article/pii/S0925231219318144

[5] Jin, X., Cai, S., Li, H. & Karniadakis, G. NSFnets (Navier-Stokes flow nets): Physics-informed neural networks for the incompressible Navier-Stokes equations. *Journal Of Computational Physics*. **426** pp. 109951 (2021)

The dynamics of nonlinear Alfvén waves in a magnetoplasma exhibit chaos and complexity

Subhrajit Roy,[1] Animesh Roy,[2] and Amar P. Misra[3]

[1] Department of Mathematics, Siksha Bhavana, Visva-Bharati University, Santiniketan-731 235, India, e-mail: suvo.math88@gmail.com

[2] Department of Mathematics, Siksha Bhavana, Visva-Bharati University, Santiniketan-731 235, West Bengal, India, e-mail: aroyiitd@gmail.com

[3] Department of Mathematics, Siksha Bhavana, Visva-Bharati University, Santiniketan-731 235, West Bengal, India, e-mail: apmisra@visva-bharati.ac.in

Abstract: We investigate the nonlinear dynamics of dispersive Alfvén wave (AW) envelopes interacting with driven ion sound waves in a uniform magnetoplasma. To capture the wave-wave interactions, we propose a low-dimensional dynamical model by focusing on a limited number of harmonic modes. Our findings reveal two subintervals of the modulation wave number, denoted as k, for the AW envelope: $(3/4)k_c$ kkkk_c and 0kkk$(3/4)k_c$ where k_c represents the critical value below which modulational instability (MI) occurs. In the former interval, characterized by a low MI growth rate, we observe periodic and/or quasi-periodic states. Conversely, in the latter interval with a high MI growth rate, chaotic states emerge. The presence of these states is confirmed through analyses of Lyapunov exponent spectra, bifurcation diagrams, and phase-space portraits of dynamical variables. Moreover, we quantify the complexity of chaotic phase spaces in the nonlinear motion using correlation dimension (CD) and approximate entropy (ApEn). We compare these measurements with those obtained from the well-known Hénon map and the Lorenz system, noting a significant qualitative agreement. The chaotic motion predicted by this low-dimensional model may serve as a precursor to the emergence of Alfvénic wave turbulence, which is relevant to the ionosphere and magnetosphere of Earth, in higher-dimensional models.

References:

[1] S. Jana, S. Ghosh, and N. Chakrabarti, Physics of Plasmas 24, 102307 (2017), https://doi.org/10.1063/1.4994118.

[2] H. Alfv´en, Nature 150, 405 (1942).

[3] S. Lundquist, Physical Review 76, 1805 (1949).

[4] J. Vogt, Surveys in Geophysics 23, 335 (2002).

[5] B. T. Tsurutani and C. M. Ho, Reviews of Geophysics 37, 517 (1999).

[6] V. Nakariakov, L. Ofman, E. Deluca, B. Roberts, and J. Davila, Science 285, 862 (1999).

[7] J. Bloxham, S. Zatman, and M. Dumberry, Nature 420, 65 (2002).

[8] P. K. Shukla, L. Stenflo, R. Bingham, and B. Eliasson, Plasma Physics and Controlled Fusion 46, B349 (2004).

[9] W. Gekelman, Journal of Geophysical Research: Space Physics 104, 14417 (1999).

[10] M. Shi, H. Li, C. Xiao, and X. Wang, The Astrophysical Journal 842, 63 (2017).

[11] K. M. Jain, M. Bose, S. Guha, and D. P. Tewari, Journal of Plasma Physics 36, 189193 (1986).

[12] F. Wang, , J. Han, and W. Duan, Plasma Science and Technology 23, 015002 (2020).

[13] E. Mjolhus and J. Wyller, Physica Scripta 33, 442 (1986).

[14] O. W. Roberts, X. Li, O. Alexandrova, and B. Li, Journal of Geophysical Research: Space Physics 121, 3870 (2016), https://agupubs.onlinelibrary.wiley.com/doi/pdf/10.1002/2015JA022248.

[15] V. M. Chmyrev, S. V. Bilichenko, O. A. Pokhotelov, V. A. Marchenko, V. I. Lazarev, A. V. Streltsov, and L. Stenflo, Physica Scripta 38, 841 (1988).

Keywords: Alfvén waves, Dynamical System, Mathematical Modelling, Chaos, Correlation dimension analysis

Subhrajit Roy

Presenting author

In-flight anomaly detection with an hybrid deep learning model using flight dynamics equations

Charles Dampeyrou[1,2,*], Martin Ghienne[1], Anita Dehoux[2], Jean-Luc Dion[1]

[1]Laboratoire QUARTZ, ISAE-Supm´eca, 93400 Saint-Ouen, France
[2]Aquila Data Enabler, 47 Rue Louis Blanc, 92400 Courbevoie, France
E-mail : charles.dampeyrou@isae-supmeca.fr

Keywords: Anomaly detection, Hybrid model, Scientific Machine Learning, Flight dynamics

* Presenting author

1 Introduction

In-flight anomaly detection is a crucial research topic for aviation safety. Among these anomalies, turbulence and icing can be particularly dangerous. Different method exist to detect anomalies in aircraft data. Oehling et al. use method based on a distance between the different datapoints to detect anomalies [1]. Isolation forest [2] is an algorithm that create an anomaly score using trees. Recently, deep learning methods have shown great results on anomaly detection tasks [3]. Hybrid models, based on deep learning and equations from the application domain, bring interpretability to the results. This approach is known as Scientific Machine Learning and is generally achieved by integrating the equations into the model's loss function.

An hybrid model is here proposed to detect anomalies. The flight dynamic equations are used. Unknown variables are estimated using deep-learning models in an unsupervised way. The data required for training are those generally recorded during flights. During inference, the equation's residues are monitored to detect and identify the anomalies.

2 Methodology

We consider the equations of the plane's dynamics, under the assumption of a rigid aircraft. These equations describe the linear and angular accelerations along the body axes.

The only unknown variables of these equations during the flight are the aerodynamic forces, the thrust and the torques due to these forces. The thrust, the torques and the aerodynamic coefficients are approximated by 7 multi layer perceptron (MLP), using their capabilities of learning patterns and relationships [4]. Each MLP takes as input the variables relevant for the prediction of the desired output. For instance, the MLP predicting the lift coefficient uses mach number, incidence and aircraft configuration as inputs. The MLPs are trained by minimizing the residue of the equations in an unsupervised manner. Once the model has been trained, the MLPs can estimate the missing terms in the equations and the residues can be calculated at any time. By monitoring these residues, it is possible to detect when flight data deviate from the training conditions. The different types of anomalies increase the residuals differently depending on the equation considered, which makes it possible to

discriminate between the anomalies.

3 Dataset

A synthetic dataset was generated to train and test the model. The simulation engine used was developped by R. Stengel [5] using the caracteristics of a real airplane. The control of the airplane was achieved by decoupling the speed, heading and altitude. The flight plans used are those of actual flights carried out by a Falcon 20 for meteorological measurements [6]. Since the data is simulated, it is possible to check the relevance of the variables estimated by the MLPs.

Two types of anomalies are generated in the data. First, turbulence is generated using a Von Karman spectral density complying with the MIL-HDBK-1798 standard [7]. The second type of anomalies considered is icing. The Lift and drag coefficients are modified in the same way as observed in real flight conditions [8].

4 Conclusion

An hybrid model is proposed to detect in-flight anomalies. MLPs estimate the missing variables in the flight dynamics equations in an unsupervised manner. The residue of the equations is monitored to detect anomalies. The model's performance is evaluated on two types of anomalies : turbulence and icing.

References

[1] Oehling et al. Using machine learning methods in airline flight data monitoring to generate new operational safety knowledge from existing data. *Safety science*, 114, 2019.

[2] Liu et al. Isolation-based anomaly detection. *ACM Transactions on Knowledge Discovery from Data (TKDD)*, 6(1):1–39, 2012.

[3] Su et al. Robust anomaly detection for multivariate time series through stochastic recurrent neural network. In *Proceedings of the 25th ACM SIGKDD international conference on knowledge discovery & data mining*, pages 2828–2837, 2019.

[4] K Hornik. Approximation capabilities of multilayer feedforward networks. *Neural networks*, 4(2):251–257, 1991.

[5] R Stengel. *Flight dynamics*. Princeton university press, 2005.

[6] Safire+ dataset. safireplus.aeris-data.fr. Accessed: 2023-05-31.

[7] *Flying Qualities of Piloted Aircraft*. Department of Defense Handbook MIL-HDBK-1797, 1997.

[8] Ide et al. The measurement of aircraft performance and stability and control after flight through natural icing conditions. In *3rd Flight Testing Conference and Technical Display*, page 9758, 1986.

Monitoring construction site situations with AI technologies

Marco Lorenzo Trani[1], Federica Madaschi [1, a], Ivan Mutis [2]
[1] A Politecnico Milano: federica.madaschi@polimi.it
[2] B Illinois Institute of Technology: imutissi@iit.edu

Activities in construction sites of buildings and or civil projects present significant risks to the workers' safety due to unanticipated hazards and often neglected safety standards and protocols. Although technology has advanced significantly to minimize safety and hazards in construction sites, there is a pressing need to address how AI affordances affect cognitive and attentional abilities as indicators of engagement for information to deter safety and hazard violations or situations that might present associated risks to workers on construction sites.

The research uses deep learning techniques to explore how users (e.g., workers and safety engineers) understand risks by presenting more relevant information, enabling a better implementation of safety standards. The study uses the researchers' extended collection of images, documents, and designs from existing and previous construction projects as datasets to train deep-learning models. The approach employs a combination of semantic segmentation techniques and transformer-based models. The aim is to enable the detection and verification of any interference between current situations and associated risks during field inspections.

The first step of the research identifies different typologies of potentially hazardous construction scenarios at the intersection of public areas and construction sites. The researchers will use an ontology built to classify and cluster-specific artifacts and scenes that present safety and hazards. By clearly describing the criteria and conditions in an ontology, the study builds a reference model to associate semantics to guide future safety and hazard machine-learning approaches.

Keywords: Deep learning, Image segmentation, Object detection, Site inspections, Safety and Health.

[a] Presenting Author

Parameter Estimation in Photonic Crystal Design Using Machine Learning Methods

Ezel Yağmur Zeydan Çelen [1, a], Sait Eser Karlık [2]

[1] Bursa Uludağ University, Bursa, 16059, Turkey, E-mail: eyzeydan@uludag.edu.tr

[2] Bursa Uludağ University, Bursa, 16059, Turkey, E-mail: ekarlik@uludag.edu.tr

Photonic crystals demonstrate periodic variations in refractive index or dielectric constant in one, two, or three dimensions. These structures allow light to propagate through the structure at specific frequencies or wavelengths while reflecting light at other wavelengths. The range of frequencies in which light propagation is prohibited is known as the "Photonic Band Gap." This band gap is critical in various optical designs, such as optical filters, lasers, and optical guide designs.

The propagation of light through a structure depends on the photonic band gap, which can be modified to a desired frequency range by adjusting the design parameters of the photonic crystal. These parameters, including the lattice constant, refractive index, radius of the dielectric rods or holes, and crystal symmetry, are vital for achieving optimal performance. Commonly, iterative methods such as "Plane Wave Expansion" and "Finite Difference Time Domain" are used to obtain the most appropriate values for each parameter. However, such methods are often time-consuming and impractical for complex crystal designs.

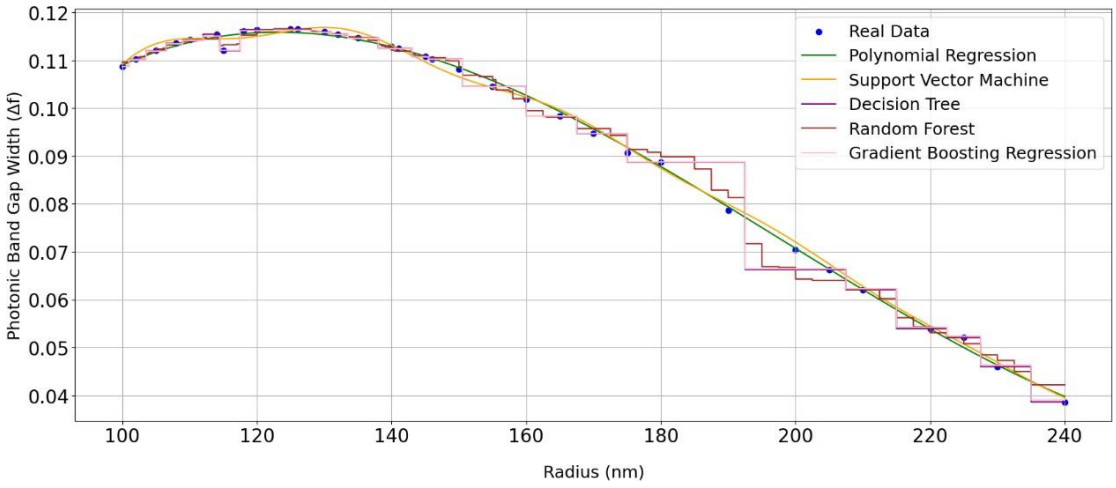


Figure 1.a: Comparison of different machine learning methods in estimating the change of photonic band gap in response to dielectric rod radius values varying between 100 nm and 240 nm in a perfect square lattice photonic crystal design.

[a] Presenting Author

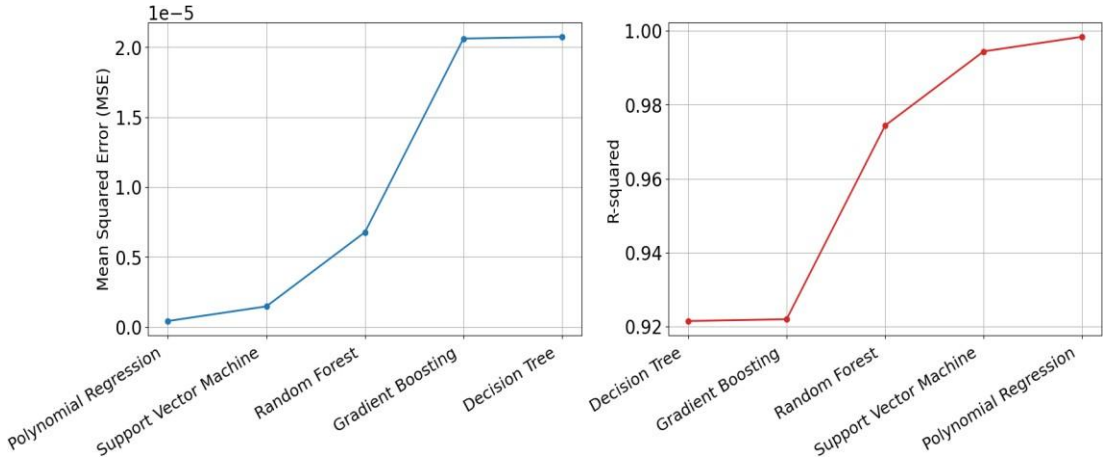


Figure 1.b: Comparison of performance metrics of different machine learning models.

This study explores machine learning methods to estimate the design parameters that can address this issue. The results of this approach are compared to those obtained by traditional methods. We have designed a perfect square lattice photonic crystal structure and have obtained this structure's photonic band gap width for different dielectric radii by conventional methods. We then have used these data as input for machine learning regression methods. We have used different machine-learning regression methods to estimate the photonic band gap width for dielectric radius values ranging from 100 nm to 240 nm. The obtained estimation results are presented in Figure 1.a. We have calculated the mean squared error and r-squared values, which include the performance metrics of different machine learning models in photonic band gap estimation depending on the radius, and the relevant metrics are given in Figure 1.b. While the mean squared error expresses the error between real data and prediction, the r-squared metric expresses the fit between the data type and the machine learning model. Support Vector Machine and Polynomial Regression models demonstrate the highest performance in this study, showing that relevant parameters of photonic crystal designs could be achieved with high accuracy.

In conclusion, this study demonstrates the effectiveness of machine learning methods in estimating the design parameters of photonic crystal structures. The results suggest this approach may be a viable alternative to traditional iterative methods for crystal designs. The implications of this study could be important for improving the efficiency and accuracy of optical designs in a wide range of applications.

Keywords: Photonic Crystals, Photonic Band gap, Machine Learning, Parameter Estimation

Activity recognition based on temporomandibular joint movement in a fertility monitoring device

Anna Wąsik*[1], Wiktor Sieklicki[2], Bartosz Reichel[3], Krzysztof Łukaszuk[4], Janusz Przewocki[1]

[1] Division of Set Theory, University of Gdańsk and Lifeconcept Ltd
[2] Institute of Mechanics and Machine Design, Gdańsk Univeristy of Technology and Lifeconcept Ltd
[3] Institute of Physics and Applied Computer Science, Gdańsk Univeristy of Technology and Lifeconcept Ltd
[4] Institute of Nursing and Midwifery, Medical University of Gdańsk and Lifeconcept Ltd

Abstract: Human activity recognition (HAR) is a well known area of research with various applications as an assistive technology in healthcare. This work is a part of a project of a fertility monitoring device. The aim of the project was to develop a new personal device (wearable) collecting and analyzing previously unconnected parameters such as body temperature, temporomandibular joint (TMJ) activity, electrodermal activity, to support female fertility and increase the chances of pregnancy. During the presentation, we would like to focus on activity recognition based on the movement of temporomandibular joint using a single accelerometer.

We have prepared several datasets with accelerometer signals. Each signal was labeled with one of the following activities: eating, drinking, speaking, or another activity. The labeling process involved pressing a corresponding button during the activity. Our goal was to create machine learning models that could classify signals according to these labels.

The first approach involved using a random forest classifier trained on various features of the signals, including Fourier transforms and recurrence plots. The second approach utilized one-dimensional convolutional neural networks. In this presentation, we will compare both types of models and present their advantages and disadvantages, along with some insights into the signal parameters that are actually utilized to accurately predict the corresponding activity.

Keywords: Signal recognition, Artificial Neural Network, fertility monitoring device, recurrence plots

* Presenting author

References

[1] D. Asso. The relationship between menstrual cycle changes in nervous system activity and psychological, behavioural and physical variables. *Biological Psychology*, 23(1):53–64, 1986.

[2] E. Fridriksdottir and A. G. Bonomi. Accelerometer-based human activity recognition for patient monitoring using a deep neural network. *Sensors*, 20(22):6424, 2020.

[3] O. D. Lara and M. A. Labrador. A survey on human activity recognition using wearable sensors. *IEEE communications surveys & tutorials*, 15(3):1192–1209, 2012.

[4] M. Straczkiewicz, P. James, and J.-P. Onnela. A systematic review of smartphone-based human activity recognition methods for health research. *NPJ Digital Medicine*, 4(1):148, 2021.

Precision in Complexity: An Evaluation Framework for Compound LLM Systems

Daniel Bretsko[1,*], Yuri Bogomolov[1], Stanislav Sobolevsky[1,2 1-]
Masaryk University, E-mail: bretsko@math.muni.cz
[2]New York University

Abstract: Large language models (LLMs) have emerged as pivotal tools in the artificial intelligence (AI) landscape, pushing the boundaries of natural language processing (NLP) and generating widespread interest across academia and industry alike. These models, capable of understanding and generating human-like text, have revolutionized how we interact with technology, offering unprecedented capabilities in a range of applications from automated content creation to complex problem-solving tasks [1].

Despite their impressive capabilities, LLMs are not without limitations. Key among these is their struggle with complex, multi-step problems or tasks requiring specialized knowledge, which are often critical for applications in advanced analytics, scientific research, and decision-making processes. This shortfall often results in responses that, while syntactically correct, lack coherence, accuracy, or depth of understanding, leading to misinformation and misinterpretation. These responses are also called hallucinations [2]. To mitigate these weaknesses, researchers have developed techniques such as Chain-of-Thought (CoT) reasoning [3, 4] and prompt chaining [5, 6], which prompts models to generate intermediate reasoning steps and enables them to use their output as an input for the next steps before arriving at a final answer. Those approaches have shown significant promise in enhancing the reasoning capabilities of LLMs, allowing them to tackle tasks requiring intricate reasoning or specialized knowledge with improved accuracy. LLMs often struggle to address the challenges associated with graph-structured data and tasks due to the intrinsic differences between graph data and the sequential data on which LLMs are typically trained. To improve graph reasoning capabilities, tools such as Graph-ToolFormer[8] have been developed, creating a compound system based on LLMs by providing the latter with mechanisms to better interact with and reason about graph-structured data.

Despite these advancements in LLMs, the evaluation of LLMs' performance on graph tasks remains an area needing further exploration. While benchmarks exist for evaluating LLMs across a broad spectrum of tasks like HumanEval [7], and also existing evaluation framework for assessing LLMs on their ability to handle graph-structured data, GPT4Graph [9], there is a scarcity of frameworks specifically designed to assess their capabilities in a CoT context for network analysis and graph-related problems. These benchmarks, while extensive, primarily focus on evaluating the end result of prompts without delving deeply into the intermediate steps that lead to the final answer which shouldn't be overlooked as even LLM ranking systems benefit from this approach [10]. It can overlook the nuanced reasoning processes critical for understanding and manipulating complex relationships and structures, particularly in graph-related tasks.

In response to this need, we introduce an evaluation framework that is designed to rigorously assess the Chain-of-Thought reasoning and prompt chaining capabilities of compound systems using LLMs within the context of network analysis and graph tasks. By leveraging an LLM with access to an extensive array of datasets and analytical tools, our framework evaluates each stage of the prompt chain decision-making process. This includes the accuracy of data selection and retrieval, the proper analytical tool chosen, as well as the accuracy of the final query result (Figure 1). This evaluation will provide a comprehensive assessment of how well novel and effective prompt engineering techniques in compound LLM systems can solve complex problems that involve graph theory, network dynamics, and related analytical challenges. By focusing on this specialized area and validating each reasoning step, our evaluation aims to push the boundaries of what LLMs-based compound systems can achieve.

Keywords: LLM, NLP, Prompt Chaining, Network Analysis

---

* Presenting author

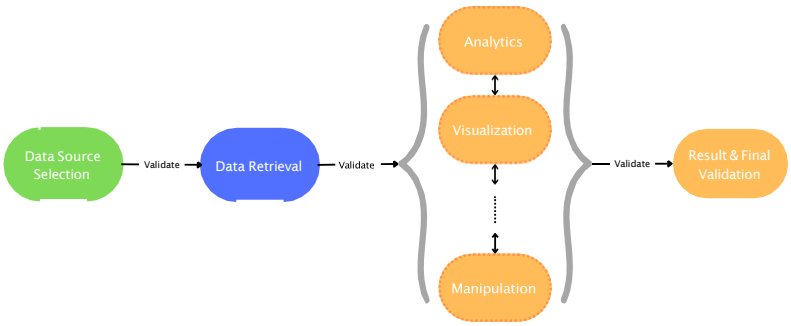


Figure 1: Validation steps in our evaluation framework for prompt chaining systems

References

[1] Zhao, W. X., Zhou, K., Li, J., Tang, T., Wang, X., Hou, Y., ... & Wen, J. R. (2023). A survey of large language models. arXiv preprint arXiv:2303.18223.

[2] Zhang, Y., Li, Y., Cui, L., Cai, D., Liu, L., Fu, T., ... & Shi, S. (2023). Siren's song in the AI ocean: a survey on hallucination in large language models. arXiv preprint arXiv:2309.01219.

[3] Wei, J., Wang, X., Schuurmans, D., Bosma, M., Xia, F., Chi, E., ... & Zhou, D. (2022). Chain-of-thought prompting elicits reasoning in large language models. Advances in Neural Information Processing Systems, 35, 24824-24837.

[4] Prystawski, B., Li, M., & Goodman, N. (2024). Why think step by step? Reasoning emerges from the locality of experience. Advances in Neural Information Processing Systems, 36.

[5] Wang, B., Deng, X., & Sun, H. (2022). Iteratively prompt pre-trained language models for chain of thought. arXiv preprint arXiv:2203.08383.

[6] Wu, T., Terry, M., & Cai, C. J. (2022, April). AI chains: Transparent and controllable human-AI interaction by chaining large language model prompts. In Proceedings of the 2022 CHI conference on human factors in computing systems (pp. 1-22).

[7] Chen, M., Tworek, J., Jun, H., Yuan, Q., Pinto, H. P. D. O., Kaplan, J., ... & Zaremba, W. (2021). Evaluating large language models trained on code. arXiv preprint arXiv:2107.03374.

[8] Zhang, J. (2023). Graph-ToolFormer: To Empower LLMs with Graph Reasoning Ability via Prompt Augmented by ChatGPT. arXiv preprint arXiv:2304.11116.

[9] Guo, J., Du, L., & Liu, H. (2023). GPT4Graph: Can Large Language Models Understand Graph Structured Data? An Empirical Evaluation and Benchmarking. arXiv preprint arXiv:2305.15066.

[10] Lightman, H., Kosaraju, V., Burda, Y., Edwards, H., Baker, B., Lee, T., ... & Cobbe, K. (2023). Let's Verify Step by Step. arXiv preprint arXiv:2305.20050.

Modeling of Data Movie in Single Molecule Localization Microscopy

Yi Sun[a]
Electrical Engineering Department, The College of City University of New York
E-mail: ysun@ccny.cuny.edu

In single molecule localization microscopy (SMLM), it is desired to build up a model of data movie to capture the effect of all parts in an SMLM system, including dynamics of photoactivatable molecules, excitation laser powers, optical lens, light diffraction, camera photosensitivity, pixel size, frame rate, autofluorescence noise, circuit noise, etc. A well-reasoned model of data movie can enable development of advanced localization algorithms. It can also be applied to generate accurate training data for AI to achieve a high quality of SMLM images. A model of data movie can be composed of two parts. One is a model of data frame, and the other is a model of emitter activation (i.e., molecule photoactivation) process. A model of data frame was developed in our previous work. In this paper, we focus on modeling of emitter activation process.

A process of emitter activation is usually modeled by a Markov chain in literature, including a Markov chain with two states of on and off, with three states of on, off, and photobleaching, and with the four states of on, meta-off, off, and photobleaching, and with $J \geq 2$ states in general. However, these previous studies are defective in two ways. First, a process of emitter activation follows the first order of kinetic law. The time of an on-state where an emitter emits photons is random and is exponentially distributed. The time of an off-state where an emitter does not emit photons before photobleaching is also exponentially distributed. A state transition either from an on-state to an off-state or converse can occur during a frame time. Thus, in a data frame where a state transition occurs, the number of detected photons, a Poisson process, has a smaller mean than that in a data frame where an on-state is kept unchanged. Moreover, the mean itself is random as well, that is, a transition can randomly occur at any time during a frame time. However, the previous models based on a Markov chain ignore the effect of the state transition during a frame. Second, all the previous models consider only the continuous illumination of emitters whereas certain SMLM systems like STORM employ cycled illuminations. The first defection is a severe flaw in previous models while the second defection is missing of model in literature. In this paper, both the defections are addressed.

First, the continuous illumination is considered. The modeling starts with a process of emitter activation in continuous time. The photoactivatable time is random and exponentially distributed. During the photoactivatable time, the on-state time and the off-state time of an emitter occur alternatively until the photobleaching. Both times are random and are exponentially distributed with means depending on the excitation laser power. The emitter state is averaged by integration over one frame after another, and the emitter state indexed by the frame time is obtained. Clearly, the emitter state in the frame time consists of three possible states, 1 denoting an on-state, 0 denoting an off-state, and a random number $r \in (0,1)$

[a] Presenting Author

denoting a random state (r-state). It is clear that the process of emitter activation indexed by the frame time cannot be modeled by a Markov chain. Based on the model of emitter activation, analyzed are the average numbers of consecutive on-states and off-states in a data movie, the mean number of 1-state emitters, and the man number of r-states in a data frame, and the corresponding formulas are obtained. Second, in the cycled illumination, pairs of conjugated activator and emitter are labeled on a biological sample. An activation laser and a deactivation laser alternatively illuminate the sample. Similarly, the process of emitter activation is modeled in continuous time and then is transferred to a discrete-time model indexed by the frame time. The model is then analyzed. Incorporating the model of emitter activation with the model of a data frame, a complete model of data movie is then obtained. Simulations for both the continuous and cycled illuminations in 2D and 3D imaging are carried out by custom MATLAB codes. The results show that the models can well synthesize a data movie of SMLM, thus broadly applicable in simulating SMLM systems, generating AI training data, evaluating quality of SMLM images, and testing performance of localization and AL algorithms.

Keywords: Single molecule localization microscopy, superresolution microscopy, fluorescence molecule, photoactivation, emitter localization.

Influence of Fluid Velocity onto the Metal Foam Screen

Mohd Azuwan bin Maoinser [1, a], Aimi Zahraa binti Zainal [2], Sofyah Anis binti Jusof [3]

[1] Universiti Teknologi PETRONAS, E-mail: mazuwan.maoinser@utp.edu.my

[2] Universiti Teknologi PETRONAS, E-mail: aimi.zainal@utp.edu.my

[3] Universiti Teknologi PETRONAS, E-mail: sofyah.jusof@utp.edu.my

Mechanical sand screens play a vital role in filtering sand particles in hydrocarbon production. Despite their importance, high sand production frequently results in screen plugging, diminishing hydrocarbon production and equipment efficiency. Metal foams offer a potential solution by enhancing screen strength while maintaining a lightweight structure. However, the effectiveness of metal foam sand screen hinges on understanding the behavior of fluids and sand particles within the structure. Yet, there is a significant gap in understanding the fluid flow behavior within these screens, as existing studies have primarily focused on metal foam heat exchangers, which may not entirely reflect the specific conditions in sand screens. This study aims to address this gap by delving into the fluid flow behavior within the metal foam structures. The study will particularly focus on the variations of fluid velocity, which exert a significant influence on fluid flow patterns and subsequently, on pressure drop. Understanding the implications of pressure drop, which can lead to screen plugging, underscores the importance of fluid flow dynamics within the metal foam structure. By focusing on fluid flow velocity, this study seeks to enhance the understanding of fluid behavior in metal foam sand screens, potentially enhancing their performance in hydrocarbon production. Subsequent studies should explore the comparative performance of metal foam screen with the conventional sand screens, such as wire-wrap and premium mesh, in terms of sand retention capabilities and screen integrity.

Keywords: sand retention, metal foam, sand screen

[a] Presenting Author

An Application of Machine Learning Techniques in Prediction of Manufacturing Quality of a Composite Wind Turbine Blade

Nihong Yang[1] [a], Qing Pan[2]

[1] University of The West of England, Bristol, UK, E-mail: nihong2.yang@uwe.ac.uk
[2] LMAT Ltd., Bristol, UK, Email: qing.pang@lmat-uk.com

Composite wind turbine blades are usually manufactured with the Vacuum Assisted Resin Infusion (VARI) technique, due to its low cost and high manufacturing rate for large composite part manufacturing. In this paper, finite element simulations are first used to model the VARI manufacturing process of a composite wing turbine blade. Four Machine Learning (ML) models, namely Decision Tree (DT), Random Forest (RF), Support Vector Machine (SVM) and Artificial Neural Network (ANN) are then developed with the manufacturing data obtained by the finite element modelling, for prediction of the manufacturing quality of the blade.

In the finite element simulations, the resin flow process is visualized and a resin fill factor, defined as the ratio of the filled nodes to the total blade nodes can be obtained for each process. A manufacturing process, specified with four manufacturing parameters, namely filling temperature, blade fabric permeability, resin flow pipe length and inlet/outlet position, is labelled as defective, if its resin fill factor is less than 99%. With the manufacturing data, the supervised machine learning classification approach is applied to obtain ML models to predict whether a process is good. The optimal models with the best hyperparameters are obtained with the specific codes from the Scikit-learn module in the Python environment. The performance of the models is then assessed and compared, according to their prediction accuracy and modelling efficiency.

It is seen that both the SVM and ANN models can achieve remarkably high prediction accuracy and have high modelling efficiency, while all four ML models yield high prediction accuracy. Within the four manufacturing parameters, the filling temperature is the parameter that strongly affects the manufacturing quality of the blade. The optimal model, developed by an appropriate ML algorithm can be used to replace FE modelling in real-time control of the process or computer assisted process optimisation to predict manufacturing quality in much lower cost and shorter time.

Keywords: Vacuum assisted resin infusion, Wind turbine blade manufacturing, Machine learning, Surrogate model, Decision tree, Random Forest, Support vector machine, Artificial neural network.

[a] Presenting Author

Physics-informed Mesh-free Deep Compositional Operator Network

Weiheng Zhong[1], Hadi Meidani[1,*]

[1]University of Illinois at Urbana-Champaign, E-mail: meidani@illinois.edu

Abstract: In numerous scientific and engineering contexts, solving parametric Partial Differential Equations (PDEs) across a broad spectrum of parameters is a critical challenge. Neural operators, which learn mappings from parameters to solutions, have recently been considered as the most promising machine-learning approach for addressing this problem. They accelerate the process of solving parametric PDEs by learning a neural operator as a mapping from the PDE parameters to the solutions of PDEs [2, 3]. However, data-driven training of neural operators often demands extensive datasets composed of parameter-solution pairs, the acquisition of which can be prohibitively expensive. Alternatively, physics-informed training presents a more cost-effective strategy for achieving high-performance neural operators. However, current physics-informed neural operators face limitations, either in handling irregular domain shapes or in mesh generalization capabilities. Physics-informed DeepONet (PI-DeepONet) [1] extends the original DeepONet framework by embedding physical laws directly into the loss function during training. With automatic differentiation, PI-DeepONet can compute the PDE residuals in any irregular domain shape. The incorporation of physical laws also enhances the learning process but, even with this advancement, physics-informed DeepONet struggles with generalization across different PDE parameter representations. On the other hand, the physics-informed Fourier Neural Operator (PI-FNO) [4] builds upon the original FNO framework, offering generalization across different PDE parameter representations while also incorporating physics-informed training methods. However, the the reliance of PI-FNO on Fast Fourier Transform (FFT) restricts its application to rectangular domains with uniform meshes since FFT depends on uniform sampling of the signal in the spatial domain. In this research, we introduce an innovative model, named Physics-informed Deep Compositional Operator Network (PI-DCON), that not only generalizes across different meshes within irregular domain shapes but also facilitates physics-informed training, eliminating the need for finite-element method computations. Our findings demonstrate that this approach enables the development of a neural operator that not only sets a new benchmark in performance but also significantly enhances training efficiency. Our proposed model is capable of generalizing across different PDE parameter representations, including those in irregular domain shapes. In this study, the irregular domain shapes are defined as those that does not belong to regular geometric forms such as rectangles, circles, or polygons. The advantage of our proposed model compared to other existing works will be presented.

Keywords: Physics-informed deep learning, Neural operator, Mesh generalization, Irregular domain shapes

* Presenting author

References

[1] Wang, Sifan, Hanwen Wang, and Paris Perdikaris. ”Learning the solution operator of parametric partial differential equations with physics-informed DeepONets.” Science

advances 7.40 (2021): eabi8605.

[2] Lu, L., Jin, P., Pang, G., Zhang, Z., Karniadakis, G. E. (2021). Learning nonlinear operators via DeepONet based on the universal approximation theorem of operators. Nature machine intelligence, 3(3), 218-229.

[3] Li, Z., Kovachki, N., Azizzadenesheli, K., Liu, B., Bhattacharya, K., Stuart, A., Anandkumar, A. (2020). Fourier neural operator for parametric partial differential equations. arXiv preprint arXiv:2010.08895.

[4] Li, Z., Zheng, H., Kovachki, N., Jin, D., Chen, H., Liu, B., ... Anandkumar, A. (2021). Physics-informed neural operator for learning partial differential equations. ACM/JMS Journal of Data Science.

An Open Source tool for Topic Modeling with Word Network Clustering

Alymzhan Toleu[1,2]*, Gulmira Tolegen[1,2], Rustam Mussabaye[1,2]

[1]Institute of Information and Computational Technologies, Almaty, Kazakhstan
[2]Satbayev University,
E-mail:atoleu@iict.kz, gtolegen@.iict.kz

Abstract:

Topic modeling (TM) is an important task in NLP that automatically uncovers hidden structures and patterns within a large collection of documents. The discovered information exhibits high interpretability and modular structural features. This implies that the topic model enables us to quickly and cost-effectively grasp the big picture of the data. The output of a topic model serves as a valuable tool for understanding the document collection and can be utilized as input variables for subsequent analyses.

One of the popular early works for probabilistic topic models is Latent Dirichlet allocation (LDA) is a two-level Bayesian generative model: i) to model topic distribution over tokens and ii) to model document distribution over topics. One assumption of LDA is to apply a prior from Dirichlet distribution to generate the distributions, which over-complicates the model when applying the Bayesian inference. Additive regularization of topic models (ARTM) is a non-Bayesian model that attempts to solve the problems in the LDA model. It considers the topic modeling as problem-oriented matrix factorization and the parameters are trained through expectation–maximization (EM) algorithm adding several task-specific regularization terms and the model parameters start with random initialization. From the ARTM view, the parameters of LDA are more likely to be initialized with Dirichlet distribution and trained with the single objective function. These approaches are trying to find two latent parameters of matrices document-topic and topic-word in a large search space: $D \times T$, $W \times T$, which is often very sparse and high-dimension in practice since these approaches utilize discrete features of documents (D, T, W refer to the size of the documents, topics, and words, respectively).

This work presents a word networks clustering approach for topic modeling [**?**] that decomposes the large search space into two sub-spaces: $T \times W$ and $D \times T$. Each of the sub-spaces cannot be very large in practice since $T \ll D$ and $T \ll W$. First of all, the topics of documents are found with a clustering algorithm in a subspace $T \times W$, and then the topic assignments in another small sub-space $T \times D$ are calculated. To uncover the thematic structure of a collection of documents, we proposed an approach based on adapting a community detection algorithm on a word network where vertices are words and edges are the distances between words.

This approach consists of the following steps: i) building word networks: word graphs were constructed with different word representations: co-occurrence, TFIDF, and word embedding-based. ii) the process can be described as follows: iii) topic assignment: Two types of topic assignments were utilized: i) Jaccard metric and ii) cosine similarity-based for calculating the distance between topics and documents.

A python library of the proposed approach was developed and it was divide into the following blocks(the developed library is available under the link https://github.com/a-toleu/WNC/):

- Pre-processing block: it involves tasks such as data cleaning, tokenization, stop-word removal, and stemming or lemmatization.
- Vocabulary extraction and optimization: it focuses on identifying and refining the set of unique words or terms in our textual dataset.
- Embedding block: it transforms text data into numerical representations.
- Word network construction: it involves creating a graph-like structure where words are nodes, and edges represent semantic relationships between them.
- Word network clustering-based TM: This approach leverages word network construction to perform topic modeling. Instead of directly clustering documents, it groups words based on their connections in the network. These word clusters then serve as topics, offering a unique perspective on topic modeling.
- Topic assignment block: it focuses on associating documents or words with specific topics.
- Evaluation block: The evaluation block assesses the quality and effectiveness of the topic modeling results.

Algorithm 1 Topic Detection algorithm

Input: a word network $G = (V, E)$.
Output: $T = (V_n, E_n)$ topics/community contains a set of words/vertices $v_i \in V$.

each word in the network $G = (V, E)$ is assigned to its own topic $t \in T$.
while true **do**
  for $v_i \in W$ **do**
    $mod_{max} \leftarrow -1$
    $mod_{original} \leftarrow$ calculate modularity for v_i remains in its original topic.
    for each neighbour v_n of v_i **do**
      $mod_{move} \leftarrow$ calculate modularity for removing v_i from its own topic and move it into v_n.
      if $mod_{move} > mod_{max}$ **then**
        $mod_{max} \leftarrow mod_{move}$
        $neighbour_{max} \leftarrow v_n$
      end if
    end for
    if $mod_{original} > mod_{max}$ **then**
      keep v_i in its original topic.
    else
      move v_i to the new topic of $neighbour_{max}$.
    end if
  end for
  $V_n \leftarrow$ newly-formed topics are become vertices.
  $E_n \leftarrow$ new edges are calculated over the topics.
  $T \leftarrow (V_n, E_n)$
  if mod_{max} is maximized and topics are stabilized **then**
    Stop the procedure;
  end if
end while

Topic coherence and the document clustering results were chosen for topic models evaluation. Several experiments were conducted to evaluate the proposed approach, and the results showed that it achieved comparable results with the current best. Evaluation results also showed that the proposed approach produces higher performance as the number of most relevant words gets larger in C_{cv} coherence score. More interestingly, the results showed the proposed approach based on co-occurrence/tfidf word network produces a better topic coherence score than the approach based on word embeddings. However, for the document clustering task, the approach based on word embeddings obtained better results than the others.

Keywords: Topic Modeling, Word Network, Clustering;

* Presenting author

Acknowledgement

The work was funded by the Committee of Science of Ministry of Science and Higher Education of the Republic of Kazakhstan under the grant BR21882268.

Ensemble Deep Learning Approach for Apple Fruitlet Detection from Digital Images

Mohamad Yusnisyahmi Yusof[1], Iskandar Ishak[1], Fatimah Sidi [1, a],
[1] Department of Computer of Science, Universiti Putra Malaysia, Malaysia.
E-mail: {GS69600, iskandar_i, fatimah}@upm.edu.my

Agriculture commodities are commodities that have a high economic worth and the potential to be developed further. The green and red apple, in instance, is one type of fruit that has the potential to be cultivated as part of agriculture. In most cases, the sorting of green apples is done manually, and individuals are the ones who make the final determinations. The process of manually identifying products can have several drawbacks, including the fact that it takes a considerable amount of time, the fact that humans can become fatigued and overworked when performing repetitive tasks, the fact that there is less variety in the products that can be identified, and so on. As a result of developments in science as well as digital image processing technology, it is now possible to automatically categorizing agricultural products and plantings. The purpose of this research is to enhance the performance of the CNN-based model in detection of apple fruitlet from apple tree images. A dataset containing 720 images of apple fruitlet is used in this project. To enhance the overall performance of the model, the revised CNN-based YOLOv5 ensemble model was implemented with the Sigmoid Linear Unit (SiLU) activation function, Batch Normalization, and SGD optimization algorithms. The combination of activation function, optimization, batch normalization, and ensemble technique are later used to enhance the YOLOv5 ensemble model with the benefits of utilizing limited resources. According to the experimental results, the accuracy of the updated ensemble model achieved 95% percent of accuracy in terms of Mean Average Precision (MAP) when compared to the benchmark model.

Keywords: Ensemble Deep Learning; CNN-based model; Detection

[a] Presenting Author