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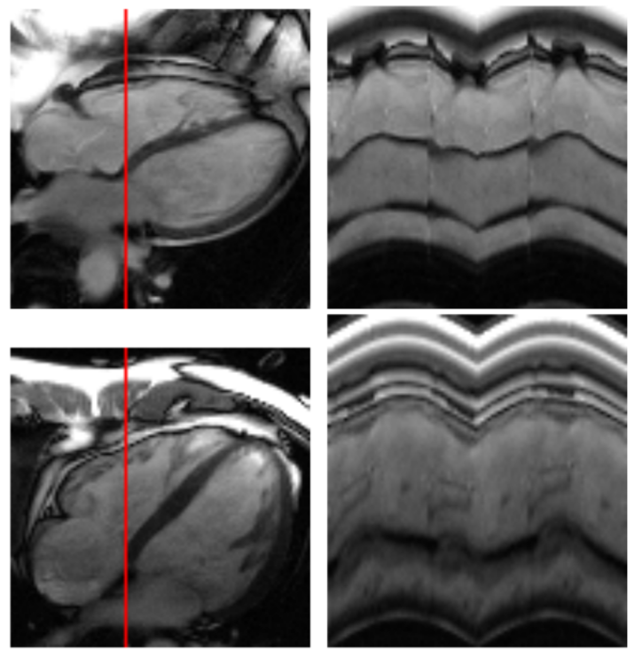
Open Student Research Projects

Project: Self gating for Cardiac MRI Data with Radial Acquisition

Background. Magnetic Resonance Imaging (MRI) is an important medical imaging technique. Image reconstruction from MR measurements is a non-trivial task, especially with dynamic data appearing in cardiac imaging. In the past years, deep learning techniques have made significant progress in MR image reconstruction, but require high-quality training data. To obtain the latter for cardiac imaging, it is necessary to obtain information on the cardiac- and respiratory states of the patient during the different time frames. Currently, this information is frequently measured with additional instruments such as ECG or respiratory belts. Obtaining this information without additional instruments would significantly simplify MR image acquisition and ultimately benefit patients and the healthcare system.



Goal. Test existing methods and develop new methods for estimating cardiac- and respiratory phases of cardiac MR data directly from the data itself.

Recommended Prerequisites.

- Knowledge in analysis and Fourier analysis, linear algebra and (Python-)programming. Experience with machine learning is an advantage. Being open to learn about MR imaging and MR physics.

Collaboration. This project will be realized in collaboration with the group of Prof. Uecker from the Institute of Biomedical Imaging of Graz University of Technology.

Contact. Univ. Prof. Dr. Martin Holler (martin.holler@uni-graz.at, +43 316 380 1645), IDea_Lab, University of Graz.

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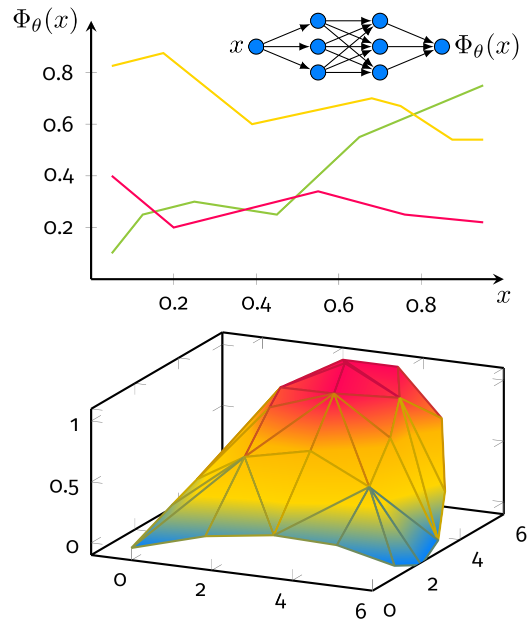
Open Student Research Projects

Project: Investigating the piecewise linear structure of ReLU neural networks

Background. Artificial neural networks play a tremendous role in modern machine learning. In particular the ReLU activation function became very popular in the last years due to its simplicity. Neural networks with ReLU activation function have a particularly interesting structure: The resulting functions are piecewise linear on polygons in the input domain. This result can be derived quite easily for shallow neural networks and can be extended to deep neural networks. For one- or two-dimensional inputs, it is possible to visualize this underlying structure and to explicitly compute the "grid" on which the function is piecewise linear. This structure reveals interesting phenomena that are also useful to better understand the behavior of neural networks with arbitrary input and output dimensions.

Output of different neural networks



The structure of ReLU neural networks might for instance be exploited in order to compute error estimates for physics-informed neural networks or to develop new initialization schemes for weights and biases.

Goal. Understand and visualize the structure of ReLU neural networks and develop algorithms to compute their underlying grids.

Recommended Prerequisites.

- Knowledge in analysis, linear algebra and (Python-)programming. Experience with machine learning, in particular neural networks, is an advantage.

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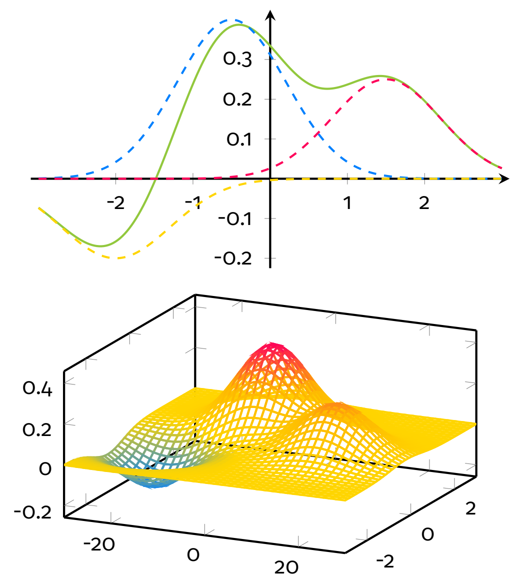
Open Student Research Projects

Project: Solving partial differential equations using deep kernel methods

Background. The solution of PDEs is an important task in scientific machine learning. Kernel methods constitute mathematically profound approaches for data and function approximation and are well-established in the machine learning community due to their rich mathematical theory and background. Recently, kernel methods have also been employed to approximately solve PDEs. However, the choice of the shape parameters in the kernel functions poses a serious difficulty in practice and often requires experience as well as a priori knowledge about the problem at hand. Deep kernel methods allow for trainable shape parameters that can be adapted towards the particular form of the function they are supposed to approximate. In particular for high-dimensional problems with an inherent low-dimensional structure, such approaches might be desirable. The considered approach builds on an energy minimization formulation of elliptic PDEs that regards the weak solution as an equivalent optimization problem.

Linear combinations of kernels



Goal. Implement and test different algorithms using deep kernel methods to solve elliptic PDEs. Numerically validate the capabilities of deep kernel methods in higher dimensions.

Recommended Prerequisites.

- Knowledge in analysis, linear algebra, numerical methods for elliptic PDEs (in particular finite elements) and (Python-)programming. Experience with functional analysis and optimization is an advantage.

Collaboration. Depending on the direction of the project, collaboration with Dr. T. Wenzel from LMU Munich is possible.

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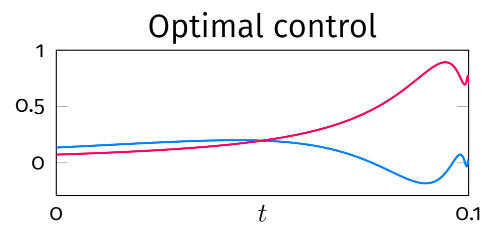
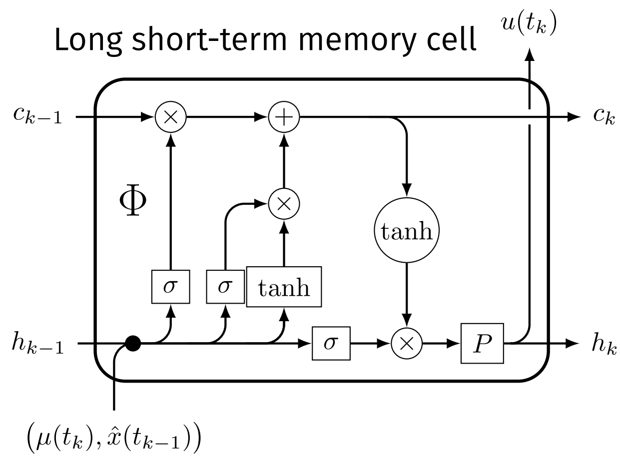
Open Student Research Projects

Project: Optimal control of dynamical systems using machine learning

Background. The field of optimal control has seen a tremendous development in recent years due to the introduction of different machine learning techniques. Moreover, the strong interactions and connections between machine learning and control theory, for instance in terms of reinforcement learning or recurrent neural networks, open several paths for improvements in both directions. Parametric dynamical systems, where the behavior of the system is influenced by certain physical parameters, constitute an additional difficulty in many practical applications. Incorporating such parametric dependencies of the optimal control problem also in the respective machine learning architectures is therefore of high interest from an algorithmic and also from a practical perspective.





Goal. Test existing and develop new machine learning architectures for optimal control problems. Extend these machine learning methods to the case of parametric dynamical systems.

Recommended Prerequisites.

- Knowledge in analysis, linear algebra, optimization and (Python-)programming. Experience with machine learning is an advantage.

Collaboration. Depending on the direction of the project, collaboration with Prof. M. Lazar from the University of Dubrovnik and Dr. C. Molinari from the University of Genova as well as participation in the COST Action “Interactions between Control Theory and Machine Learning (InterCoML)” is possible.

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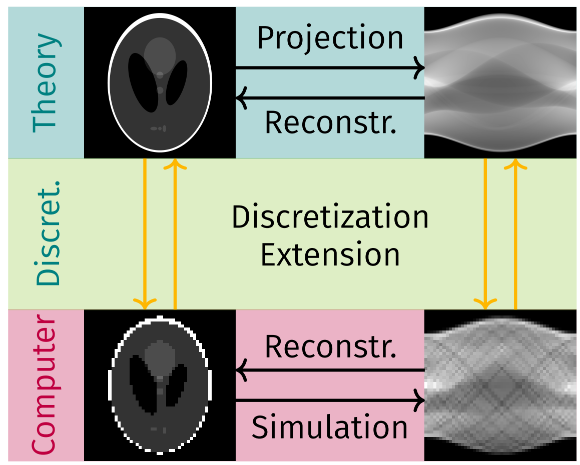
Open Student Research Projects

Project: Connecting theoretical tomography with the world of computer implementations



Background. Tomographic methods offer a non-invasive way to visualize a patient's interior features, and are thus of fundamental importance in medicine. Despite the long-running interest in the inverse problems of tomographic reconstruction, a suitable choice of discretization schemes remains a topic of debate that is dominated by anecdotal reports with little mathematical rigor. Key questions are how to design discretizations and their impact on the reconstruction process. Rigorous mathematical investigations can connect theoretical (infinite-dimensional) considerations with the concrete work done by computers, hence offering the potential to answer these questions and infer improved discretization schemes. Conversely, convincing more applied researchers – that will be the ultimate beneficiaries of the described research – of these theoretical results requires validation via simulation studies.

Goal. Develop, analyze and implement discretization schemes for tomographic operators and investigate their impact on tomographic reconstructions. Dependent on the student researcher's interest, the task can range from more abstract convergence investigations to more applied software development related tasks.

Recommended Prerequisites.

- Interest and knowledge in numerical analysis, functional analysis and programming.
- Experience in Python and PyTorch would be greatly appreciated but are not a must.

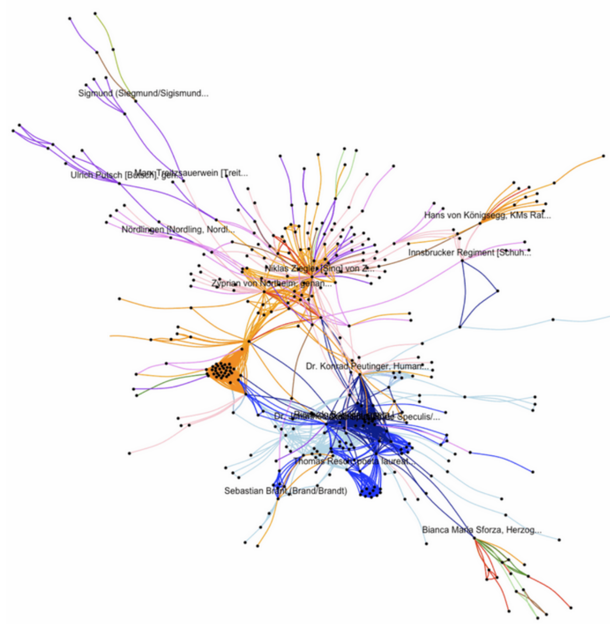
Collaboration. Dependent on the direction of the project, collaboration with Prof. Kristian Bredies and Dr. Benjamin Hackl (Institute for Mathematics and Scientific Computing, University of Graz) on the Gratopy toolbox (https://gratopy.readthedocs.io) are possible.

Contact. Dr. Richard Huber (richard.huber@uni-graz.at, +43 316 380 1651), IDea_Lab, University of Graz.

Open Student Research Projects

Project: Completing knowledge graphs that represent historical data

Background. Knowledge graphs are a well-established approach for representing diverse types of data in a structured format that facilitates data analysis and machine learning applications. In the project Managing Maximilian of the Department of Digital Humanities, University of Graz, knowledge graphs are employed to store and represent historical data about Maximilian of Habsburg (1459–1519). However, historical data is often incomplete, with certain gaps being readily apparent to human observers who understand the semantics of the data. Automatically filling these gaps presents a significant challenge, which this project aims to address using graph-based machine learning techniques.



Goal. Implement and test machine learning methods to complete the knowledge graph as provided by the Department of Digital Humanities. Numerically validate the capabilities of developed methods.

Recommended Prerequisites.

- Knowledge analysis, linear algebra and (Python-)programming, basic knowledge of graph theory. Experience with machine learning is an advantage. Being open to interdisciplinary collaboration.

Collaboration. This project will be realized in collaboration with the group of Prof. Vogeler from the Department of Digital Humanities, Univeristy of Graz.

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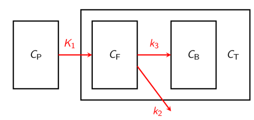
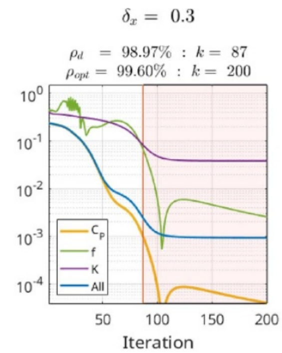
Open Student Research Projects

Project: Reconstructing physiological parameters from image-based PET

Background. Positron Emission Tomography (PET) is a powerful imaging technique that provides insights into the functional processes of the body by mapping the time-space distribution of a radiotracer. While reconstructing high-quality images from PET data is already a complex and computationally demanding task, the clinical utility of PET often extends beyond image generation. Physicians frequently seek to extract specific physiological parameters from these images, as these parameters can offer critical insights into the presence and progression of certain diseases. The process of inferring physiological parameters from PET images introduces additional challenges. It requires not only accurate modeling of the underlying identification problem but also the development of robust and efficient reconstruction algorithms. These algorithms must bridge the gap between the raw PET data, the reconstructed images, and the physiological parameters of interest, all while maintaining reliability and clinical relevance.



$$\begin{cases} \frac{\mathrm{d}}{\mathrm{d}t} C_F = K_1 C_P - (k_2 + k_3)\, C_F, & t > 0 \\ \frac{\mathrm{d}}{\mathrm{d}t} C_B = k_3 C_F, & t > 0 \\ C_F(0) = 0, \ C_B(0) = 0 \end{cases}$$



Goal. The goal is to develop and numerically validate a reconstruction method capable of reliably identifying physiological parameters from image-based PET measurements. This involves formulating an appropriate mathematical model for the identification problem and designing a reconstruction algorithm that is both accurate and computationally efficient.

Recommended Prerequisites.

- Knowledge in analysis, linear algebra and (Python-)programming. Experience with ML and optimization is an advantage.

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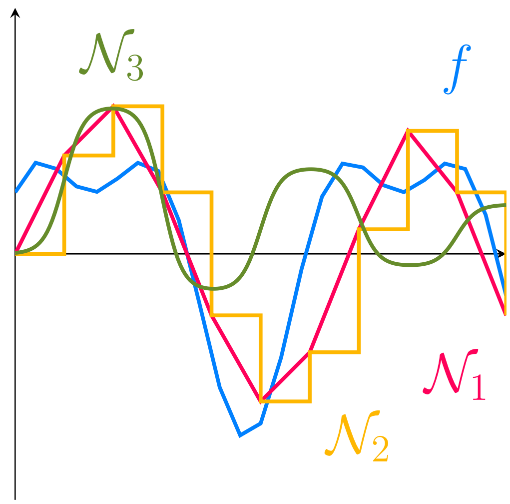
Open Student Research Projects

Project: Investigating approximation properties of neural networks in practice



Background. The success of neural network-based machine learning methods can be attributed, in part, to their ability to approximate a wide range of functions with high precision. This can be achieved by increasing the complexity of the neural network architecture, which is typically characterized by parameters such as network width, depth, and the total number of weights. However, this increased complexity comes at a cost. Training highly complex networks often requires significantly more computational resources and time, and it can lead to challenges such as overfitting. Another critical factor influencing the practical performance of neural networks is the choice of activation function(s) which is crucial for the network's expressiveness. Understanding how these factors, network complexity and activation functions, interact in practice is essential for designing efficient and effective neural network architectures.

Goal. This project aims to explore approximability by neural networks numerically, shedding light on how their theoretical properties translate into practice.

Recommended Prerequisites.

- Knowledge in analysis, linear algebra and (Python-)programming. Experience with ML and optimization is an advantage.

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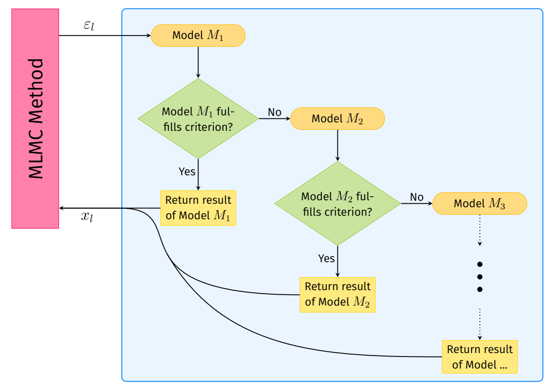
Open Student Research Projects

Project: Application of model hierarchies in multilevel Monte Carlo methods



Background. Uncertainty quantification typically requires the repeated execution of complicated and costly numerical simulations for many different parameters of the underlying model. In this context, multilevel Monte Carlo (MLMC) methods constitute an approach to reduce the computational costs by replacing the majority of costly simulations by cheaper evaluations of approximate models with different "levels" of accuracy. MLMC methods allow for a rigorous convergence analysis and are a well-established tool to compute expectations in stochastic simulations. Recently, adaptive model hierarchies were discussed extensively in the context of parametric problems. Such model hierarchies combine models with different approximation qualities and construct them adaptively, tailored to the parameters of interest, while making use of the cheaper models whenever possible. The goal of this project is to bring together both concepts – MLMC methods and adaptive model hierarchies – on a practical level.

Goal. Implement a combination of MLMC methods and adaptive model hierarchies (building on existing software packages).

Recommended Prerequisites.

- Knowledge in analysis, linear algebra and (Python-)programming. Moreover, a sound foundation in probability theory or statistics is beneficial.

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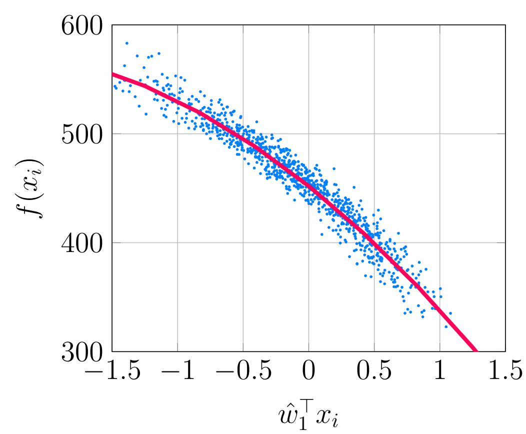
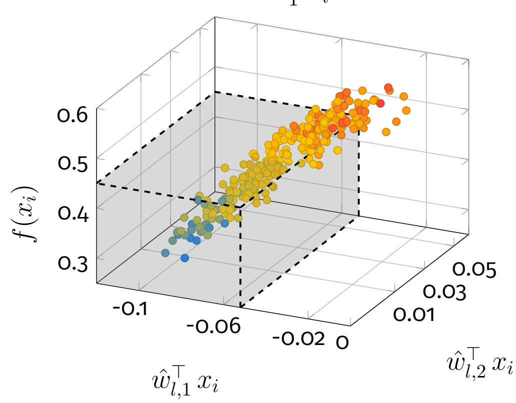
Open Student Research Projects

Project: Analyzing high-dimensional data using active subspaces





Background. Scalar-valued data with high-dimensional input spaces often appears in practical applications. For instance, it is possible to model the infection with HIV over time as a dynamical system depending on several parameters. However, only certain linear combinations of the input parameters have a significant impact on the behavior of the disease whereas many directions in the parameter space are negligible. In this project, the goal is to identify such unimportant parts of the input space from data in order to simplify the model and to facilitate the analysis of high-dimensional data. Potential directions of interest might include the theoretical investigation of active subspaces or their practical implementation in different application scenarios. Moreover, a combination for instance with optimization algorithms is possible.

Goal. Investigate the approach of active subspaces and obtain an understanding of their theoretical foundation as well as practical matters. Depending on the student's interest, the focus of this project can either be on theoretical questions or on practical applications.

Recommended Prerequisites.

- Knowledge in analysis and (numerical) linear algebra. Depending on the direction of the project, knowledge of (Python-)programming might be important. Moreover, a sound foundation in probability theory or statistics is beneficial.

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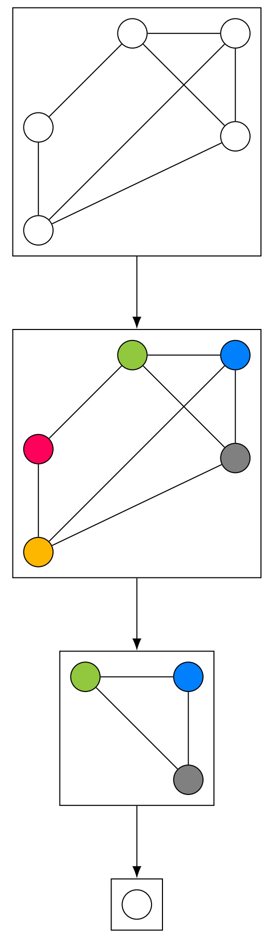
Open Student Research Projects

Project: Graph neural networks and group equivariance



Background. In many practical applications, the underlying structures can be encoded as graphs consisting of vertices that are connected via edges. Both of these components – vertices and edges – can carry information. For instance, images can be seen as graphs where the vertices correspond to the pixels of the image whereas the edges encode information of adjacency of pixels respectively vertices. More complicated graphs with an irregular structure can for example be used to represent intricate chemical molecules. In the past years, neural networks that act on graphs – so called graph neural networks – have been of growing interest due to their wide applicability. In the context of graph neural networks, it is important to ensure that the output of the network is in a sense independent of the ordering of the vertices as long as the connectivity and the information associated to corresponding vertices and edges is the same. Using the concept of group equivariances, it is possible to extend this idea to different "invariances" (or equivariances to be more precise) by adding suitable layer structures. In this project, we make ourselves familiar with graph neural networks and group equivariant versions thereof. Both, a theoretical or a practical investigation of the concepts is possible.

Goal. Understand the main concepts for graph neural networks and group equivariances. Examine these ideas either on a theoretical level or consider group equivariant graph neural networks in practical applications.

Recommended Prerequisites.

- Knowledge in analysis and linear algebra. In case of a more application-driven direction of the project, basic knowledge in (Python-)programming is advantageous. Moreover, first experience with neural networks or graph theory is beneficial.

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Open Student Research Projects

Project: Reliable Medical Image Segmentation via Conformal Prediction

Background. State-of-the-art Convolutional Neural Networks (CNNs) achieve outstanding performances in classification tasks, but lack rigorous reliability guarantees necessary for critical applications, such as medical imaging. Conformal prediction (CP) is a technique to obtain such guarantees in the form of error bounds via a calibration procedure. Most importantly, those error bounds can be obtained for any black box machine learning method and are statistically guaranteed to hold with high probability. By extending its error-bounding capabilities to segmentation tasks, conformal prediction can provide confidence maps that highlight regions of uncertainty, enabling more informed decision-making. This added layer of reliability ensures that segmentation models are not only accurate but also trustworthy, paving the way for their safe deployment in real-world high-stakes scenarios.

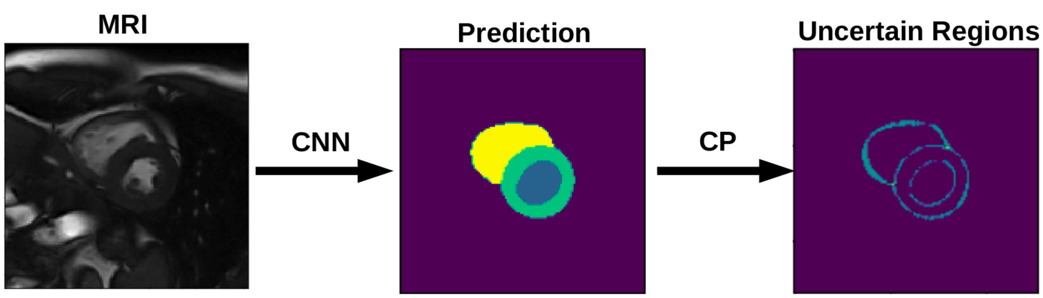

Figure 1: Workflow of MRI segmentation with post-processed conformal prediction: a CNN segments the medical image, while conformal prediction quantifies and highlights uncertain regions in the segmentation mask.

Goal. Analyze and implement different techniques of conformal prediction for image medical image classification/segmentation.

Recommended Prerequisites.

- Knowledge in (Python-)programming, Deep Learning and statistics.

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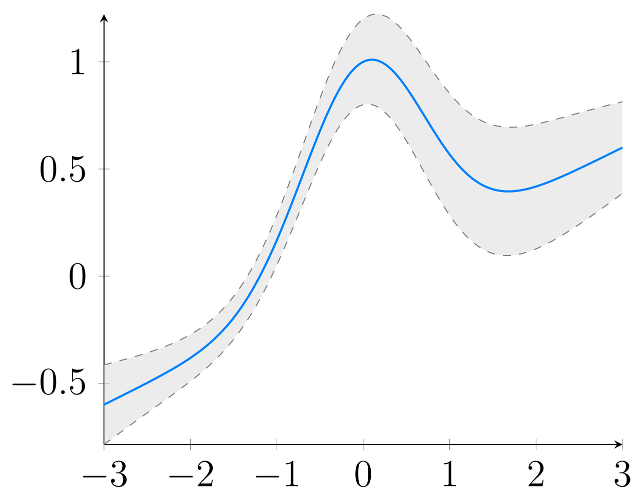
Open Student Research Projects

Project: Error bounds for deep learning methods via conformal prediction

Background. State of the art deep learning methods often achieve unprecedented practical performance in classification and regression tasks, but lack rigorous reliability guarantees necessary for critical applications. Conformal prediction is a technique to obtain such reliability guarantees in the form of error bounds via a calibration procedure. Most importantly, the obtained error bounds can be obtained for any black box machine learning method and are statistically guaranteed to hold with high probability.

Prediction with Error Bounds



Goal. Analyze and implement different techniques of conformal prediction for image classification.

Recommended Prerequisites.

- Knowledge in statistics, probability theory and (Python-)programming. Experience with machine learning is an advantage.

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