DAAD GSSP - Stipendienausschreibung

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Learning Deep Insights into Hydrological Processes using Bayesian Neural Hydrology

Keywords: Hydrological modelling, Model development, Deep learning, Neural Ordinary differential equations, Bayesian inference, Knowledge infusion

Introduction / Background:
The study of hydrological processes is of paramount importance in understanding and effectively managing our water resources. However, the complex and interconnected nature of these processes often presents challenges in modelling. Fully-blown models based on physical hydrosystem considerations and partial differential equations are extremely hungry for input data, parameter values and geometries. Fully lumped rainfall-runoff models contain little physical principles and are strongly simplified, but can be computed very fast and require much less data for model building. However, their prediction quality is limited by their inherent simplifications. Some model classes exist in between that strike the one or other compromise.

Lately, there has also been the branch of neural hydrology, where hydrological models are directly leaned from data via machine learning (e.g. LSTM neural networks,[1]). Initially, no physical background and absolutely no interpretability was warranted, but neural hydrology has advanced, e.g., to copy the model structure from rainfall-runoff models, but then to machine-learn the fluxes between the lumped storage units. A downside of machine learning is typically its limited interpretability, and the limited ability of users to insert and re-use the existing domain knowledge.

Research goals:
We are convinced that neural hydrology can be advanced even further by moving it to the Bayesian framework. Not only would the Bayesian framework allow for a meaningful quantification of uncertainties. It would also allow to express and integrate soft and hard knowledge on hydrological processes. The latter would constrain the machine-learned models to be more efficient in data-limited situations. Also, it will make the learned models compatible with – and formulated on the level of – human understanding. From this, we expect deep insights, not just deep learning by some machine that can only predict without understanding. In other words: our research goal is to develop Bayesian Neural Hydrology as new cutting-edge approach that holds the potential to revolutionize our understanding of hydrological systems. Existing understanding can be extended by combining models, data and machine learning within a clear framework of scientific inference. This approach shall not only provide us with more precise modelling capabilities, but also offers a unique lens

through which we can uncover hidden patterns and dependencies within hydrological systems.

Methods to be used:
The work will explore system-specific architectures of deep learning, such as neural ordinary differential equations [2] or neural delay differential equations. These approaches express dynamic systems while admitting that the dependencies between the model's state variables and their temporal evolution (i.e. the right-hand sides of ordinary differential equations) still needs to be learned. The definition of state variables can be selected in analogy to existing conceptual hydrological rainfall-runoff models, such as HBV. But the storage terms and fluxes as function of current model states will be learned by neural networks. All these functions to be learned will be viewed as random functions parameterized by the weights and biases of the used neural networks (or by other forms of parametrization such as Gaussian Processes with inducing points).

In order to copy existing knowledge into this learning, Bayesian priors will be expressed, e.g. stating that evapotranspiration rises monotonically with soil increasing soil moisture, or that mass balances are approximately closed (up to the imprecision and incompleteness of model input data and model output data). Then, appropriate algorithms for Bayesian inference will be applied (or adapted if necessary), such as Markov-Chain Monte Carlo samplers that can work with gradient information (from the backpropagation in neural networks).

In order to demonstrate and test this framework, selected case studies will be implemented, and compared to suitable baseline models (e.g., standard HBV, or non-Bayesian neural hydrological models). This selection of methods is not final, but finding a most suitable combination is the very core of the proposed research topic.

Research Environment:
This research will be embedded into the Chair of Stochastic Simulation and Safety Research for Hydrosystems (LS^3) at the IWS, Faculty of Civil and Environmental Engineering. Depending on qualification of the candidate, a formal association of the project to the SC SimTech and the Cluster of Excellence in Data-Integrated Simulation Science is possible and advisable.

References:

[2] Kratzert, Frederik, et al. "Rainfall–runoff modelling using long short-term memory (LSTM) networks." *Hydrology and Earth System Sciences* 22.11 (2018): 6005-6022.
[1] Chen, R. T., Rubanova, Y., Bettencourt, J., & Duvenaud, D. K. (2018). Neural ordinary differential equations. *Advances in neural information processing systems*, *31*.

Prerequisites:
- MSc in hydrology, environmental sciences, hydrogeology, water management (or similar) or in data sciences, statistics, applied mathematics.
- Skills in programming (e.g. python, matlab, julia)
- Skills at scientific writing and presentation
- Ability to work independently and in a team
- Willingness to learn new concepts and methods
- Experience (e.g., coursework, thesis work) in hydrological modelling or in machine learning is desirable
- Willingness to contribute to the goals and culture of the research group