Workshop

Machine Learning in Earth system science

February 3-4, 2020

German Climate Computing Center (DKRZ)
Hamburg, Germany

**Programme,
Book of Abstracts
and Participants**

Introduction

To overcome limitations in computing and data analytics related to Earth System science, the uptake of artificial intelligence (AI) and machine learning (ML) methodologies is currently being explored. Multiple initiatives are now emerging to tackle open challenges such as subscale parametrization, detection of patterns and in-situ analysis, adoption of ML for alternative process models or dedicated fast prediction systems to address specific end-user needs. This also leads to further concerns that need to be addressed with regard to the verifiability and reproducibility of results, efficient and effective use of computing and storage resources and the necessary practical software environments.

Among these initiatives, the Helmholtz Association initiated the Helmholtz Artificial Intelligence Cooperation Unit (HAICU). From the beginning of 2020 on, HAICU will form a strong collaboration across multiple disciplines to bring AI into practice. It will develop, implement, and disseminate methods of Artificial Intelligence for purposes including the analysis of complex systems in the fields of health, energy, transport and earth and environment. Specific to Earth sciences, the Helmholtz Digital Earth project has also already paved the ground for large-scale data analytics and initiated actions to foster AI adoption.

With Digital Earth, HAICU and other initiatives, there is now an accelerating momentum to tackle these challenges with a diverse set of approaches and stakeholders, which opens up a rich area of future opportunities for collaboration. This workshop will bring multiple key stakeholders together, exchange current experiences, and foster further community actions.

The workshop is planned as a 1.5-day event in Hamburg. The first day will introduce the scope and challenges through a series of short talks, while the second day will provide a forum for interactive discussion. A poster reception to which all participants are invited to contribute is planned for day 1. The goals of the workshop are to assess the state of the art, identify gaps in knowledge or services, and build future community collaborations.

We welcome you to Hamburg, and look forward to a successful workshop!

Corinna Schrum (HZG)
Tobias Weigel (DKRZ)
Fabian Reith (GEOMAR)
Laurens Bouwer (HZG/GERICS)

Programme:

Day 1 - February 03, 2020 (Monday)	
08:30-09:00	Registration
09:00-09:15	**Welcome and introduction:** ● Corinna Schrum (HZG) ● Thomas Ludwig (DKRZ / Universität Hamburg)
09:15-09:30	Introduction to AI in Earth & Environment (Frederik Tilmann, GFZ)
09:30-10:30	**Session 1: Domain challenges and approaches** Keynote presentations (30 min. each) ● Markus Reichstein (MPI-BGC Jena): Linking Machine Learning and physical-biological System Modelling ● Kristian Kersting (TU Darmstadt): The Third Wave of AI: Closing the Gap between AI and the Domain Experts *(remote)*
10:30-11:00	Coffee break
11:00-12:30	**Session 2: Domain challenges and approaches** Keynote presentation (30 min.) ● Jakob Runge (DLR / Universität Jena): Perspectives for causal inference on time series in Earth system sciences and beyond Short presentations and discussion (15 min. each) ● Julia Fuchs (KIT): Applications of machine learning techniques to satellite observations of the cloud environment ● Peter Dueben (ECMWF): Deep learning for weather predictions
12:30-13:30	Lunch break
13:30-15:00	**Session 3: Building bridges between AI and domains** Keynote presentation (30 min.) ● David Greenberg (HZG): Fitting Interpretable Scientific Models with Machine Learning Short presentations and discussion (15 min. each) ● Christopher Kadow (DKRZ): AI reconstructs missing climate information ● Hanna Meyer (WWU): Machine learning applications in environmental remote sensing – Moving from data reproduction to spatial prediction
15:00-15:30	Coffee break
15:30-17:00	Introduction to interactive part of the workshop (10 min.) ● How will the breakouts work: Rapporteur and moderator role ● Open options for future activities **Session 4: Breakout groups** ● Science questions A - e.g., modelling, parametrizations, parameter estimation, uncertainty quantification

	● Technical topics - e.g., GPUs, Python usage, I/O and storage
17:00-17:30	Day 1 wrap-up: ● Reporting of day 1 breakouts
17:30-19:30	**Poster reception and Dinner**

Day 2 - February 04, 2020 (Tuesday)	

08:30-09:30	**Session 5: Domain challenges and approaches, uncertainty and explainability**
	 ● Welcome and recap of day 1 (5 min.)
	 ● Short talks (15 min.)
	  ○ Peter Braesicke (KIT): On the Role of Stratospheric Ozone in the Interactive Chemistry-Climate System
	  ○ Dim Coumou (VU): Machine Learning in climate science: Finding causal connections and improving seasonal forecasts
	  ○ Maria Moreno de Castro (DKRZ): Uncertainty Quantification, Machine Learning Interpretability, and Explainable Artificial Intelligence

09:30-09:45	Short break
09:45-10:45	**Session 6: Breakout groups** ● Science questions B – time series analysis, causality, data-assimilation, statistical prediction ● AI/ML methodology gaps - e.g., uncertainty, reproducibility
10:45-11:15	Coffee break
11:15-12:15	**Session 7: Breakout groups** ● Software frameworks, services and infrastructures ● Applications beyond Earth and environment ● Community building, synergies of existing national initiatives, funding opportunities
12:15-13:30	**Breakouts day 2 wrap-up** **Workshop wrap-up** ● Lessons learned and major outcomes ● Ideas for a follow-up workshop ● Overview on other relevant activities: Workshops, trainings, networking opportunities
13:30	Lunch and farewell

Logistics

The workshop takes place at the German Climate Computing Centre (DKRZ) in Hamburg.

Deutsches Klimarechenzentrum (DKRZ)
Bundesstraße 45a
20146 Hamburg

The workshop takes place mainly in room 034, directly at the main entrance. Registration starts Monday 08:30. Information how to reach DKRZ is available on the websites:
https://www.dkrz.de/about-en/contact/directions

A list of hotels in the vicinity can be found on the MPI-M websites:
http://www.mpimet.mpg.de/en/institute/visitor-information/hotel-list/

If you are giving a poster presentation, please bring your poster already printed in the right format. The poster boards are vertical, roughly 120x150 cm. The posters will be presented during the reception on Monday evening. They can be put up just before the reception.

In case of questions, contact Tobias Weigel (weigel@dkrz.de).

Abstracts – Talks

Peter Braesicke (KIT): On the Role of Stratospheric Ozone in the Interactive Chemistry-Climate System

Stratospheric ozone protects life from hard UV radiation and determines important aspects of the thermal structure of the atmosphere. In classic climate simulations, ozone is prescribed as a boundary condition. However, we know that the interaction of (stratospheric) ozone, radiation and circulation can be central for some aspects of climate change.

Over the years, different groups have constructed models with interactive composition (including stratospheric ozone), investigating mechanisms in which ozone changes are central to climate change signals that would not be captured when prescribing a climatology. However, comprehensive composition simulations can be computationally very expensive. Thus, a number of approximations exist to simulate stratospheric ozone in simplified ways. Here, we will discuss such approximations and how machine learning can help to provide reliable implementations of simplified stratospheric chemistry.

For a certain class of simulations, we conclude that composition(chemistry)-climate models (e.g. ICON-ART) are indispensable tools to understand certain aspects of climate change. We can meet the challenge of modelling across scales and in-depth validation with highly resolved measurement data with new modelling systems that include simplified stratospheric ozone.

Dim Coumou (VU): Machine Learning in climate science: Finding causal connections and improving seasonal forecasts

Summer, with most biological and agricultural production, is probably the season when future changes in extremes will have the most-severe impacts on humanity. Summer extremes are particularly devastating when they persist for several days: Many consecutive hot-and-dry days causing harvest failure, or stagnating wet extremes causing flooding. Often such situations are related to quasi-stationary waves in the Jetstream. Despite this importance, we are far from a comprehensive understanding of the physical mechanisms involved in creating such quasi-stationary waves, nor how they will change with future warming.

Using machine learning techniques based on causal inference we can understand and quantify the drivers and causal pathways that influence jet dynamics. I will present several examples of how causal inference techniques can disentangle cause from effect to provide insights into the dynamics of the large-scale atmospheric circulation and teleconnections. Understanding the physical pathways in atmosphere by quantifying causal links can help improving forecasts on seasonal to sub-seasonal timescales including prolonged extremes like heat waves and droughts. Some of these data-driven forecasts using machine learning outperform operational forecasts based on dynamical models. Ultimately we aim for developing hybrid forecast methods to improve early warning of extreme weather events.

Peter Dueben (ECMWF): Deep learning for weather predictions

This talk will discuss different approaches to use deep learning to improve weather and climate predictions that are investigated at ECMWF across the workflow of numerical weather predictions. The approaches may speed-up simulations, help to improve models, or enhance the usefulness of model output in the future.

In particular, I will talk about the emulation of model components, downscaling of model output, improvements of uncertainty quantification in ensemble predictions, and the use of machine learning to learn the equations of motion in atmosphere and ocean.

Julia Fuchs (KIT): Applications of machine learning techniques to satellite observations of the cloud environment

Understanding clouds, aerosols, their interactions with the land surface and large-scale dynamics is essential for the understanding of our climate system. However, multiple covariations within the climate system complicate the identification of e.g. cloud-relevant influences and the quantification of the aerosol-cloud relation.
In our studies we conduct satellite-based analyses of cloud properties and aerosol patterns and their sensitivities to their meteorological environment. Our foci include stratocumulus cloud properties in the Southeast Atlantic and comparable regions, European fog distribution and aerosol patterns over Germany. The effect of multiple geophysical parameters is investigated based on ensemble-based machine learning approaches such as Gradient Boosting Regression Trees using a combination of satellite and reanalysis data. Comprehensive analyses of these climate drivers are performed and lead to an improved knowledge of the interactions of clouds and their environment from regional to global scales.

David Greenberg (HZG): Fitting Interpretable Scientific Models with Machine Learning

For many important models across the natural sciences, running simulations with known parameters is easy but assigning parameters to data is difficult. However, recent work combining machine learning with mechanistic modeling shows that neural networks can be trained to solve this inverse problem, effectively assigning model parameters based on incomplete or noisy observations. By using simulations as training data, this strategy can be used to identify parameters even when the simulator has non-differentiable outputs, intractable likelihood or millions of hidden internal variables. It can also recover the full range of parameter sets consistent with experimental observations, allowing parameter uncertainty to be incorporated into predictions of future observations. In applying this approach to earth system science, major challenges arise due to the size and complexity of models and data, but advances in neural network architectures and density estimation can help address them.

Christopher Kadow (DKRZ): AI Reconstructs Missing Climate Information

Nowadays climate change research relies on climate information of the past. Historic climate records of temperature observations form global gridded datasets like HadCRUT4, which is investigated e.g. in the IPCC reports. However, record combining data-sets are sparse in the past. Even today they contain missing values. Here we show that artificial intelligence (AI) technology can be applied to reconstruct these missing climate values. We found that recently successful image inpainting technologies, using partial convolutions in a CUDA accelerated deep neural network, can be trained by 20CR reanalysis and CMIP5 experiments. The derived AI networks are capable to independently reconstruct artificially trimmed versions of 20CR and CMIP5 in grid space for every given month using the HadCRUT4 missing value mask. The evaluation reaches high temporal correlations and low errors for the global mean temperature.

Lydia Keppler (MPI-Met): A SOM-FFN approach to map monthly dissolved inorganic carbon from sparse ship data

I present a 2-step neural network method to obtain a global monthly climatology of dissolved inorganic carbon (DIC) in the upper 2000 m of the ocean, based on direct measurements. The method first clusters the ocean into regions of similar biogeochemical and physical properties using self-organizing maps (SOMs) and then runs a feed-forward network (FFN) in each cluster to establish and apply statistical relationships between the global fields of physical and biogeo-chemical properties and available DIC measurements from the GLODAPv2.2019 database. I tested the method using synthetic data from a global hindcast simulation of an ocean biogeo-chemistry model, an existing time-mean climatology, and independent time-series and biogeo-chemical float observations. I found that the surface seasonal cycle of DIC in the high northern latitudes of the Pacific Ocean (north of ~30°N) and the eastern equatorial Atlantic have the larg-est amplitudes (~30 to >50 μmol kg-1 and ~40 μmol kg-1, respectively), while most of the re-maining ocean has a weaker amplitude ranging from 5 to 20 μmol kg-1. The months with the highest surface DIC concentrations tend to be in spring when vertical mixing dominates the sea-sonal maximum.

Kristian Kersting (TU Darmstadt): Making Clever Hans Clever: Humans Revise Learning Machines for Plant Phenotyping

Current machine learning techniques have shown excellent performances in many real-world applications such as plant phenotyping. Particularly, deep neural learning has become a popular method of choice. Unfortunately, they might be making use of confounding factors within datasets to achieve high prediction rates, resulting in not trustworthy decisions. Rather than discarding the trained models or the dataset, we show that interactions between the learning system and the human user can correct the model. Specifically, we revise the models decision process by adding annotated masks during the learning loop and penalize decisions made for wrong reasons. In this way the decision strategies of the machine can be improved, focusing on relevant features, without considerably dropping predictive performance.

Hanna Meyer (WWU Münster): Machine learning applications in environmental remote sensing – Moving from data reproduction to spatial prediction

Machine learning finds frequent application for spatial predictions of environmental variables. In a typical prediction task, remote sensing data are related to observations of an ecological target variable to model its spatial distribution. However, the characteristics of spatial data, especially spatial autocorrelation, are widely ignored in machine learning applications in remote sensing.

We hypothesize that this is problematic and results in models that can reproduce training data but are unable to make spatial predictions beyond the locations of the training samples. We assume that against the opinion that machine learning algorithms are robust to uninformative predictors, spatial dependencies can lead to considerable misinterpretations by the algorithm. We suggest that predictors need to be tested for their spatial contribution in the model and misleading variables need to be excluded.

We use two case studies aiming at predictions of land cover as well as leaf area index. As predictors we use remote sensing data (aerial images, Sentinel-2) but we also present terrain-related and geolocation variables to the models which feature high spatial autocorrelations. Random Forest, as one of the most frequently applied algorithms in environmental remote

sensing, is used to train models and we compare how spatial variable selection affects the predictions and the estimated model performance.

Our findings confirm that spatial cross-validation is essential in preventing overoptimistic model performance estimates. We further show that highly autocorrelated predictors can lead to considerable overfitting and result in models that can reproduce the training data but fail in making spatial predictions. The problem becomes apparent in the visual assessment of the spatial predictions that show clear artefacts that can be traced back to a misinterpretation of the spatially autocorrelated predictors by the algorithm. The proposed spatial variable selection could automatically detect and remove such variables that lead to overfitting, resulting in reliable spatial prediction patterns and improved statistical spatial model performance.

We finally conclude that spatial machine learning applications require that spatial characteristics are taken into account to produce reliable models that can advance our knowledge in environmental science.

Maria Moreno de Castro (DKRZ): Uncertainty Quantification, Machine Learning Interpretability, and Explainable Artificial Intelligence

State-of-the-art machine learning and deep learning algorithms are developed to always predict an output (even if the input has nothing to do with the training set) and have originally been designed for interpolation rather than extrapolation. Moreover, with the increase of data volume and model complexity, their predictions can be very accurate but prone to rely on spurious correlations, encode and magnify bias, and draw conclusions that do not incorporate the underlying dynamics governing the system. Because of that, the uncertainty of the predictions and our confidence in the model are difficult to estimate and the relation between inputs and outputs becomes hard to interpret.

While many promising proof-of-concept examples are being developed in Earth System modelling, little attention has been paid to uncertainty quantification (UQ), machine learning interpretability (MLI), and explainable artificial intelligence (XAI). In fact, most of machine learning and deep learning applications aim to optimize performance metrics (for instance accuracy, which stands for the times the model prediction was right), which are rarely good indicators of trust (that is, why these predictions were right?).

We will explain the intuition behind the most popular techniques of UQ, MLI, and XAI: (1) the Permutation Importance and Gaussian processes to explore the input space, (2) the Monte-Carlo Dropout, Deep ensembles, Quantile Regression, and Gaussian processes to explore the model space, (3) Conformal Predictors to provide a confidence interval on the outputs, (4) the Layerwise Relevance Propagation (LRP), Shapley values, and Local Interpretable Model-Agnostic Explanations (LIME) to visualize what data were relevant for a particular prediction, and (5) some best-practices, like the detection of anomalies in the training data before the training, the implementation of fallbacks when the prediction is not reliable, and physics-guided learning by including constraints in the loss or reward function to avoid inconsistencies, like the violation of conservation laws.

Abstracts – Posters

Julianna Carvalho Oliviera (HZG): Neural interpretation of European summer climate ensemble predictions

Predicting European summer climate is a complex problem, and current state-of-the-art dynamical seasonal prediction systems still show very limited skill. To overcome this problem, we propose a neural network-based classification of individual ensemble members at the initialisation of summer climate predictions with MPI-ESM-MR, prior to performing a skill analysis. Different from European winter climate, largely dominated by the North Atlantic Oscillation, predictability of European summer climate has been associated with several physical mechanisms, including teleconnections with the tropics. Recent studies have shown that forecast skill improves when the dominant physical processes in a given season are identified at the initialisation of a prediction. Each of these dominant physical process is associated with large-scale circulation patterns, often depicted by modes of Empirical Orthogonal Functions (EOF). We argue that Self-Organising Maps (SOM) can provide further insight on interpreting the forecast skill of MPI-ESM-MR, by identifying which circulation patterns lead to more predictable states than others. We first perform a SOM analysis on sea level pressure fields of ERA-20C reanalysis for the summer season (June to August) covering the period of 1900-2010. We identify 25 large-scale circulation regimes, further reduced to 4 main classes after performing Hierarchical Agglomerative Clustering. We compare the SOM-derived modes with variability modes derived from traditional analyses, and perform a composite analysis on surface air temperature and precipitation, in order to characterise each class of circulation regime. This analysis is then used to distinguish different classes of forecasts with two different sets of MPI-ESM-MR initialised simulations with 10 and 30 members, covering the period of 1902-2008 and 1982-2016, respectively. We then discuss the differences and advantages of performing a neural interpretation of the skill of an ensemble forecast, over traditional skill analysis.

Tobias Finn (University of Hamburg): Inferring the unknown: Unifying statistical pre- and post-processing in meteorology with amortized variational inference

Three problems, one latent state, which we want to infer, but three different solution. That is the usual case in meteorology. Observations are processed with their own pipeline, and used by data assimilation. But how to incorporate these observations into a statistical post-processing pipeline, like model output statistics? One could argue that this unsolved problem hinders the evolution of numerical weather prediction. Here, I propose a unified framework for seamless inference, going from observations, over data assimilation to model output statistics. This unified framework is based on recent advances in statistical methods (variational inference) and deep neural networks. I cast the three different problems into a variational inference problem, where we want to get an unknown latent state based on perturbed observational representations. To solve this variational inference problem, we have only to construct a decoder, also called observation operator, and a prior for the latent state. It is often much easier to construct these two ingredients than solving the inference problem. These two ingredients are then used to train deep neural networks in a fully unsupervised framework called amortized variational inference. I show that this procedure can be used for observational data cleaning (weather radar processing), but it can be also used for fully bayesian and gridded model output statistics (statistical post-processing). In my last example, I demonstrate how this framework can be combined with Generative Adversarial Networks for implicit and non-linear data assimilation. These examples show that it is possible to use recent developments in unsupervised deep learning to solve long-standing problems in meteorology.

Sarah Hallerberg (HAW Hamburg): Predictability of Critical Transitions and Perturbation Growth

Critical transitions occur in a variety of dynamical systems. Here we employ quantifiers of chaos to identify changes in the dynamical structure of complex systems preceding critical transitions. As suitable indicator variables for critical transitions, we consider changes in growth rates and directions of covariant Lyapunov vectors. Studying critical transitions in several models of fast-slow systems, i.e., a network of coupled FitzHugh-Nagumo oscillators, models for Josephson junctions, and the Hindmarsh-Rose model, we find that tangencies between covariant Lyapunov vectors are a common and maybe generic feature during critical transitions. We further demonstrate that this deviation from hyperbolic dynamics is linked to the occurrence of critical transitions by using it as an indicator variable and evaluating the prediction success through receiver operating characteristic curves. In the presence of noise, we find the alignment of covariant Lyapunov vectors and changes in finite-time Lyapunov exponents to be more successful in announcing critical transitions than common indicator variables as, e.g., finite-time estimates of the variance. Additionally, we propose a new method for estimating approximations of covariant Lyapunov vectors without knowledge of the future trajectory of the system. We find that these approximated covariant Lyapunov vectors can also be applied to predict critical transitions.

Marcel Nonnenmacher (HZG): Machine Learning Tools for fitting Interpretable Models to Data

Scientific models incorporate concepts, hypotheses and established knowledge, while their free parameters represent knowledge gaps and can be adjusted to match data. Compared to the purely statistical "black-box" models commonly used in machine learning, scientific models offer much higher interpretability and require fewer parameters. On the flipside, inferring free parameters from data is typically much more challenging for scientific models because they seldomly allow tractable likelihoods.

Likelihood-free methods allow approximate Bayesian inference for any model that can be repeatedly simulated, without relying on internal details of the model or its implementation. With this, we can also for complex scientific models study the full space of free parameters consistent with given observations. As we demonstrate on several application, likelihood-free methods based on deep learning can infer parameters from hand-selected data features, or automatically learn informative features from high-dimensional observations. These methods have a strong potential to facilitate and improve parameter tuning for earth system models.

Timm Schöning (GEOMAR): Marine Image Analysis

Optical imaging is a common technique in ocean research. Diving robots, towed cameras, drop cameras and TV-guided sampling gear: all produce image data of the underwater environment. Technological advances like 4K cameras, autonomous robots, high-capacity batteries and LED lighting now allow systematic optical monitoring at large spatial scale and shorter time but with increased data volume and velocity. Volume and velocity are further increased by growing fleets and emerging swarms of autonomous vehicles creating big data sets in parallel. This generates a need for automated data processing to harvest maximum information. Systematic data analysis benefits from calibrated, georeferenced data with clear metadata description, particularly for machine vision and machine learning. This presentation will focus on data workflows, at-sea high-performance computing and unsolved challenges in automated understanding of marine imagery.

Hui Tang (GFZ): Deriving discharge thresholds for runoff-generated debris flow using process-based models and machine learning methods

Debris flows threaten life and infrastructure in areas close to steep mountain fronts. Currently employed rainfall intensity-duration (ID) thresholds are empirical and developed with historical data, and therefore most applicable to those settings where debris flows have been recorded in the past. We propose a method that combines process-based numerical models and machine learning to derive critical values of dimensionless discharge for runoff-generated debris flows in a variety of settings. By using a support vector machine method, we train logistic regression functions using a combination of monitoring data and hydrologic modelling of debris flows. Our training dataset includes post-wildfire debris flows in the Fish Fire, California, USA, the Pinal Fire, Arizona, USA, the Buzzard Fire, New Mexico, USA, runoff-generated debris flows in Chalk Cliffs, Colorado, USA, and runoff events in the Venetian Dolomites, Italy. Our proposed approach is based on a slope-dependent dimensionless discharge threshold that can be used to estimate rainfall ID thresholds in areas with no historical data on runoff-generated debris flow occurrence. This results in a dimensionless discharge threshold that is consistent with previously derived discharge thresholds for post-fire debris flows in southern California.

Frederik Tilmann (GFZ): Low uncertainty multi-feature magnitude estimation with 3D corrections and boosting tree regression: application to North Chile

Magnitude estimation is a central task in seismology needed for a wide spectrum of applications ranging from seismicity analysis to rapid assessment of earthquakes. However, magnitude estimates at individual stations show significant variability, mostly due to propagation effects, radiation pattern and ambient noise. To obtain reliable and precise magnitude estimates, measurements from multiple stations are therefore usually averaged. This strategy requires good data availability, which is not always given, e.g. for near real time applications or for small events. We developed a method to achieve precise magnitude estimations even in the presence of only few stations. We achieve this by reducing the variability between single station estimates through a combination of optimization and machine learning techniques on a large catalog. We evaluate our method on the large scale IPOC catalog with $> 100, 000$ events, covering seismicity in the northern Chile subduction zone between 2007 and 2014. Our aim is to create a method that provides low uncertainty magnitude estimates based on physically meaningful features. Therefore we combine physics based correction functions with boosting tree regression. In a first step, we extract 110 features from each waveform, including displacement, velocity, acceleration and cumulative energy features. We correct those features for source, station and path effects by imposing a linear relation between magnitude and the logarithm of the features. For the correction terms, we define a non-parametric correction function dependent on epicentral distance and event depth and a station specific, adaptive 3D source and path correction function. In a final step, we use boosting tree regression to further reduce inter-station variance by combining multiple features. Compared to a standard, non-parametric, 1D correction function, our method reduces the standard deviation of single station estimates by up to 57%, of which 17% can be attributed to the improved correction functions, while boosting tree regression gives a further reduction of 40%. We analyze the resulting magnitude estimates regarding their residuals and relation to each other. The definition of a physics-based correction function enables us to inspect the path corrections and compare them to structural features. By analyzing feature importance, we show that envelope and P wave derived features are key parameters for reducing uncertainties. Nonetheless the variety of features is essential for the effectiveness of the boosting tree regression. To further elucidate the information extractable from a single

station trace, we train another boosting tree on the uncorrected features. This regression yields magnitude estimates with uncertainties similar to the single features after correction, but without using the earthquake location as required for applying the correction terms. Finally, we use our results to provide high precision magnitudes and their uncertainties for the IPOC catalog.

Andrey Vlasenko (HZG): Ability of Neural Network in reproducing Chemical Transport Model Estimates based on meteorological data.

The presence of volatile chemicals in the atmosphere affects air quality and, as a consequence the health of the population. As a result, there is a need for robust air quality simulations and future scenarios to investigate the effects of emission reduction measures. Due to high computational costs, the prediction of concentrations of chemical substances using discretized atmospheric chemistry transport models (CTM) remains a big challenge. Neural network (NN) is an alternative to cumbersome numerical estimates since it can approximate any limited continuous function (i.e., concentration time series) with reasonable accuracy requiring much less computational resources. Thus, the NN trained on the CTM estimates should be able to forecast concentrations of chemical substances similar to CTM. We test the ability of a NN to reproduce CTM concentration estimates with the example of daily mean summer NO_2 and SO_2 concentrations. In these tests check how accurate NN reproduces the CTM estimates and what is the corresponding gain in saving of the computational resources. Note that after a spin-up time, CTM estimates are independent of the initial conditions. We show that similar spin-up time exists in NN, which allows it and predict atmospheric chemical state without having input concentration data.

Kathrin Wahle (HZG): Feed-forward backpropagation Neural Network

Feed-forward backpropagation Neural Networks can be applied to a broad range of problems occuring in Earth system science, such as data analysis, module (function) emulation and data assimilation. We will give an overview of our previous results in these fields.

Jan Walda (University of Hamburg): Unsupervised seismic attribute interpretation using deep learning

Machine learning, in particular deep learning, has become a vital factor in pattern recognition and repetitive tasks, outperforming humans regularly. Seismic interpretation is often associated with finding specific patterns of interest and can depend on the interpreters involved. We aim to provide consistent automatic interpretation of seismic data, that assist interpreters. In order to do so, we combine deep learning with traditional machine learning techniques for automatic interpretation of seismic attributes using 3D data seismic field data. A major difficulty of seismic interpretation is the way of dealing with the richness of seismic attributes (up to hundreds), which results in a multidimensional problem. Usually, the amount of seismic attributes is reduced, e.g. by principle component analysis, before interpretation. In order to analyze the most important spatial information from two sets of attributes containing six attributes each, we use a 3D convolutional autoencoder. The autoencoder aims to find a reduced representation of the data. To verify, whether the found representation is reasonable, we reconstruct the original data and evaluate the misfit of reconstructed and original data. Once the misfit is sufficiently small, we cluster the reduced representation (encoding) to obtain a feature cube that contains a label for each sample. This process reduces the multidimensional information of multiple seismic attributes and their spatial distribution to one label for each sample in the 3D spatial volume. The found labels can be interpreted

instead of the numerous seismic attributes, which eases and accelerates interpretation and reduces cost. Furthermore, human interpreters might overlook features of interest, such as faults, salt or horizons in the seismic attributes, which can be revealed by our unsupervised deep learning approach.

Eduardo Zorita (HZG): Application of Machine Learning methods for reconstructions of past climate

Reconstructions of past climates are based on proxy indicators, such as tree-rings or lake sediments, that contain information about past environmental conditions, but that also are influenced by other non-climatic factors. The extraction of the climate signal is achieved so far by statistically calibrating there proxy records against available observations. Machine Learning methods are beginning to be applied for climate reconstructions, but it is not yet clear if they can outperform the classical statistical methods. We will present here a few applications.

One application is focused on the reconstructions of the sea-surface-temperatures in the North Atlantic over the past millennium from the information contained in terrestrial proxies located along the Atlantic coasts. The applied method is Gaussian Process Regression. Traditionally, these type of reconstructions have been performed with ordinary linear regression, possibly after a pre-filtering by Principal Components Analysis. This approach leads to the underestimation of past variability. A straightforward application of Gaussian Process Regression also suffers from this deficiency. However, a rearranging of the predictors and predictand phase space can substantially ameliorate this problem.

The second example is focused on the reconstruction of the atmospheric circulation over the past centuries based on precipitation sensitive proxies. The method here is the k-nearest neighbour, Spatial patterns of reconstructed precipitation are compared with those simulated in long climate simulations, selecting thereby the most similar. The simulated atmospheric circulation in those most similar instances is then identified as the reconstructed atmospheric circulation. This method can be further refined by a subsequent correction using a Kalman Filter, to reduce existing biases and standard deviation of the estimation.

Participants

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1	Alexander Winkler	MPI-Met
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30	Lennart Schmidt	UFZ
31	Lydia Keppler	MPI-Met
32	Mahyar Valizadeh	HMGU
33	Marcel Nonnenmacher	HZG
34	Maria Moreno de Castro	DKRZ
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44	Oliver Bothe	HZG
45	Peter Braesicke	KIT
46	Peter Dueben	ECMWF
47	Rami Sonal Pravinbhai	AWI

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51	Sofiane Bendoukha	DKRZ
52	Thomas Ludwig	DKRZ
53	Timm Schoening	GEOMAR
54	Tobias Finn	University of Hamburg
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56	Viktoria Wichert	HZG