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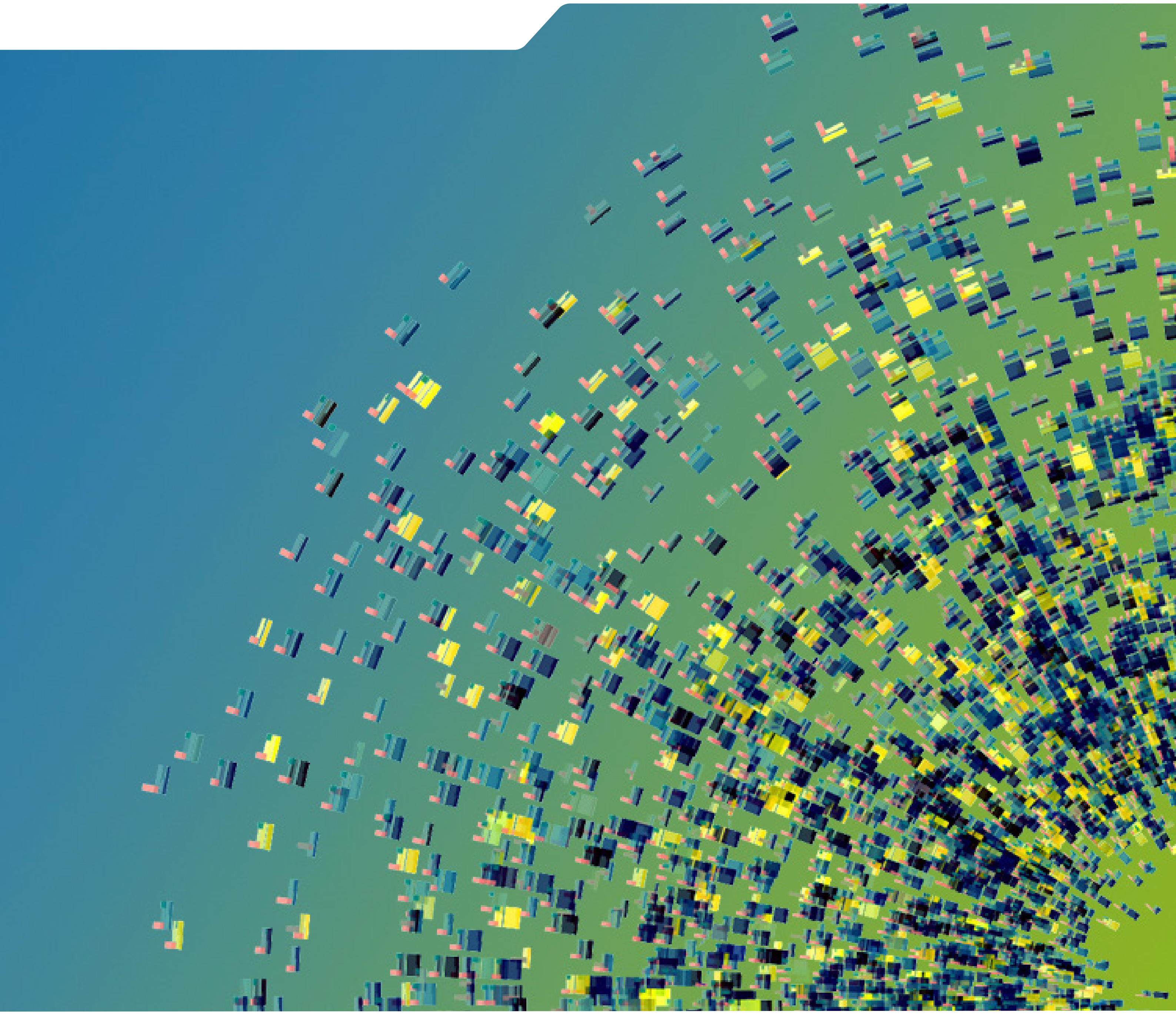

VIRTUAL CONFERENCE

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ABSTRACT BOOK

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MODELS AND INFRASTRUCTURE

HELMHOLTZ AI COMMUNITY

Computational Mapping of the Human SARS-CoV-2 Protein-RNA Interactome

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The SARS-CoV-2 pandemic is still affecting the lives of billions of people worldwide. It is known that viruses make extensive use of the host cell‘s machinery, hijacking it for the purpose of viral replication and interfere with the activity of master regulatory proteins. This includes RNA binding proteins (RBPs), which are key regulators of the cell's RNA metabolism. Often, targets of RBPs share at least one common local sequence feature – a so-called motif – which facilitates the recognition of the RNA by the RBP. Host RBPs are critical factors for viral replication and have been shown to influence viral RNA stability, replication and escape of host immune response.

While current research efforts have been centered around identifying mechanisms of host cell-entry, the role of host RBPs in context SARS-CoV-2 replication is still not understood. Although some experimental studies have started mapping the SARS-CoV-2 RNA-protein interactome, computational approaches are able to screen large numbers of RBPs for putative interactions with the viral RNA and are crucial to prioritize candidates for further experimental investigation. Here, we investigate the role of RBPs in context of SARS-CoV-2 by constructing an in-silico map of human RBP / viral RNA interactions. Our framework is based on pysster, a deep learning method which learns sequence preferences of given RBPs. Models were trained using eCLIP datasets for > 150 RBP from human cell lines and applied cross-species to predict RBP-binding across the SARS-CoV-2 RNA. After validation of trained models, we generate binding profiles across different SARS-CoV-2 variants, to address the questions of (1) evolutionary conservation of binding, (2) differential binding across strains and (3) gain and loss of binding in novel mutants.

We believe that identifying viral RBP binding sites will give valuable insights into the mechanisms of host-virus interaction and will deepen our understanding of the life cycle of SARS-CoV-2.

Keywords: Deep Learning, Convolutional Neural Networks, SARS-CoV-2, RNA Biology, RNA-Binding Proteins

Deep Learning Based Time-to-Event Prediction for a Large Multicentric Cohort of H&N Cancer Patients

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Recent studies have shown that convolutional neural networks (CNNs) are able to predict clinical outcomes after radiotherapy (RT) for cancer patients, using only their segmented pre-treatment CT images. The aims of this study were to build 2D/3D CNNs for distant metastasis (DM) prognosis of H&N cancer patients, to extend the models by incorporating censoring information to produce time-dependent predictions and to assess their performance using several independent testing cohorts. We implemented image based 2D and 3D-CNNs, a clinical covariates based artificial neural network (ANN) and 2D/3D CNNs combined with clinical covariates (CNN+Clinical). All models were extended with a previously published survival model for neural networks to incorporate censoring information and output distant DM-free probability curves for every patient. CTs from 294 patients in four different Canadian hospitals, available on the cancer imaging archive (TCIA), were used for training and 3-fold cross-validation (CV). As independent testing cohorts, we used 136 patients treated at MAASTRO clinic (from TCIA), 497 patients treated at Princess Margaret Cancer Center (PMH) (from TCIA) and 110 patients treated at Centro di Riferimento Oncologico (CRO). All networks achieved good Harrell's concordance index (HCI) on two out of three testing sets, being able to reproduce the good performance reached on the Canadian CV cohort. Results on the PMH cohort were significantly better than 0.5 but at best 0.69, which might be explained with certain unknown clinical background for this cohort, e.g. missing information on surgery. Regarding stratification capability in high and low-risk patient groups, the best CNN models in terms of average testing HCI (2D-CNN+Clinical and 3D-CNN) and the baseline ANN were able to significantly stratify all testing cohorts. However, as visible in the Kaplan-Meier plots, the difference between high and low-risk groups is less visible for the ANN compared to a CNN.

Keywords: Radiomics, Predictive Modelling, Outcome Prediction, Personalised Medicine, Head and Neck Cancer, Distant Metastasis

Noise2NAKO: AI Methods Linking Environment and Health - a Large-Scale Cohort Application

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The environment has major impacts on human health which requires sophisticated models to better reflect life exposures and to determine the long-term impacts of environmental factors on health. Thus, advanced statistical and data science approaches are needed to understand the complex interplay between the environment and population health. Existing models are hampered by the trade-off between complexity, interpretability and the biased nature of population-based data. Studies reported adverse impacts of noise on human health, mainly for cardiovascular outcomes, e.g. hypertension. Several studies also found a systematic bias w.r.t. social status. In this project, we aim at developing beyond state-of-the-art ML methods to advance existing noise maps, improve the quantification of noise impacts on health and delineate the complex interplay between environmental, socio-economic and health data. As a basis, we compile extensive German-wide noise maps applying data augmentation and deep CNN to overcome the spatial limitations of existing maps. Next, the noise data will be linked to socio-economic and demographic data from participants of the German national cohort (NAKO). In a first prediction task, we will identify German-wide vulnerable clusters in terms of noise and neighborhood factors for the risk of hypertension employing Distribution Regression Networks. In a second task, we will enhance this network by individual socio-economic and health data to investigate the interplay of different risk factors on hypertension. That is, we test and expand interpretable ML techniques e.g. AdaBoost, random forest and QRF to our setting and compare them to traditional models, e.g. additive logistic regression. To enhance the quality of data, we consider pre-processing methods, e.g. standardization, normalization and imputing missing values. Moreover, we will employ effective feature selection approaches, e.g. correlated features or information theoretic-based algorithms.

Keywords: Ensemble Learning, Deep Learning, Distribution Regression Network, Regression, Deep Regression Model, Deep Neural Network, Ensemble Methods, Interpretable AI/ML, Earth Observation, Satellite, Noise, Health, NAKO Cohort, Hypertension

Designing 3D Protein Descriptors for Use in Convolutional Neural Networks

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When a protein functions improperly or is used by virulent species against our body, it can cause great harm. Therefore, it is essential to understand target proteins to design new therapeutics. In our research, we aim to learn the properties of proteins from the representation of the local chemical environment. We show the descriptor and network design required to research this topic. To achieve this, a structure database of unique enzyme representations is created. The enzyme is treated as a data object from which the chemically interesting parts are extracted. Furthermore, we map chemical features to enrich the data. From this information, 3D descriptors are built as voxelized- or point cloud-objects for use in convolutional neural networks. For the neural network, we show two important factors in our design: rotational invariance and the molecular attention transformer.

Keywords: Proteins, Medicine, 3D Convolution, Descriptors, Learning Methods, Convolutional Neural Networks

Predicting T Cell Activation for Mutational Epitopes

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Epitope recognition by T cells plays a crucial role in the adaptive immune system of vertebrates. Pathogen- or tumor cell-derived epitopes are bound to the Major Histocompatibility Complex, a peptide-presenting surface protein, and interact with the CDR3 region of the T cell receptor (TCR). In principle, there are 1020 possible TCRs in nature and every human harbors at least 108 different TCRs. T cells whose TCR recognizes their cognate epitope are activated and initiate an adaptive immune response. Understanding and predicting the TCR-epitope interaction is thus of fundamental interest in basic immunological research and directly benefits the development of immunotherapies. However, due to the immense diversities of TCRs and epitopes, computational models are urgently needed. In this project, we analyzed a novel dataset of 5.472 unique pMHC-TCR interactions consisting of T cell activation to single-amino acid mutations (altered peptide ligands) of the SIINFEKL epitope. The percentage of T cell activation was experimentally determined for 20 murine TCRs from a naive and 16 TCRs from an educated (i.e., previously exposed) repertoire. The availability of CDR3 regions and activation for each of the 152 mutations allowed us to build predictive models of T cell activation within and across TCRs of unprecedented accuracy.

Keywords: Random Forests, UMAP, T Cell Activation Prediction, T Cell Receptor, Epitope Recognition, Adaptive Immune System

FedPerl: Peer Learning in Semi-Supervised Federated Learning for Skin Lesion Classification

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Globally, Skin carcinoma is among the most lethal diseases. Yearly, millions of people are diagnosed with skin cancer. Fortunately, detecting this cancer in the early stages decreases the medication cost and mortality rate substantially. The recent improvement in the automated cancer classification using deep learning methods has reached a human-level performance. While this achievement requires a large amount of annotated data assembled in one location, finding such conditions usually is not feasible. Recently, federated learning has acquired a lot of interest. The main idea of federated learning is to train decentralized machine learning models in a privacy-preserved fashion, making federated learning fits the medical setting. Still, federated learning depends on labeled data at the client side, which is most of the time not available and costly. To address this, we propose FedPerl, a semi-supervised federated learning method. Our method is inspired by peer learning from educational psychology and ensemble averaging from committee machines. FedPerl builds communities based on clients‘ similarities. Then encourages its members to learn from each other to generate more accurate pseudo labels for the unlabeled data. We also proposed the peer anonymization (PA) technique to hide the clients‘ identities and preserve privacy. As a core component of our method, PA reduces the communication cost while enhances performance. We validate our method on 71,000 skin lesion images collected from 5 publicly available datasets. With few annotated data, FedPerl outperforms state-of-the-art SSFL and the baselines by 1.8% and 15.8%, respectively. Also, it generalizes better to an unseen client while less sensitive to noisy ones.

Keywords: Skin Cancer Classification, Semi-Supervised Learning, Federated Learning, Peer Learning, Peer Anonymization

Deep Learning Model Predicts Water Interaction Sites on the Surface of Proteins

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We develop a residual deep learning model, hotWater (https://pypi.org/project/hotWater/), to identify key water interaction sites on proteins for binding models and drug discovery. This is tested on new crystal structures, as well as cryo-EM and NMR structures from the PDB and in crystallographic refinement with promising results.

Keywords: Water Binding Sites, Protein Structures, Structural Biology

Multi-Modal Network Analysis to Identify Host Factors Important for Covid-19 Infection

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Deeper insights into disease pathophysiology can be gained in biomedical questions when using information from all 'omic' layers, comprising the whole set of e.g. genes, genetic variation as well as clinical features of patients. State-of-the-art analysis is often performed layer-wise due to the high complexity of data, however, potentially missing the whole picture. For this purpose, we developed 'Knowledge gulded Multi-Omics Network Inference' (KiMONo) which leverages prior information from experimentally validated databases while using sparse-group-lasso to build a multi-modal network. To obtain an understanding of the complex molecular interactions during COVID-19, we used KiMONo for data integration of all available 'omic' layers in the Genotype-Tissue Expression (GTEx) Project. Our main goal was to find tissue specific genes that interact with viral proteins found from previous studies that explain the heterogeneity of symptoms during infection. Additionally, we aimed to identify genes which are associated with genetic predisposition of a severe disease course. This will be done by including polygenic risk scores into the network models. These genes will then be analysed in COVID-specific cohorts.

Keywords: Network Biology, Multi-Omic, Disease

Annotation-Efficient Classification Combining Active Learning, Pre-Training and Semi-Supervised Learning for Biomedical Images

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Deep learning based biomedical image classification typically requires large annotated datasets. On the other hand, the manual annotation process by experts is expensive, time-consuming and hence scarce. Active learning, pre-training and semi-supervised learning aim to increase the classification performance with a limited number of annotated images. However, these methods are mostly benchmarked on natural image datasets. In addition, it is not clear which combination of the aforementioned methods yields the best performance on biomedical image datasets. In this paper, we performed an extensive grid-search with four-fold cross validation based on eight active learning algorithms, four pre-training methods and three training strategies on four biomedical image datasets in nine iterations. We found that the state-of-the-art active learning algorithms tend to perform similarly on biomedical image datasets. On the other hand, combining the correct pre-training and semi-supervised learning proved to be more effective than the active learning choice. In particular, ImageNet pre-training and pseudo-labeling showed superior performance in all cases from the first iteration. Finally, we found that combination of BADGE (active learning), ImageNet initialization (pre-training) and pseudo-labeling (training strategy) as the most stable annotation-efficient combination for similar tasks.

Keywords: Biomedical Images, Deep Learning, Active Learning, Semi-Supervised Learning, Self-Supervised Learning

Alternaria Spores Detection in BAA-500 Images with U-Net

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Around 30% of the European population suffers from pollinosis. Pollinosis is commonly known as allergy to airborne pollen/ fungal spores. One of these airborne fungal spores is the genus Alternaria, which is widely spread. Alternaria has two peaks during the year: in summer and in the early autumn. Pollen and spores have been monitored since the 1950's using manual procedures. In the last years new technologies have been developed to automate the monitoring process. Our work is based on pictures taken from airborne samples of the BAA-500 (Hund Ghmb) pollen monitor. This device counts pollen but it is not able to count Alternaria spores. Here we present the workflow developed based on the U-net which allows the detection of the fungal spores.

Keywords: Pollinosis, Alternaria, Detection, Air Monitoring, Convolutional Neural Network, U-Net

Attention Based ML for Fast Analysis of GISAXS and PDE Learning

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Machine learning is widely used in the field of fast analysis of physics data. Variety of architecture has been adopted, eg. DenseNet for Grazing Incidence Small Angle X-ray Scattering (GISAXS) data, MultiLayer Perceptron (MLP) for Small Angle X-ray Scattering (SAXS) data and Partial Differential Equation (PDE) learning. However, the existing classical networks are designed for nature images. That has a huge difference with physical one. On the other hand, the handcraft network is not easy to design for a specific application, especially to physical researchers. Thus, it's very necessary to develop an auto designed network and a plug-in module to help the network to adapt into any specific situation.

Neural Architecture Search (NAS) has been widely studied and successfully applied in many fields, such as, nature image classification and object detection. It is a research field concerned with utilizing optimization algorithms to design optimal neural network architectures. In the PhD project, the gradient based NAS will be first introduced to optimize the current network in PDE learning. By introducing a score or a factor to diversify the network, the network can be more powerful.

Analysis of scattering data is a very time-consuming process, as it requires solving an ill-posed inverse problem to infer properties describing the imaged object. Scattering patterns are complex, thus make the data analysis challenging, even for the simulation data. Attention modules, especially spatial and channel-wised attention can help the network to focus on in-plane and out-of-plane signals, which is important for recognizing patterns of different kinds of target parameters, easy to plug in the network and can adapt the network to any specific tasks.

Keywords: Attention, Neural Architecture Search, GISAXS, PDE Learning

Hybrid Modelling via Analytical Model Predictions Corrected with Machine Learning towards High-Fidelity Simulation Solutions

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Machine learning predictions within the fields of material mechanics are usually performed based on relationships along the process-structure-property-performance chain. The exploitation of physical laws besides data can enable low prediction errors in comparison to predictions that are only based on data. Since physics-based models usually contain assumptions and simplifications, prediction deviations to reality may occur. In contrast, purely data-driven models typically rely on substantial amounts of data because physical relationships are not provided explicitly. Despite these respective drawbacks of both model types, a synergetic combination of both can be reached when physics-based predictions with deviations to a reference solution are corrected by a data-driven model which maps those deviations. This yields a hybrid model that is both physics-related as well as data-driven and shows low prediction errors even in scarce data settings. In this poster presentation, a hybrid model is composed of a physics-based analytical model that is corrected by an artificial neural network. In particular, a semi-analytical model serves as a low-fidelity model, where predictions outside its calibration domain show prediction errors that are corrected towards the desired high-fidelity solution provided by finite element simulations. As a result, the applicability range of the semi-analytical model is enhanced while its prediction errors are reduced and the efficiency is maintained. As an example use-case, residual stresses induced by Laser Shock Peening are predicted. Dimensionless inputs and outputs lead to low prediction errors and to an expansion of the process parameter space of the training region when remaining within the trained range of corrections. Ultimately, the hybrid model outperforms a purely data-driven model in a benchmark comparison and shows lower predictions errors, even when available data is scarce as often the case when using experimental data.

Keywords: Hybrid Modelling, Machine Learning, Analytical Model, Finite Element Model, Artificial Neural Networks, Model Correction, Physics-Based, Data-Driven, Laser Shock Peening, Residual Stresses

AlphaNumerics Zero: First Steps, First Results, First Mysteries

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The spectral deferred correction method is an iterative solver for time-dependent partial differential equations. It can be interpreted as a preconditioned Picard iteration for the so-called collocation problem. The key to an efficient method is the choice of the preconditioner: It defines the speed of convergence and the level of parallelism. While the de-facto standard is a fast-converging, serial preconditioner, our goal is to use reinforcement learning techniques to find a fast-converging, parallel one. We look at a simple test equation and train a phasic policy gradient (PPG) agent to pick favorable, diagonal preconditioners depending on the parameter of the equation. For small dimensions of the collocation problem, PPG is indeed able to yield very promising results. This does not hold for larger dimensions, though. When successful, however, the trained network can be used directly to pick parallel preconditioners for more complex problems, where the parameters describe stiffness, largest eigenvalue or other characteristics of the differential equation. This work is a prototype problem for the Helmholtz AI AlphaNumerics Zero project, where reinforcement learning is used to learn on-average optimal numerical solutions for a given simulation problem.

Keywords: Reinforcement Learning with Phasic Policy Gradient, Ordinary Differential Equations, Iterative Solver, Preconditioning

Surrogate Modelling of Ion Acceleration and Overdense Laser-Plasma Interactions

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Interaction of an overdense plasma with ultra-intense laser pulses represents a promising route to enable the development of compact ion sources. Prospective applications of high-energetic protons and ions include, but are not limited to, medical applications, materials science and nuclear fusion. However, current records for maximum proton energies (94 MeV, Higginson Nat Commun 9, 724 2018) are still well below the required values for many applications (typically 150-250 MeV) and many challenges remain unsolved to this day. In particular, a high-dimensional parameter space, as well as considerable effort per observation, make it impossible to uniformly sample the parameter space by means of simulations, let alone experimentally, while simultaneously strong nonlinearities limit the coarseness of the grid. Consequently, a combination of modern sampling approaches, optimized simulation codes and powerful data-based methods are essential for building realistic surrogate models. More specifically, we want to employ invertible neural networks (Ardizzone arXiv:1808.04730, 2018) for bidirectional learning of input and output, and convolutional autoencoder (Vincent J. Mach. Learn. Res. 11, 12 2010) to reduce intermediate field data to a lower-dimensional latent representation.

Keywords: Laser-Plasma, Ion Acceleration, Computational Physics, Simulations, Surrogate Modelling, Neural Networks, Inverse Problems

Simulation-Based Inference of Beamline Characteristics at BESSY

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Monitoring, updating and controlling Beamline Parameters to deliver high-quality beam characteristics is a challenging task. Today, it requires heuristics and experiences from years of operations brought in by beamline scientists to do well. In this poster, we present current efforts to use modern methods of statistical learning to invert a simulation of a beamline in order to obtain the simulation parameters that correspond to the state of the beam given a beamline profile only. We use recently published techniques to perform the likelihood-free estimation given the simulation to estimate a solution to this inverse problem. Preliminary and pre-alpha stage results are shown.

Keywords: Regression, Inverse Problems, Simulation-Based Inference, Likelihood Free Inference, Conditional Invertible Neural Networks, Accelerators, Synchrotron Sources

Machine Learning to Prevent Dangerous Consequences of Solar Storms

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Solar storms are hazardous events consisting of a high emission of particles and radiation from the sun that can have adverse effects both in space and on Earth. In particular, the satellites can be damaged by energetic particles through surface and deep dielectric charging. The Prediction of Adverse effects of Geomagnetic storms and Energetic Radiation (PAGER) is an EU Horizon 2020 project, which aims to provide a forecast of satellite charging through a pipeline of algorithms connecting the solar activity with the satellite charging. The plasmasphere is a region of cold plasma surrounding the Earth and its modeling is an essential component of the PAGER pipeline, as it controls the growth of waves and how waves interact with particles. Successful machine learning models of the plasma density in the plasmasphere have been already developed, however, in the context of the PAGER project one is constrained to use a specific set of features, whose forecasts are provided by other components of the pipeline. Here, we develop a machine learning model of the plasma density in the plasmasphere restricting exactly to these features and we validate it by measuring its performance in particular during solar storms. We tackle in particular the challenge of reproducing fine spatial structures which appear during the rarer times of solar storms.

Keywords: Neural Networks, Solar Storms, Plasmasphere Density, Spatial-temporal Predictions, Rare Events

Prediction and Understanding of the Earth's Ionosphere Using Machine Learning

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Earth's ionosphere represents a complex and dynamic region characterized by increased concentration of charged particles. Changes in ionospheric density can affect the propagation of electromagnetic signals thus disrupting navigation and positioning. The existing models of ionospheric density rarely meet the accuracy requirements due to being either only climatological (physical models), or using the time and spatial averaging (empirical models). Here we present a continuous empirical three dimensional (3D) model of electron density at heights 130-900 km. Since the ionosphere is a data rich environment it is essential to use all of the collected observations. We use the radio occultation data from various spacecraft, together with in situ data by CHAMP and CNOFS missions and observations from GRACE-KBR, for over 18 years of data. We discuss the application of deep learning to efficiently handle the entire dataset comprising billions of data points. In order to analyze, which features result in the best model performance, we employ a number of ML-based feature selection techniques and discuss the optimal combination of inputs, and their physical meaning. The resulting model gives accurate predictions of electron density in the Earth's ionosphere and yields >90% correlation on the validation data. The model has a wide range of applications for scientific purposes, space weather monitoring and industrial applications such as positioning and navigation.

Keywords: Ionosphere, Big Data, Space Physics, Environment, Radiation, Plasma Physics

Intelligent Road Survey Based on Improved Foreground-Aware Network Segmentation

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Road information is one of the most basic components of a geographic database. Extracting road information plays an important role in city planning etc. However, different from the ordinary image segmentation tasks, inherent characteristics of roads bring us challenges, such as connectivity and large spans. This study focuses on trying to extract roads accurately using various models, including traditional ones (LinkNet, DLinkNet) and new ones (FarSeg, DFarSeg), and make a comparison among them. A practical example with real world data from GF1 will also be given at the end.

Keywords: Foreground-Aware Network, LinkNet, Image Segmentation, Road Extraction, Deep Learning, LinkNet, FarSeg, Intelligent Road Survey

Understanding "Cosmic-Ray" Composition at IceCube Observatory, Using Graph Neural Networks

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IceCube Observatory is a cubic-km physics detector which is concealed deep under the South Pole Antarctic Ice at the Amundsen–Scott South Pole Station in Antarctica. With its thousands of sensors located under the Antarctic ice, it is used to detect high-energy particles from cosmic events. This provides us with new insights into their fundamental behavior and the dynamics of their astrophysical sources. For the purpose of cosmic ray detection, we can use the in-ice part of the IceCube detector, in addition to the cosmic-rays detection dedicated surface component of the detector, called as IceTop. Understanding the mass composition of cosmic-rays is extremely important since it possibly holds the secrets to their origin and their sources. However, their composition analysis is still prone to large systematic uncertainties. There is a significant dependence of expected particle-flux and primary-particle mass on the hadronic-interaction model one chooses to interpret the air-shower measurements. Current „Deep Learning" based methods (based on MLPs or CNNs) implemented in IceCube are either inherently over-simplistic or are inflexible to the proposed detector upgrades. This opens an opportunity to implement the domain flexible Graph Neural Networks. Preliminary tests have shown promising results for an improved sensitivity over the previous methods for composition analysis. This will possibly help establish IceCube as a unique three-dimensional cosmic-ray detector, providing improved sensitivities for detailed physics analysis.

Keywords: Cosmic Rays, IceCube Observatory, Graph Neural Network, Extensive Air Showers, DL, ML, Cosmic Ray Composition

Investigating Role of Globally Available Label Datasets for Flood Detection Using Synthetic Aperture Radar (SAR) Data and Deep Learning

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Flood is one of the most widespread and frequent natural disasters. Deriving accurate and rapid cartographic information on flood extent is essential to help manage the situation. Satellite remote sensing is now widely used for near real-time flood monitoring as it provides large scale detection in a time- and cost-efficient manner. Optical satellite imagery is employed as important tools for flood mapping due to easier interpretability and high spatial resolution. However, cloudy weather associated with floods are a great obstacle to optical sensors for flood monitoring. In contrast, Synthetic Aperture Radar (SAR) allows observation of wide areas across near all-weather conditions and plays a significant role in operational services for flood management. Although in many cases smooth water surfaces can be easily extracted from SAR imagery, it is subjected to overestimation of flooded areas especially in the arid and semi-arid regions since the complex interactions between SAR characteristics and environmental conditions.
Advanced machine learning and deep learning approaches have demonstrated large potential to overcome the problem by learning features directly from images which requires a large number of labeled samples for training and validation. Therefore, some public georeferenced dataset to train and test deep learning flood algorithms are being produced.
To investigate the role of globally available label datasets in obtaining reliable flood maps using SAR data and deep learning approaches, we tried one of the open access dataset, Sen1Floods11, which is a surface water dataset. We trained, validated and tested a ResNet50 model to segment flood water using a subset of this dataset.The classification results of flood water have obtained an overall accuracy of 89.5% for the test dataset in India and 78.9% for the test dataset in Pakistan. Results show the potential of the flood water dataset to better detect the flooded area.

Keywords: FCNN, ResNet50, Flood Mapping, Sentinel-1, Synthetic Aperture Radar (SAR), Convolutional Neural Networks, Water Bodies

Vehicle Detection in Satellite Video

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Vehicle detection in remote sensing imagery is challenging, as vehicles appear with limited appearance and with four to ten pixels very tiny compared to the overall size of satellite images which are usually much larger than one megapixel. Standard object detection fails for this problem due to the violation of implicit assumptions such as rich texture and small to moderate ratios between image size and object size. A fundamental limit to detecting tiny objects is the ground sampling distance of optical sensors. In contrast, satellite video introduces temporal consistency as inductive bias which promises to overcome this limit and the resulting lack of visual information in still images. Current approaches to vehicle detection in satellite video use either background subtraction, frame differencing or subspace methods showing moderate performance (0.26 - 0.82 F1 score). We apply recent work on convolutional neural networks (FoveaNet) for wide-area, aerial motion imagery (WAMI) to satellite video. We suggest a transfer learning approach and adaptions to the network architecture and to the final segmentation of the heatmap. The proposed neural network (FoveaNet4Sat) is trained on an existing large-scale, aerial WAMI dataset (WPAFB'09) and is fine-tuned on labelled satellite video. Our experiments show clearly that FoveaNet4Sat outperforms FoveaNet when applied to satellite video (0.75 - 0.89 F1 score) and outperforms the state-of-the-art on the publicly available SkySat-1 Las Vegas video. Our work also shows additional experiments on new video data and new manual ground truth (15k labels) taken from the city of Karthoum. Despite a reduced pre-processing (video stabilisation only), the results (0.88 F1 score) promise a practical method for the detection of moving vehicles in satellite imagery.

Keywords: Supervised Learning, Transfer Learning, Spatiotemporal Neural Network, Convolutional Neural Network, Tiny Object Detection, Moving Object Detection, Object Detection, Satellite Video Processing

Data quality affects deep-learning-based air quality forecasts

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“Air pollution has a $2.9 trillion economic cost.“ Reliable pollutants forecasts, especially PM2.5 and Ozone, will contribute to a reduction of such costs and an improvement of public health. The state-of-the-art air quality forecasting based on a 3D numerical model tends to underestimate high concentrations. Moreover, it is very computationally expensive. We aim to improve PM2.5 and Ozone forecasting with deep learning techniques. In this paper, we develop 14 deep neural networks – two dense neural networks, one CNN (convolutional neural network), ten variants of LSTMs (long short-term memory), and a Seq2Seq model. We evaluate these models on three datasets with distinct patterns: relatively clean, heavily polluted, and clean but with rare high peaks. We achieved around 15% MAPE (mean absolute percentage error) given a long period of data collection including pollutants concentration and meteorological measurements. Our experimental results indicate that a single-layer LSTM outperforms multi-layer LSTM and CNN for a 26-year dataset with stable temporal patterns. However, it performs worse to capture the rare high peaks due to wildfire. It suggests that we need an air quality forecasting framework that consists of multiple deep learning methods instead of a single model system to provide the best performance at all sites. In the future, we will explore more data sources and better evaluation metrics for optimized forecasts across sites.

Keywords: Air Quality Forecast, Time Series, Deep Learning, LSTM

Using Minimal Spanning Tree Based ICA Optimization for Volcanic Unrest Determination

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Repeated Synthetic Aperture Radar (SAR) acquisitions can be utilized to produce measurements of ground deformations and associated geohazards, such as it can be used to detect signs of volcanic unrest. Existing time series algorithms like Permanent Scatterer (PS) analysis and Small Baseline Subset (SBAS) are computationally demanding and cannot be applied in near real time to detect subtle, transient and precursory deformations. To overcome this problem, we have adapted a minimum spanning tree (MST) based spatial independent component analysis (ICA) method to automatically detect sources related to volcanic unrest from a time series of differential interferograms. We utilize the algorithm's capability to isolate signals of geophysical interest from atmospheric artifacts, topography and other noise signals, before monitoring the evolution of these signals through time in order to detect the onset of a period of volcanic unrest, in near real time. In this work we first demonstrate our approach on synthetic datasets having different signal strengths and temporal complexities. Then we apply the approach to the new volcanic unrest of Mt. Thorbjörn on the Reykjanes Peninsular in Iceland in 2020 and also on the volcanic unrest of the Colima volcano in Mexico from 2017 to 2019.

Keywords: Sentinel-1, Interferometric Synthetic Aperture Radar (InSAR), ICA, Minimal Spanning Tree, Volcano, Iceland, Mt. Thorbjorn, Mexico, Volcan de Colima

FedDis: Disentangled Federated Learning for Unsupervised Brain Pathology Segmentation

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In recent years, data-driven machine learning (ML) methods have revolutionized the computer vision community by providing novel efficient solutions to many unsolved (medical) image analysis problems. However, due to the increasing privacy concerns and data fragmentation on many different sites, existing medical data are not fully utilized, thus limiting the potential of ML. Federated learning (FL) enables multiple parties to collaboratively train a ML model without ex- changing local data. However, data heterogeneity (non-IID) among the distributed clients is yet a challenge. To this end, we propose a novel federated method, denoted Federated Disentanglement (FedDis), to disentangle the parameter space into shape and appearance, and only share the shape parameter with the clients. FedDis is based on the assumption that the anatomical structure in brain MRI images is similar across multiple institutions, and sharing the shape knowledge would be beneficial in anomaly detection. In this paper, we leverage healthy brain scans of 623 subjects from multiple sites with real data (OASIS, ADNI) in a privacy- preserving fashion to learn a model of normal anatomy that allows to segment abnormal structures. We demonstrate a superior performance of FedDis on real pathological databases containing 109 subjects; two publicly available MS Lesions (MSLUB, MSISBI), and an in-house database with MS and Glioblastoma (MSI and GBI). FedDis achieved an average dice performance of 0.38, outperforming the state-of-the-art (SOTA) auto-encoder by 42% and the SOTA federated method by 11%. Further, we illustrate that FedDis learns a shape embedding that is orthogonal to the appearance and consistent under different intensity augmentations.

Keywords: Federated Learning, Unsupervised Learning, Brain MR Anomaly Segmentation

Contrastive Representation Learning for Whole Brain Cytoarchitectonic Mapping in Histological Human Brain Sections

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Cytoarchitecture is defined by the spatial arrangement of neuronal cell bodies into layers and columns with respect to cell density, orientation and presence of certain cell types. It allows to segregate the brain into distinct areas, which link structure with connectivity and function and provide a microstructural reference for brain atlases. Recent work provided methods for automatic segmentation of cytoarchitectonic areas in the visual system using Convolutional Neural Networks. Envisioning a solution for mapping the complete human brain, we extend this approach to become applicable to a wider range of brain areas. We propose a contrastive learning task for encoding microscopic image patches into robust microstructural features, which are efficient for classification of cytoarchitectonic areas. A model pre-trained using this task outperforms a model trained from scratch, as well as a model pre-trained on a recently proposed auxiliary task. Cluster analysis in feature space shows that learned representations form anatomically meaningful groups.

Keywords: Convolutional Neural Networks, Contrastive Learning, Human Brain, Mapping, Deep Learning, Contrastive Learning

Precise Quantification of Adipose Tissue Using Deep Learning-Based Image Segmentation

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The German National Cohort (GNC) is the largest population-based cohort study in Germany. Its main objective is to investigate the cause of chronic diseases (e.g. diabetes mellitus) and to identify lifestyle, socioeconomic and environmental factors. A subset of approximately 30000 participants is included in a whole-body magnetic resonance imaging (MRI) sub-study. Abdominal obesity, as manifested by increased visceral adipose tissue (VAT), shows a strong correlation to insulin resistance and is a key condition of the metabolic syndrome which is associated with the risk of developing type 2 diabetes. Chemical shift selective MRI using Dixon based techniques is regarded as a gold-standard for the quantification of adipose tissue. Segmentation of fat compartments, i.e. VAT and subcutaneous adipose tissue (SAT), in MR images is used for volumetric quantification. As manual segmentation is time-consuming, costly and therefore not feasible in a large cohort study, segmentation using deep learning is applied. A stratified (age, gender, BMI) sample of n=30 manually segmented MR data sets from the GNC is used to train a U-Net model (nnU-Net) to perform segmentation of VAT and SAT. The model is trained using 5-fold cross-validation providing the mean of the five separate U-Nets as a segmentation result. As a measure for segmentation uncertainty mean pairwise Dice scores are used. Mean Dice similarity coefficients for VAT (0.947) and SAT (0.973), corresponding to a mean absolute deviation of fat volume of -18.4 ml and 47.9 ml respectively, on the validation sets indicate high precision of the segmentation model. On a stratified (age, gender, BMI), unlabeled test set of n=10 data sets from the GNC, high consistency in terms of mean pairwise Dice score between the different folds of training is found: 0.991 (VAT) and 0.987 (SAT). Automated segmentation using nnU-Net provides precise quantification of body fat compartments and will be applied on a large data set of n>11000.

Keywords: Semantic Segmentation, Deep Learning, Adipose Tissue Quantification, Medical Image Segmentation, German National Cohort

DeGeSim and the High Granularity Calorimeter for the CMS Experiment at the Large Hadron Collider

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We present the beginning work on fast simulations for the new High Granularity Calorimeter (HGCal), which will become part of the CMS experiment at the Large Hadron Colider (LHC) at CERN/Geneva. It will replace the current end-cap calorimeters for data acquisition in 2027. The design of the new calorimeter is driven by the increased particle density following the High Luminosity Upgrade of the LHC. This enforces a complex geometry of the active sensor and a massive increase from about 7k currently to more than 3 million individual channels for each of the two future end-cap calorimeters. Traditionally, particle physics has used detailed simulations of detectors and physics. These simulations are of high precision and can describe minute details. The price for this precision is a large computational power requirement. Since the predicted computational resources will not be sufficient for the traditional stepwise simulations, we will explore deep learning techniques combining fast inference with generative models, e.g., physics-informed GANs-VAEs hybrids for simulations. In particular, Graph Neural Networks are a promising candidate to describe the complex geometry of the new detector. This project is part of the Helmholtz AI funded project DeGeSim.

Keywords: GAN, GNN, Generative Modeling, Detector, Simulation, Calorimeter, Particle Physics, HEP, CMS, LHC

Contour Proposal Networks for Biomedical Instance Segmentation

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We present a conceptually simple framework for object instance segmentation called Contour Proposal Network (CPN), which detects possibly overlapping objects in an image while simultaneously fitting closed object contours using an interpretable, fixed-sized representation based on Fourier Descriptors. The CPN can incorporate state of the art object detection architectures as backbone networks into a single-stage instance segmentation model that can be trained end-to-end. We construct CPN models with different backbone networks, and apply them to instance segmentation of cells in datasets from different modalities. In our experiments, we show CPNs that outperform U-Nets and Mask R-CNNs in instance segmentation accuracy, and present variants with execution times suitable for real-time applications. The trained models generalize well across different domains of cell types. Since the main assumption of the framework are closed object contours, it is applicable to a wide range of detection problems also outside the biomedical domain. An implementation of the model architecture in PyTorch is freely available.

Keywords: Instance Segmentation, Cell Segmentation, Cell Detection, Object Detection, Fourier, CPN, U-Net, Mask R-CNN, PyTorch

InstantDL: An Easy-to-Use Deep Learning Pipeline for Image Segmentation and Classification

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Deep learning contributes to uncovering molecular and cellular processes with highly performant algorithms. Convolutional neural networks have become the state-of-the-art tool to provide accurate and fast image data processing. However, published algorithms mostly solve only one specific problem and they typically require a considerable coding effort and machine learning background for their application.
We have thus developed InstantDL, a deep learning pipeline for four common image processing tasks: semantic segmentation, instance segmentation, pixel-wise regression and classification. InstantDL enables researchers with a basic computational background to apply debugged and benchmarked state-of-the-art deep learning algorithms to their own data with minimal effort. To make the pipeline robust, we have automated and standardized workflows and extensively tested it in different scenarios. Moreover, it allows assessing the uncertainty of predictions. We have benchmarked InstantDL on seven publicly available datasets achieving competitive performance without any parameter tuning. For customization of the pipeline to specific tasks, all code is easily accessible and well documented. With InstantDL, we hope to empower biomedical researchers to conduct reproducible image processing with a convenient and easy-to-use pipeline.

Keywords: Segmentation, Classification, Machine Learning, Bioinformatics, Image Processing

EchoMouseNet, a Deep Learning Framework Uncovers New Echocardiography Phenotypes

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In this project, we delivered a deep learning based framework which i) assesses the acquisition quality of transthoracic echocardiography images of mice and ii) automatically extracts heart-related features from these images. The pipeline is currently being used to analyse a large pool of data available the German Mouse Clinic, and has already helped to discover new cardiac phenotypes previously overlooked with manual procedures.

Keywords: Echocardiography, Quality Classification, Heart Segmentation

Learning Anatomical Segmentations for Tractography from Diffusion MRI

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Diffusion MRI guided tractography enables connectivity analyses of the brain valuable for clinical and research studies. Tractography usually requires an anatomical segmentation based on a T1-weighted image, e.g. with FreeSurfer. However, the segmentation workflow takes several hours and involves an error-prone registration. We improve and accelerate this workflow with the learning-based FastSurfer-CNN which is an U-Net-based neuroimage segmentation network validated extensively on MRI datasets. Specifically, we segment 170 brain regions in a fraction of the time (32 seconds) natively in diffusion-weighted image space without the need for a T1-w image and the registration. Since a direct approach to segment a stack of diffusion-weighted images (DWIs) does not generalize, we investigate DWI representations that can and find that they provide suitable alternatives. Our segmentations feature a high agreement with reference segmentations based on T1-w images and accelerate the tractography workflow while maintaining the quality of tract estimates.

Keywords: Deep Learning, Segmentation, Diffusion MRI, Tractography

Parameter Space CNN for Cortical Surface Segmentation

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Spherical coordinate systems have become a standard for analyzing human cortical neuroimaging data. Surface-based signals, such as curvature, folding patterns, functional activations, or estimates of myelination define relevant cortical regions. Surface-based deep learning approaches, however, such as spherical CNNs primarily focus on classification and cannot yet achieve satisfactory accuracy in segmentation tasks. To perform surface-based segmentation of the human cortex, we introduce and evaluate a 2D parameter space approach with view aggregation (p^{3}CNN). We evaluate this network with respect to accuracy and show that it outperforms the spherical CNN by a margin, increasing the average Dice similarity score for cortical segmentation to above 0.9.

Keywords: Cortical Segmentation, Geometric Deep Learning, Semantic Segmentation

Machine-Learned 3D Building Vectorization from Satellite Imagery

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We propose a machine learning based approach for automatic 3D building reconstruction and vectorization. Taking a single-channel photogrammetric digital surface model (DSM) and panchromatic (PAN) image as input, we first refine the building shapes of input DSM with a conditional generative adversarial network (cGAN). The refined DSM and the input PAN image are then used through a semantic segmentation network to detect edges and corners of building roofs. Later, a set of vectorization algorithms are proposed to build roof polygons. Finally, the height information from the refined DSM is added to the polygons to obtain a fully vectorized level of detail (LoD)-2 building model. We verify the effectiveness of our method on large-scale satellite images, where we obtain state-of-the-art performance.

Keywords: DSM Refinement, Semantic Segmentation, Vectorization, 3D Building Reconstruction

FedNorm: Federated Learning with Modality-Based Normalization

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Organ segmentation is an important task in medical image analysis, which can be performed by deep learning models to assist physicians with their diagnosis. However, due to lack of labelled data in many hospitals and privacy regulations, it would be helpful to train such models in a decentralized manner, where training data from different modalities and multiple hospitals contributes to the training process. In this work, we focus on multi-modal liver segmentation with CT and MRI data using federated learning. We present a novel federated learning algorithm, FedNorm, which uses a normalization technique based on the modalities of the data. Furthermore, we demonstrate the ability of our approach to successfully generalize to unseen multi-modal data. We show that FedNorm can outperform other federated learning approaches on unseen MRI data by a large margin.

Keywords: Federated Learning, Liver Segmentation, Medical Imaging

A Group Based Anomaly Detection Approach to Discover Abnormal Phenotypes in Knockout Studies

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In this work, we have analyzed the auditory brainstem response (ABR) waveforms of genetic knockout mice for abnormalities. To this end, we developed a group based anomaly detection algorithm to detect groups of mice (sharing a mutation) whose ABR phenotype is significantly different from that of control mice. In contrast to a standard approach to outlier detection, the group-based algorithm finds groups that are abnormal in their entirety, rather than just individual abnormal mice. Thus, the group-based algorithm for anomaly detection can also be used to identify a group whose individual mice are not significant outliers at all, but the sum of the deviation together is prominent. In this way, even much more subtle deviations can still be detected.

Keywords: ABR, Anomaly Detection, Statistics, Mutants, Unsupervised Learning, Mice, Auditory Brainstem Response, Hearing, Health

PySDDR: A Python Package for Semi-Structured Deep Distributional Regression

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Here we introduce PySDDR: a python package used for regression tasks, which combines statistical regression models and neural networks into a general single framework that can deal with multi-modal data (e.g. tabular and image data). The implementation consists of (1) a modular neural network building system for the combination of various statistical and deep learning approaches, (2) an orthogonalization cell to allow for an interpretable combination of different subnetworks as well as (3) a user-friendly manner to define models using distribution definitions. The package‘s modular design and functionality provides a unique resource for rapid and reproducible prototyping of complex statistical and deep learning models while simultaneously retaining the indispensable interpretability of classical statistical models.

Keywords: Regression, Deep Learning, Additive-predictors, Effect-decomposition, Orthogonal-complement

Comparative Fitness Landscape Analysis for Neural Architecture Search

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Neural Architecture Search (NAS) is a promising branch of AutoML dedicated to automating the design of Neural Network models. This field is rapidly growing, with a surge of methodologies ranging from Bayesian Optimization, Neuroevolution, to Differentiable Search and applications in various contexts. As these advances are happening, the efforts invested in studying or understanding the difficulty of performing NAS itself remain lacking. On the other hand, the field of Optimization has developed methods ‚highlighting' keys aspects to describe Optimization problems. The Fitness Landscape Analysis (FLA) stands out when it comes to characterize reliably and quantitatively Search Algorithms. We propose to use FLA to study a NAS problem. We show insights and findings provided by FLA on the two large-scale image classification datasets of CIFAR-10 and the Real World Remote-Sensing dataset of LCZ-42. Tools such as measuring a Fitness Landscape Profile, its Ruggedness, or an enumeration of Local optima help us get a sense of the difficulty of Performing NAS on those two tasks, given a Search Space. We also introduce the framework of Fitness Landscape Footprint as an aggregation of eight (8) metrics to synthesize an FLA in NAS. We provide insights for helping improve baseline algorithms on both datasets from such footprints.

Keywords: Neural Architecture Search, Fitness Landscape Analysis

Feature Selection Combining Neural Network and Genetic Algorithm for Metabotype Discrimination between Prediabetic and Healthy Subjects

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High-resolution non-targeted mass spectrometry methods (for example, Fourier Transform-Ion Cyclotron Resonance Mass Spectrometry (DI-FT-ICRMS)), output datasets with a large number of features (many thousands), while the number of samples is much lower. This imbalance creates a challenge for the analysis of non-targeted metabolomics datasets and means that we need to develop custom methods to unearth information that was not always visible by classical statistical techniques. We have applied a novel convolutional neural network together with a genetic algorithm, in one pipeline for the purpose of feature selection. The output of our pipeline is a set of features, selected by analyzing the classification model trained on the target dataset. The classification has been performed by a neural network and selecting the most relevant features has been done by a genetic algorithm. The neural network classification model on which the feature selection method is based achieved a precision-recall (PRC) score of over 0.95 on the test set, and this result allows us to subsequently use it for feature selection. The output of the developed pipeline contains approximately 200 features with high predictive scores, thus describing a metabolic fingerprint of the prediabetic condition on the dataset and potentially identifying some latent patterns. Our framework could, with minor modifications, be applied to diverse metabolomics datasets (with the exception that they must contain timepoints), which would allow us to analyze complex datasets and questions and utilize the advantages of neural networks for analyzing high resolution mass spectrometric data.

Keywords: Feature Selection, Metabolomics, Diabetes, Neural Networks

Aerial Scene Understanding in the Wild: Multi-Scene Recognition via Prototype-Based Memory Networks

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Aerial scene recognition is a fundamental visual task and has attracted an increasing research interest in the last few years. Most current researches mainly deploy efforts to categorize an aerial image into one scene-level label, while in real-world scenarios, there often exist multiple scenes in a single image. Therefore, in this paper, we propose to take a step forward to a more practical and challenging task, namely multi-scene recognition in single images. Moreover, we note that manually yielding annotations for such a task is extraordinarily time- and labor-consuming. To address this, we propose a prototype-based memory network to recognize multiple scenes in a single image by leveraging massive well-annotated single-scene images. The proposed network consists of three key components: 1) a prototype learning module, 2) a prototype-inhabiting external memory, and 3) a multi-head attention-based memory retrieval module. To be more specific, we first learn the prototype representation of each aerial scene from single-scene aerial image datasets and store it in an external memory. Afterwards, a multi-head attention-based memory retrieval module is devised to retrieve scene prototypes relevant to query multi-scene images for final predictions. Notably, only a limited number of annotated multi-scene images are needed in the training phase. To facilitate the progress of aerial scene recognition, we produce a new multi-scene aerial image (MAI) dataset. Experimental results on variant dataset configurations demonstrate the effectiveness of our network. Our dataset and codes are publicly available on https://github.com/Hua-YS/Prototype-based-Memory-Network.

Keywords: Convolutional neural Networks (CNN), Multi-Scene Recognition in Single Images, Memory Network, Multi-Scene Aerial Image Dataset, Multi-Head Attention-Based Memory Retrieval, Prototype Learning

Exploring Chemical Space Using Computational Methods

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As the lightest structural engineering metal, magnesium (Mg) is a promising base material for the development of advanced technologies in transport, medical as well as in battery applications. A prerequisite to unlock the full potential of Mg–based materials is gaining control over their corrosion behaviour due to the relatively high chemical reactivity of Mg whereas each application field imposes unique requirements on this challenge. Corrosion prevention is essential in transport applications to avoid material failure. Bone implants require a degradation rate that is tailored to a specific injury whereas constant dissolution of the anode material is required to boost the efficiency of Mg-air primary batteries. Fortunately, small organic molecules have shown great potential to control the dissolution properties of pure Mg materials and its alloys. [1] However, the vast space of small molecules with potentially useful dissolution modulating properties (inhibitors or accelerators) renders conventional experimental discovery methods too time- and resource-consuming. Consequently, computer-assisted selection prior to experimental investigations of the most promising candidates is of great benefit in the search for effective corrosion modulating additives. [2,3] Here, we demonstrate how unsupervised clustering of potential Mg dissolution modulators based on structural similarities and sketch-maps can quantitatively predict their experimental performance when combined with a kernel ridge regression (KRR) model. [3] Furthermore, we confirm the robustness of our data-driven model by blind prediction of the dissolution modulating performance of 10 untested compounds. Finally, a workflow is presented that facilitates an automated selection of compounds with promising properties by screening of a large database comprised of commercially available substances. [1] Corros. Sci. 2017,128, 224. [2] npj. Mater. Degrad. 2021, 5, 2. [3] Corros Sci. 2020, 163, 108245.

Keywords: Magnesium, Corrosion Control, Dissolution Modulators, Quantitative Structure-Property Relationships, Dimensionality Reduction, Database Screening

One Year of AI Consulting for Earth and Environment - Lessons Learned

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After one year of providing AI services to the Earth and Environment research community ranging from technical implementation to methodological guidance, it is evident that some challenges, pitfalls and solution paths are recurring across support projects independent of thematic setting. This is likely true also beyond the domain of Earth and Environment as far as service building and technical solutions are concerned. This presentation will summarize these first insights and motivate discussions of future service shaping. In particular, it will shed light on the relation between effort spent on data tuning, machine learning code optimization and workflow automation, discuss balances between the technical extravagance and simplicity, and motivate agility in consulting.

Keywords: ANN, Decision-Trees, AI in Practice, Digital Services, Consulting

Research on AI at ITAS

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Scientific and technological progress affect almost all areas of our lives, although frequently they are associated with unexpected and often undesirable side-effects. Motivated by the need to ensure that research and innovation activities are societally desirable, ethically acceptable and sustainable, technology assessment (TA) studies assume an important role due to its specific combination of knowledge production (concerning the development, consequences and conditions for implementing technology), the evaluation of this knowledge from a societal perspective, and the recommendations made to politics and society. The Institute for Technology and Systems Analysis (ITAS), of the KIT is the leading and most long-standing scientific institution in Germany (and beyond) dealing with TA and systems analysis, in theory and practice. ITAS investigates scientific and technological developments with a focus on their impacts and possible systemic and unintended effects. It produces analytical knowledge and assessments of socio-technical developments, also to provide policy and design options for decision-makers. Since the 1990s, ITAS has also increasingly been involved in stakeholder and public engagement activities and is now a major player in this area in Germany. With more than 100 scientific staff members from a wide variety of disciplines, ITAS is conducting a wide range of research activities in third party funded projects and contract work. Important external clients and funding partners are the German and the European parliaments, the European Commission, and federal and state ministries and agencies. Private sector entities are among its clients too. The aim of the poster is to present an overview of the research conducted at ITAS on AI. We hope that our visual mapping can be a promoter for interaction and discussion with participants of the event.

Keywords: Trustworthiness, Democracy, Values, Social Acceptance, Ethics, Risks, Responsible Research and Innovation, Vision Assessment, Knowledge Transfer, Policy Implications

Data Science for Terramechanics

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One major challenge for extraterrestrial mobile robotics is a safe traversal of soft regolith. Due to the complex behavior of regolith, the prediction of a rover's locomotion is challenging. Currently, various conventional modeling approaches are used to describe wheel soil interaction, ranging from detailed discrete element methods to simpler empirical models. The Terramechanics Robotics Locomotion Laboratory at DLR, a robotic single wheel test facility, designed to automatically perform wheel soil interaction experiments, already provides data for model validation. With the tradeoff between model precision and computational speed, currently, no methods for high-quality onboard predictions are available. Further simulation studies using conventional models are usually computationally expensive and are thus limited in scope. To solve these problems, the goal of the project is to explore the usage of machine learning and data science methods to combine data generated by the testbed with already existing models and modeling knowledge. By using a multi-fidelity approach combining data from the testbed with data generated by existing mathematical models, a model will be synthesized that should capture most patterns while being more computationally efficient. To combine the different sources, respective weights, derived from their fidelity levels, are assigned to them. The forces and torques acting on the wheel are predicted using the wheel velocity as well as surface geometry as input. Various regression models can be applied for this task. Surface geometry is treated as images and convolutional neural networks are applied to estimate an interaction direction. To capture the dynamic wheel behavior, models like recurrent neural networks or Hidden Markov models are used. Considering all mentioned above, experimental and simulated data can be used to extract insightful statistical patterns and use them to increase the prediction quality for rover locomotion.

Keywords: Terramechanics, Robotics, Locomotion

Munich School for Data Science (MUDS)

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The Munich School for Data Science (MUDS) trains the next generation of data scientists at the interface of data science and four application domain sciences: biomedicine, plasma physics, earth observation, and robotics. Our research school strengthens the domain-driven research within the Helmholtz Association by teaching methodological data science skills in an interdisciplinary and application-oriented fashion. MUDS offers joint research projects designed by two partners, a domain-specific application partner and a methodological partner, both supervising the PhD student and therefore ensuring methodological as well as application specific education. At the metropolitan region of Munich, the universities TUM and LMU, and three regional Helmholtz centers, HMGU, IPP, DLR, joined forces for an internationally visible and highly attractive consortium at a prime location for computational sciences in Germany. Additionally, MUDS is cooperating with Roche Penzberg and Boehringer Ingelheim to promote application-oriented PhD projects in biomedicine, and is a member of the Helmholtz Information & Data Science Academy (HIDA).

Keywords: Research School, PhD, Data Science, Biomedicine, Plasma Physics, Earth Observation, Robotics

Helmholtz AI Local Unit For Matter at Helmholtz-Zentrum Dresden-Rossendorf

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This poster provides a tip of the iceberg view of the activities by the Helmholtz AI local unit for matter at HZDR. The poster selects 3 topics of each sub-group and highlights them briefly. The poster is meant as a teaser for any discussion.

Keywords: YIG, Consultant Team, Surrogate Models, Denoising, Normalizing Flows, Invertible Neural Networks, Anomaly Detection

Helmholtz AI consulting

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Helmholtz AI consulting offers scientists from all Helmholtz centres of the Helmholtz Association the opportunity to receive support from AI method specialists to leverage (underused) data sets and to disseminate know-how. To facilitate access and user-friendliness, a web-based submission system (based on the open-source software Zammad) was set up in close cooperation with all six local units of Helmholtz AI and implemented together with HIFIS.

Keywords: Voucher system, AI, Consulting

ELLIS Munich

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In December 2018 the 'European Laboratory for Learning and Intelligent Systems' (ELLIS) was founded to create a diverse European network to promote cutting-edge research and breakthroughs in ML, to train the next generation of ML researchers and to drive economic growth in Europe through the use of ML technologies.
To foster European excellence in the highly competitive field of ML, research programs, a pan-European PhD program and a network of ELLIS units have been formed. The ELLIS Munich unit was proposed by the Technical University Munich (TUM) and Helmholtz Munich and selected as the only Bavarian ELLIS unit after a rigorous, highly competitive review. The Helmholtz AI local unit is the founding partner of ELLIS Munich at HMGU. Out of the 15 outstanding researchers forming the founding faculty of ELLIS Munich, Xiaoxiang Zhu and Fabian Theis represent regional Helmholtz AI prowess and Eleftheria Zeggini Helmholtz Munich. The unit is deeply integrated in the ELLIS programs on Computer Vision, Health, Earth & Climate and Semantic, Symbolic & Interpretable ML. The main goal of ELLIS Munich is to develop novel methods of ML and to apply them in the fields of biomedicine, computer vision and earth observation. Machine learning is the basis of these application areas. ELLIS Munich scientists work in a truly communal environment demonstrating impact on the application areas, training the next generation of interdisciplinary scientists by contributing to the ELLIS PhD program, promoting industrial collaborations and startups to advance ML as a core research field.

Keywords: ELLIS, ELLIS Munich, Machine Learning, Biomedicine, Computer Vision, Earth Observation, Networking

HAICORE - Helmholtz AI Computing Resources

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To provide the Helmholtz AI community with easy access to federated computing resources, the Helmholtz AI Computing Resources (HAICORE) was initiated at the end of 2019 as part of the Helmholtz Incubator. It includes Helmholtz funding of €2.5 million, mainly for GPU hardware installed and managed at Forschungszentrum Jülich (FZJ) and Karlsruhe Institute of Technology (KIT). The resources are available to the entire AI community within the Helmholtz Association. To enable open, fair, low-threshold and community-based access to HAICORE resources, the HAICORE access board was established, consisting of guests and deputies from the computing centers and the various Helmholtz platforms. For the ramp-up phase, the HAICORE access board decided to split the HAICORE resources into two usage modalities: 1) ad-hoc usage for initial playing with the data and/or AI methods with up to 10 GPU/h per day at KIT, and 2) lightweight projects with a maximum of 5,000 GPU/h per year at FZJ. Access to both modalities is available on the Helmholtz AI website. The HAICORE access board monitors the usage of HAICORE and will adapt the policy if necessary.

Keywords: Supercomputing, High-Performance Computing, HPC, GPUs, Computing Resources

Helmholtz AI Central Unit & Local Unit Health

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Helmholtz Zentrum München (HMGU) is home to the central unit of Helmholtz Artificial Intelligence Cooperation Unit (Helmholtz AI), which also covers the local unit for health. With its strong and expanding array of computationally-focused institutes (ICB), a dynamically growing digital health environment (ITG), and the bioengineering and imaging-focused HPC, HMGU is an ideal and well-connected host for the central unit.
The Helmholtz AI science management team at the central unit is integral to implementing and running Helmholtz AI, with its science and outreach managers, coordinating platform activities and projects across all Helmholtz AI units and within the Helmholtz Association that ensure wide dissemination of methods and that increase international visibility. The team is responsible for outreach and events, the Helmholtz AI voucher system and project calls, as well as facilitating the meetings of the Helmholtz AI steering board (SB), the HAICORE access board and the scientific advisory committee (SAC). Through liaison with the Association‘s head office, its various bodies and other platforms of the Incubator Information and Data Science the science management team ensures a seamless flow of information, alignment with overall strategy and concise reporting. Helmholtz AI central unit also includes a team of health-focused AI consultants (led by Marie Piraud) that will provide scientific machine learning support to researchers across the Helmholtz Association through the voucher system, and currently four research labs (led by Niki Kilbertus, Heidi Seibold, Tingying Peng and Shadi Albarqouni) who work on new scientific topics and strategies in AI for health.
The website www.helmholtz.ai serves as the central portal providing information on science, events, projects and funding calls, as well as the latest news (also on Twitter: @helmholtz_ai) and job offers at all units.

Keywords: Coordination, Outreach, Projects, Vouchers, Strategy, Health

Helmholtz AI Cooperation Unit

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Our ambition at the Helmholtz AI cooperation unit is to reach an internationally visible leadership position in applied Artificial Intelligence (AI) / Machine Learning (ML) by combining unique research questions, data sets and expertise with newly developed AI/ML-based tools and democratize access to them in an open and dynamic community. We are a research-driven hub for applied AI that i) fosters cross-field creativity, ii) identifies and leverages similarities between applications, iii) integrates field-specific excellence and AI/ML prowess, iv) improves the quality, scalability and timely availability of emerging methods and tools and v) empowers and trains the current and next generation of scientists. We are structured as a hub-and-spoke model with six units across the Helmholtz Association; these units fund research groups and employ Helmholtz AI consultant teams, ensuring a strong anchoring of our activities in all research fields. The central unit coordinates platform strategy and activities, particularly outreach, the voucher system and Helmholtz AI project calls, a funding line for collaborative projects.
Our goal is to enable the efficient and agile development and implementation of AI/ML assets across the whole Helmholtz Association.

Keywords: AI, Cooperation, Research, Projects, Outreach

Helmholtz AI at Forschungszentrum Jülich: Human Brain Models and AI Methods on High Performance Computing Systems

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Helmholtz AI at Forschungszentrum Jülich (FZJ) addresses digital transformation especially at the overlap of AI with innovative high-performance computing (HPC), and neuroscience. FZJ adopts an interdisciplinary approach based on domain-specific research questions intertwined with applied AI techniques. At FZJ, Helmholtz AI is embedded into one of the largest research centers in Europe, focusing on brain research, HPC, renewable energy and energy systems, atmosphere, and bioeconomy science, to lay the foundation for key technologies of tomorrow and work on viable solutions for complex questions facing society today. Jülich's Helmholtz AI unit is built on an intense interdisciplinary partnership between Juelich Supercomputing Centre (JSC) and Institute of Neuroscience and Medicine which has already become the main driver of the European research flagship 'Human Brain Project' (HBP). The focus of Jülich's Helmholtz AI unit is on robust deep learning methods for microscopic image analysis, as well as on large-scale, active continual learning transferable across different tasks and domains. Driven by high-throughput data acquisition and the ambition to quickly transfer knowledge across tasks and scientific domains, the implementation of AI methods on HPC systems is a key aspect of this work.

Keywords: Brain-inspired AI, Human Brain Organisation, Large-Scale Continual Learning, Transfer Learning, Supercomputing for Distributed Training

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