AKPIK 1: Reservoir Computing & Neural Networks

Time: Tuesday 9:30–11:00 Location: MAR 0.002

AKPIK 1.1 Tue 9:30 MAR 0.002

Minimal Reservoir Computing — •Haochun Ma[1], Davide Prosperino[1], and Christoph Räth[2] — [1]Allianz Global Investors, risklab, Seidlstraße 24, 80335, Munich, Germany — [2]Deutsches Zentrum für Luft- und Raumfahrt (DLR), Institut für KI Sicherheit, Wilhelm-Runge-Straße 10, 89081 Ulm, Germany

Reservoir computers are powerful machine learning algorithms for predicting nonlinear systems. However, the traditional reservoir computer uses random matrices to define the underlying recurrent neural network and has a large number of hyperparameters to optimize.

Here, we show that a few simple modifications to the traditional reservoir computer architecture, which eliminate randomness and minimize computational resources, lead to significant and robust improvements in short- and long-term predictive performance compared to similar models, while requiring minimal amount of training data. Specifically, the adjacency matrix of the reservoir becomes a block diagonal matrix, where each block is the same matrix with all elements being one. Further, we omit the nonlinear activation function. The nonlinearity is only introduced by also taking higher powers of the reservoir response. Thus, this new architecture open new avenues to explainable and interpretable reservoir computing.

For certain parameterizations, we find that the predictions are accurate for more than 10 Lyapunov times and that ordinary least squares regression directly on the embedded data can predict the long-term climate of chaotic systems [1].

[1] H.Ma et al., Sci. Rep., 13, 12970 (2023)

AKPIK 1.2 Tue 9:45 MAR 0.002

Novel implementations for reservoir computing – from spin to charge — •Atreya Majumdar[1], Karin Everschor-Stte[1], Katharina Wolk[2], and Dennis Meier[2,3] — [1]Faculty of Physics and Center for Nanointegration Duisburg-Essen (CENIDE), University of Duisburg-Essen, 47057 Duisburg, Germany — [2]Department of Materials Science and Engineering, Norwegian University of Science and Technology (NTNU), Trondheim 7034, Norway — [3]Center for Quantum Spintronics, Norwegian University of Science and Technology (NTNU), Trondheim 7034, Norway

Magnetic and ferroelectric materials are emerging as promising candidates for unconventional computing and next-generation information technology. We review and explore the potential of nanoscale topological textures, focusing on magnetic skyrmions and ferroelectric domain walls, for use in reservoir computing [1] a scheme that allows transforming non-linear tasks into linearly solvable ones. We highlight the essential characteristics needed for physical reservoirs, outlining the advantages of topological textures, such as the increased complexity and flexible input and output options. We provide insights into how topological textures in magnetic and ferroelectric systems can serve as an avenue for enhancing reservoir computing and, more generally, broadening the scope of in-materio computing.

[1] K. Everschor-Sitte, A. Majumdar, K. Wolk, D. Meier, arXiv:2311.11929

AKPIK 1.3 Tue 10:00 MAR 0.002

Analyzing phase transitions in minimal reservoir computers — •Davide Prosperino[1], Haochun Ma[1], and Christoph Räth[2] — [1]Allianz Global Investors, risklab, Seidlstraße 24-24a, 80335, Munich, Germany — [2]Deutsches Zentrum für Luft- und Raumfahrt (DLR), Institut für KI Sicherheit, Wilhelm-Runge-Straße 10, 89081 Ulm, Germany

Minimal reservoir computers are powerful machine learning algorithms that can accurately predict nonlinear systems [1]. They differ from traditional feedforward neural networks by not relying on randomness but instead utilizing linear optimization, which enables them to operate on small training datasets and requires minimal computational resources.

Additionally, they can make accurate predictions for over ten Lyapunov times with certain parameterizations. However, we discovered that for certain parametrizations, the prediction fails. With only a few parameters, the phase transition between various parameterizations can be analyzed to comprehend the reasons behind the success of a prediction. We do that by analyzing the reconstructed, underlying equations.

[1] H. Ma, D. Prosperino, et al., Sci. Rep., 13, 12970 (2023)

AKPIK 1.4 Tue 10:15 MAR 0.002

Image reconstruction with diffusion models for accelerated magnetic resonance imaging — •Christine Müller[1], Vanya Saksena[2], Florian Knoll[2], and Bernhard Kainz[1] — [1]Image Data Exploration and Analysis Lab, Friedrich-Alexander-Universität Erlangen-Nürnberg — [2]Computational Imaging Lab, Friedrich-Alexander-Universität Erlangen-Nürnberg

Magnetic resonance imaging (MRI) is a widely used non-invasive imaging technique in medical practice. However, conventional MRI acquisitions are often time-consuming, limiting their applicability in clinical settings. Accelerated MRI techniques reduce scan time but come at the expense of image quality. Diffusion models are a recent promising class of generative models for image reconstruction in MRI [1,2]. These models learn to generate high-quality images from undersampled MRI data by gradually denoising a noisy image.

In this work, we evaluate the performance of a score-based diffusion model that was trained on brain MRI data from the publicly available fastMRI dataset [3]. It employs a predictor-corrector sampling step and combines parallel imaging and compressed sensing techniques. A learned score function is utilized as a prior to guide the reconstruction process, enabling the generation of realistic content, especially at high acceleration rates. Diffusion models offer the potential to improve the quality of reconstructed images and reduce scan time, making MRI more accessible and efficient.

[1] DOI: 10.1016/j.media.2022.102479, [2] DOI: 10.1016/j.media.2023.102846, [3] DOI: 10.1148/RYAI.2020190007

AKPIK 1.5 Tue 10:30 MAR 0.002

Performance of RBM neural quantum states from the perspective of the quantum geometric tensor — •Sidhartha Dash[1], Filippo Vicentini[2,1], Michel Ferrero[2,1], and Antoine Georges[1,2,3] — [1]Collège de France, Université PSL, 11 place Marcelin Berthelot, 75005 Paris, France — [2]CPHT, CNRS, École polytechnique, Institut Polytechnique de Paris, 91120 Palaiseau, France — [3]Center for Computational Quantum Physics, Flatiron Institute, New York, New York, 10010, USA

There have been a lot of recent advances in using artificial neural networks, as variational ansätze (Neural quantum states), to approximate the ground states of quantum systems. Various neural network architectures including RBMs, RNNs, CNNs, and Transformers have been successfully used to approximate the ground states of many quantum spin models with a reasonable accuracy. However, the practical limit of the representation power of such ansätze is far from being understood. The universal approximation theorems only guarantee that the RBM can represent any distribution with an arbitrary accuracy, given a sufficient number of hidden units which is exponential in system size. In this work, we systematically study the accuracy of RBMs for representing the groundstate of spin-1 models. We use the quantum geometric tensor at convergence to characterize the performance of the ansatz for various spin-1 models, and for various densities of the network.

AKPIK 1.6 Tue 10:45 MAR 0.002

Physics-Informed Deep Learning to Couple Reactive Diffusion and Swelling in Cellulose-based Porous Media — •Alexandra Serebrennikova[1], Maximilian Fuchs[1], Raimund Teubler[2], and Karin Zojer[1] — [1]Institute of Solid State Physics, TU Graz, Graz, Austria — [2]Institute of Analytical Chemistry, TU Graz, Graz, Austria

Simulating the reactive diffusion of fluids through porous media presents significant challenges due to the intricate geometries of real-world systems, particularly when the porous media itself undergoes changes, such as swelling of the solid matrix. Traditional numerical solvers often struggle to represent these complex details accurately and feasibly. Based on state-of-the-art extended physics-informed neural networks (PINNs), this contribution focuses on creating a mesh-free modeling framework for studying the reactive transport of volatile organic compounds (VOCs) through the complex microstructure of paper. PINNs serve us to implicitly incorporate the experimentally observed evolution of geometrical features of paper matrix into the formulation of the governing partial differential equations. This approach enables to study the spatio-temporal evolution of VOC concentrations in the porous environment of paper, while the geometry of the material

dynamically adapts itself through swelling or shrinking as response to the current state of adsorption.

To our knowledge, this is the first contribution that applies PINNs to consider adaptive geometries during transport.