Deep Chaos ODE for Advanced Hydrological Modelling: Integrating Deep Learning and Polynomial Chaos into Data-Driven Hydrology

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Introduction / Background:

The majority of hydrological models rely heavily on the principle of mass balance, often represented through Ordinary Differential Equations (ODEs). These models encapsulate the conservation of mass within hydrological systems, ensuring that the inflows, outflows, and storage changes are accurately accounted for. This fundamental principle, coupled with assumed relationships between various components of the hydrological cycle (such as precipitation, evapotranspiration, runoff, and infiltration), forms the core of traditional hydrological modeling approaches. However, these assumed relationships, often coded as linear forms, do not offer the flexibility needed to capture the non-linear and dynamic interactions present in real-world hydrological systems.

Lately, there has also been the branch of neural hydrology, where hydrological models are directly learned from data via machine learning (e.g., LSTM neural networks, [1]). Initially, these models ignored all physical background knowledge and did not necessarily conserve mass, as they used black-box model structures far away from that of rainfall-runoff models. For these reasons, neural hydrology is often criticized by the conventional hydrological community. Alternatively, it is well known that Neural ODEs [2] are capable of representing dynamic systems that are coded in ODEs. They can encapsulate the complex temporal dependencies and dynamics inherent in hydrological systems, offering a promising direction for integrating machine learning with physical modeling. The potential of neural ODE models in hydrology has been discussed in [3].

However, long-term predictions using Neural ODEs may not be reliable for highly nonlinear systems due to the mathematical structure of the involved neural networks. Recent research in our department has demonstrated that arbitrary Polynomial Chaos ODEs (Chaos ODEs), which utilize the orthonormal decomposition of aPC [4], outperform Neural ODEs and as well Gaussian Process Emulator ODEs in terms of accurately capturing the complexity of dynamic processes. Moreover, further extension of Chaos ODEs to Deep Chaos ODEs by using Deep arbitrary Polynomial Chaos Neural Networks (DaPC NN, [5]) may offer significant additional advantages: By combining polynomial chaos expansion with neural network structures, the DaPC NN is more flexible in modelling higher-order interactions, while performing better in predictions outside the available training data.

Research Goals

Our primary goal is to improve the accuracy and prediction reliability of hydrological models. Hence, we propose methodological research to exploit Chaos ODEs for hydrological modelling, and to develop the concept of Deep Chaos ODE. By doing so, we seek to allow for the model flexibility that made neural hydrology so successful, while maintaining the fundamental mass balance relationships and while utilizing hydrological knowledge even in machine-learned models.

Additionally, following the recent advances of aPC, the framework could be extended to include Bayesian, sparse, and other features, providing a versatile and powerful toolset for various modeling scenarios. This new approach offers a unique perspective, enabling us to uncover hidden patterns and dependencies within hydrological systems, thereby advancing both theoretical understanding and practical applications.

Methods to be used

The research will explore system-specific architectures of deep learning, focusing on the formulation suggested in [2] and the structure in [5], resulting in the desired Deep Chaos ODEs. These methodologies will be employed to model dynamic systems, where the dependencies between state variables and their temporal evolution will be learned. State variables will be defined similarly to those in existing conceptual hydrological rainfall-runoff models, such as HBV. However, the storage terms and fluxes, as functions of the current model states, will be learned using Deep Chaos ODE, which inherently follows the principle of mass balance.

To validate and test the proposed framework, selected case studies will be implemented and compared against suitable baseline models, such as standard HBV and traditional neural hydrological models. The selection of methods and case studies will be tailored to identify the most effective combination for addressing the challenges posed by the proposed research. This methodological flexibility is crucial for optimizing the model's performance and ensuring its applicability to real-world hydrological systems. The Deep Chaos ODE approach aims to provide a more accurate and robust representation of the underlying processes, offering significant improvements over existing methods.

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:

[1]. Kratzert, F., Klotz, D., Brenner, C., Schulz, K., & Herrnegger, M. Rainfall–runoff modelling using long short-term memory (LSTM) networks. *Hydrology and Earth System Sciences*, 22(11), 6005-6022. (2018).
[2]. Chen, R. T., Rubanova, Y., Bettencourt, J., & Duvenaud, D. K. Neural ordinary differential equations. *Advances in Neural Information Processing Systems*, 31. (2018).
[3]. Höge, M., Scheidegger, A., Baity-Jesi, M., Albert, C., & Fenicia, F. Improving hydrologic models for predictions and process understanding using neural ODEs. *Hydrology and Earth System Sciences*, 26(19), 5085-5102. (2022).
[4]. Oladyshkin, S., & Nowak, W. Data-driven uncertainty quantification using the arbitrary polynomial chaos expansion. *Reliability Engineering & System Safety*, 106, 179-190. (2012).
[5]. Oladyshkin, S., Praditia, T., Kroeker, I., Mohammadi, F., Nowak, W., & Otte, S. The deep arbitrary polynomial chaos neural network or how Deep Artificial Neural Networks could benefit from data-driven homogeneous chaos theory. *Neural Networks*, 166, 85-104. (2023).

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
- Willingness to contribute to the goals and culture of the research group