Scientific Computing in Computer Science
Department of Informatics
Technische Universität München

Harmonic AI

# PhD Position: Machine Learning with Linear Operators

## Brief description

Simulating complex, highly interconnected systems such as the climate, biology, or society typically involve methods from the "traditional" field of scientific computing. These methods are usually reliable and explainable through their foundations in rigorous mathematics. Examples are efficient space discretization schemes such as sparse grids and scalable, parallel solvers for partial differential equations. Unfortunately, most of them are not immediately applicable to the extremely high-dimensional, heterogeneous, and scattered data where neural networks are usually used. Those methods employed in the AI community, on the other hand, are typically not reliable or explainable in the traditional sense, and pose problems illustrated through adversarial examples and brittle generalization results.
Towards the goal of explainable, reliable, and efficient AI, two PhD projects are embedded in an Emmy Noether research group from Dr. Felix Dietrich[1] that connects the two worlds of scientific HPC and deep learning, forming a concept we call “Harmonic AI”. Specifically, we will combine linear operator theory and deep learning methods through harmonic analysis. The benefit of such a link between AI and linear operators is bi-directional. Inference, classification, and training of neural networks will be understood mostly in terms of linear algebra. This will open the field to much more mathematical rigor and enable more mathematicians to work on AI methods. Simultaneously, applied AI researchers obtain reliable methods that can currently only be found for problems outside the field, such as Finite Element Methods or iterative Newton-Raphson solvers.
The PhD projects are devoted to explainability of AI by bridging the gap to rigorous mathematics: Leveraging the common principles between the Laplace operator [5], Gaussian processes [16], and neural networks, the first PhD project will connect AI and linear algebra. The second PhD project in the group will combine ideas from the Neural Tangent Kernel [9] and the Koopman operator [3, 6] toward a dynamical systems interpretation of iterative AI methods, including training and data processing in neural network layers.

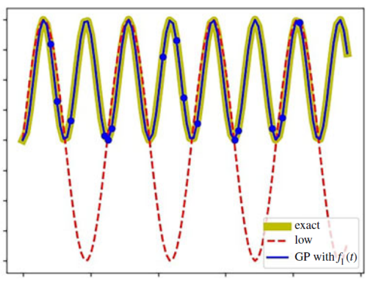


Figure 1 from [11]: Multi-fidelity modeling with Gaussian processes.

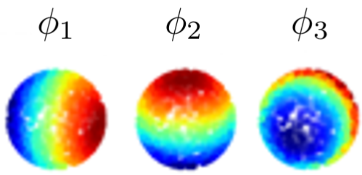


Figure 2: Three eigenfunctions of the Laplace-Beltrami operator on a sphere, approximated with Diffusion Maps [5] and `datafold` [13].

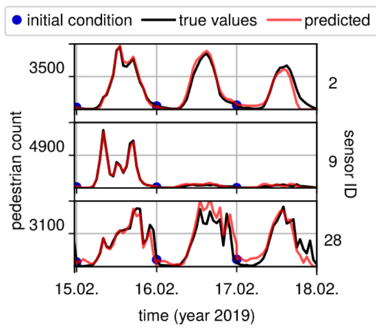


Figure 3: Koopman operator approximation and prediction of crowd measurements in Melbourne, Australia [12].

[1] See https://www.in.tum.de/en/news-single-view-en/article/neue-emmy-noether-forschungsgruppe-um-dr-f-dietrich-bewilligt0/

## Time line

The project is designed to be completed in three years. Adjustments are possible.

## Requirements

The following items are sufficient to start and successfully complete the project.

- Minimum degree: Master in Informatics, Mathematics, or related (minimum GPA 2.5/5 or better).
- Knowledge about Machine Learning (neural networks, Gaussian processes), Scientific Computing (matrix approximations), Linear operator theory (ideally: Laplace/Koopman operators).
- Experience with TensorFlow, PyTorch, or similar software is ideal, but not necessary.
- Soft skills: analytical thinking, structured and organized work, intrinsic motivation.

## Tasks and Details

You can apply to one or both of the projects available. One of them is focused on the Laplace operator, the other on the Koopman operator.
The Laplace-Beltrami operator is a core object in harmonic analysis. It is intimately connected to stochastic calculus, its eigenfunctions have a multiscale structure that is related to spatial discretisation schemes such as sparse grids [4], it is the main object employed by spectral approximation and classification methods [1], and is the generator of Gaussian (diffusion) processes [17]. Algorithms to approximate the operator are available, for example "Diffusion Maps" formulated by our collaborator R. R. Coifman [5] and implemented in our software `datafold`[2].
The other linear operator, for the second PhD project, was first studied by B. Koopman [10]. This "Koopman operator", albeit linear, captures the dynamics of nonlinear systems, and allows researchers to predict the evolution of observables [3]. Essentially, the Koopman operator is to dynamical systems what the Laplace operator is to geometry: these operators encode everything about the system or object under study, and numerical approximations of them can therefore be used to access, process, store, and analyse all properties that are important to the respective application [2, 6, 14].
We already develop a code base called `datafold`[3] for efficient approximation of linear (Laplace and Koopman) operators on point clouds in our research group [13], in collaboration with Prof. Gerta Köster. Gaussian Processes can be approximated on images with the kernel from [8], several codes to approximate landmarks on manifolds (the codes from [15, 7] and other, more efficient methods) are also available.
Throughout the project, to disseminate, demonstrate, and test the new methods in a proof of concept, we will collaborate with the simulation groups from Prof. Christian Mendl (Quantum Computing Group at TUM[4]) studying quantum dynamics and from Prof. Gerta Köster (Crowd Simulation group[5], Department of Computer Science and Mathematics, University of Applied Sciences Munich) studying human crowds.

[2] See https://datafold-dev.gitlab.io/datafold/index.html
[3] See https://datafold-dev.gitlab.io/datafold/index.html
[4] See https://www5.in.tum.de/~quanTUMcomputing/
[5] See https://www.cs.hm.edu/die_fakultaet/ansprechpartner/professoren/koester/index.de.html

## How to apply

Please apply by filling out the form at the following URL, and refer to this project in the section on "topic suggestion":

https://www5.in.tum.de/lehre/thesis-application/

TUM has been pursuing the strategic goal of substantially increasing the diversity of its staff. As an equal opportunity and affirmative action employer, TUM explicitly encourages nominations of and applications from women as well as from all others who would bring additional diversity dimensions to the university's research and teaching strategies. Preference will be given to disabled candidates with equal qualifications. International candidates are also highly encouraged to apply.

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