Robust data-driven uncertainty quantification in water cycle extreme predictions

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Science Challenge

Climate experts apply global climate models to predict the future climate, informing decisions and adaptations. Uncertainty plays a fundamental role in this process (particularly for the water cycle simulation, the most relevant but least well-simulated). For many aspects of the water cycle there are disagreements for future climate projections, reflecting the significant uncertainty in model formulation. Also, the chaotic nature of climate dynamics, as well as indeterministic future projection emission scenarios, contribute to the uncertainty in climate predictions. New AI methods that are beginning to be adopted by the climate community have the power to improve predictions of water cycle extremes. The crucial question is how to capture all sources of uncertainty in a systematic way in order for the predictions from the AI models to be maximally leveraged by decision makers [1].

Rationale

AI is demonstrating its ability to improve climate predictions, especially in the case of water cycle extremes where traditional approaches using global climate models have fallen short [2]. However, improved predictive capability often comes with increased complexity of the AI model, which in turn makes quantifying uncertainties more challenging. AI approaches can improve water cycle extreme predictions, for example by incorporating observations to capture the relevant physics missing from the global climate models or by imposing various dynamical or physical constraints. Uncertainties are crucial for predictions to be meaningful in a decision making context, yet they are currently not systematically considered when deploying AI methods in climate science. While novel AI methods can improve predictive capabilities, limitations of the AI models must be understood, and a quantitative measure of the uncertainty in their prediction must be made.

Narrative

There are many ways in which uncertainty can be quantified in predictions from AI models. Here we identify one such approach using Bayesian neural networks (BNNs). BNNs offer a robust, fully probabilistic approach to address uncertainty in predictive AI models. Instead of yielding a deterministic prediction like most neural networks, the output from a BNN is a posterior predictive distribution, fully characterizing the uncertainty in the prediction. Their uncertainty estimates reflects how confident the model is in its predictions in various spatiotemporal regimes. For example, in data-sparse spatial locations, or when predicting in a regime (e.g. the

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future climate) where we have no data (temporal extrapolation), prediction uncertainties will be higher. BNNs have been used to predict river streamflow [3], and were also recently used to improve prediction accuracy and incorporate spatiotemporally varying uncertainty from a chemistry-climate model [4].

In the domain of climate research, more advanced AI methods are being developed for earth system prediction. Although these AI methods could have the power to achieve huge leaps forward in predictive capability, it is not clear yet how to incorporate these more complicated AI architectures and methods into a fully Bayesian framework. Here we outline some of the important components that need to be addressed.

1) AI models that have been transfer-learned with observations

Uncertainty arising from the model itself is often referred to as epistemic uncertainty. Epistemic uncertainty reduces with more data and so the more data we can provide the AI model with, the more we can reduce its epistemic uncertainty. It is crucial to quantify this uncertainty, especially in regimes where limited data is available, since uncertainties in those regimes may be too large to be trusted for decision making purposes. Observational data can be leveraged by AI models to improve their predictive capability by capturing missing physics from the climate models they were trained on [5]. But we must ensure that we 1) correctly handle the integration of multiple observational datasets and their associated uncertainties into the AI model, and 2) understand how the observational data uncertainty propagates to the overall uncertainty in the predictions made by the AI model. Prediction uncertainties will vary as a function of spatial location (e.g. predictions in regions that have more observational data should correspondingly have smaller prediction uncertainties.) BNNs offer a potential approach to integrate observational data in a systematic way.

2) Incorporation and propagation of aleatoric uncertainties in AI models

AI approaches can incorporate uncertainty arising from “noise”, so-called heteroscedastic aleatoric uncertainty, which in our case arises from unresolved atmospheric processes, but also includes other types of irreducible uncertainties. There are also homoscedastic aleatoric uncertainties that must be incorporated. An approach to addressing aleatoric uncertainties were recently addressed in [2] using approximate Bayesian methods. Leveraging BNNs could enable us to understand and account for the many different sources of aleatoric uncertainty in climate predictions.

3) Uncertainty aware physics-informed AI models

AI models can be made more predictive by enforcing various constraints and otherwise making them more “physics-informed”, however how these constraints or modifications then propagate to the uncertainty in the AI model prediction must be considered. How do we address uncertainties in these complex architectures? Can this be done in a fully Bayesian approach?

4) Climate change uncertainty for annual to decadal AI model predictions

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How to capture the uncertainty due to the non-stationary climate system when making predictions using AI models on timescales greater than seasonal. Can this signal be incorporated into a fully Bayesian framework?

The vision of this whitepaper is to have end-to-end, robust AI workflows with built in uncertainty quantification (UQ) that accounts for all sources of uncertainty. A critical need for robust UQ arises in the case of the often data-sparse water cycle extreme event prediction on near-term timescales (i.e seasonal to decadal) where a quantification of uncertainty is crucial for decision making. A robust Bayesian (probabilistic) framework can naturally account for and quantify different uncertainty sources, but this can be challenging for more complex architectures.

Currently, a key barrier to the implementation of fully Bayesian neural networks is their sheer computational expense arising from probability distributions over each node in the neural network. While approximate Bayesian methods exist, a challenge with approximate methods is that we don't know whether we can trust their posterior predictions, as the approximations are very often inaccurate and/or miscalibrated. Significant advances in computational abilities expected over the coming decade could enable the development of high-dimensional, fully-Bayesian, scalable, uncertainty-aware AI models that provide accurate and calibrated uncertainties on their predictions.

References

[1] Begoli, E., Bhattacharya, T. & Kusnezov, D. The need for uncertainty quantification in machine-assisted medical decision making. *Nat Mach Intell* **1,** 20–23 (2019). https://doi.org/10.1038/s42256-018-0004-1

[2] Pan, B., Anderson, G. J., Goncalves, A., Lucas, D. D., Bonfils, C. J., & Lee, J. (2020). Improving seasonal forecast using probabilistic deep learning. arXiv preprint arXiv:2010.14610.

[3] Zhang, X., F. Liang, R. Srinivasan, and M. Van Liew (2009), Estimating uncertainty of streamflow simulation using Bayesian neural networks, Water Resour. Res.,45, W02403, doi:10.1029/2008WR007030.

[4] Sengupta, U., et al. "Ensembling geophysical models with Bayesian Neural Networks." Advances in Neural Information Processing Systems (NeurIPS) 2020.

[5] Pan, B., Anderson, G. J., Lucas, D. D., Goncalves, A., Bonfils, C., Lee, J., & Tian, Y. (2020, December). Identifying and correcting climate projection biases using artificial intelligence. In AGU Fall Meeting 2020. AGU.