Physics Guided Machine Learning Methods for Hydrology

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Abstract

Streamflow prediction is one of the key challenges in the field of hydrology due to the complex interplay between multiple non-linear physical mechanisms behind streamflow generation. While physically-based models are rooted in rich understanding of the physical processes, a significant performance gap still remains which can be potentially addressed by leveraging the recent advances in machine learning. The goal of this work is to incorporate our understanding of physical processes and constraints in hydrology into machine learning algorithms, and thus bridge the performance gap while reducing the need for large amounts of data compared to traditional data-driven approaches. In particular, we propose an LSTM based deep learning architecture that is coupled with SWAT (Soil and Water Assessment Tool), an hydrology model that is in wide use today. The key idea of the approach is to model auxiliary intermediate processes that connect weather drivers to streamflow, rather than directly mapping runoff from weather variables which is what a deep learning architecture without physical insight will do. The efficacy of the approach is being analyzed on several small catchments located in the South Branch of the Root River Watershed in southeast Minnesota. Apart from observation data on runoff, the approach also leverages a 200-year synthetic dataset generated by SWAT to improve the performance while reducing convergence time. In the early phases of this study, simpler versions of the physics guided deep learning architectures are being used to achieve a system understanding of the coupling of physics and machine learning. As more complexity is introduced into the present implementation, the framework will be able to generalize to more sophisticated cases where spatial heterogeneity is present.

Introduction

Streamflow prediction is one of the key tasks for effective water resource management. A number of physics based models have been developed over the decade to model different aspects of the hydrological cycle using physical equations. A major drawback of these models is that they require extensive effort to calibrate for any given geography of interest (Arnold et al. 2012, Shen, Chen, and Chen 2012). Moreover, in some cases, we don’t have a complete understanding of the underlying physics which impacts their ability to predict the physical quantities (fluxes) of interest. In recent years, deep learning techniques have shown tremendous success in a number of computer vision and natural language processing applications. These techniques are increasing becoming popular in earth science applications including hydrology (Nearing et al. 2020, Shen et al. 2018, Boyraz and Engin 2018, Fan et al. 2020, Hu et al. 2020, Ni et al. 2020, Kratzert et al. 2018, Kratzert et al. 2019, Yang et al. 2020, Feng, Fang, and Shen 2019, Hu et al. 2018, Fu et al. 2020, Shen 2017). However, a vast majority of existing research in hydrology rely on off-the-shelf deep learning solutions to model streamflow using weather inputs. While, these solutions show promise, their efficacy is limited because of the dependence on large amounts of data for training. Furthermore, the assumptions made by these techniques are more suited for computer vision and natural language processing applications which limits their performance for hydrology applications.

In this paper, we propose a new physics guided machine learning framework that aims to address the aforementioned issues. Specifically, the proposed framework aims to incorporate physical principles in the network architecture and introduces modifications to existing components such as LSTM to incorporate assumptions that are applicable for hydrological processes.

The hydrological cycle has strong temporal structure and thus time aware deep learning techniques such as RNNs can be used to model different output variables using weather inputs. However, the mapping from weather inputs to variables of interest is very complex, and hence a traditional deep learning approach would required large amounts of data to train. For example, streamflow is connected to weather inputs through a number of inter-connected processes as shown in Figure 1. Moreover, the hydrological system has states that acts as a memory of the system. These states play a significant role in the response of different processes to weather inputs. For example, for a given amount of rainfall, the amount of surface run-off will depend on how much water is already present in the soil. In other words, if the soil is very wet before rainfall occurs, it will lead to more surface run-off compared to the scenario when the soil is dry. Simi-
larly, for any given temperature distribution over the day, the amount of water available through snow melt will depend on how much Snowpack is already present.

Hence, a framework that captures these relationships has the potential to perform better than directly mapping weather inputs to streamflow. In this paper, we propose a hierarchical deep learning architecture that explicitly models intermediate states and fluxes to incorporate the physical relationships between different hydrological processes. The efficacy of the proposed framework is evaluated using a 200 year simulation dataset created from SWAT model. Our preliminary analysis shows the promise of the proposed architecture and provide insights for future directions.

Methodology

Given a timeseries of weather inputs, our goal is to predict streamflow for each timestep. The most intuitive architecture would be a RNN with LSTM (or other variants) in a many-to-many prediction setup. In other words, use a single LSTM to directly map weather inputs to streamflow. We propose to add intermediate tasks that model fluxes (e.g. Evapotranspiration, surface run-off) and memory states (e.g. Soil Water and Snowpack) which are then fed as input (together with weather inputs) to the final task of streamflow prediction. Figure 3 shows the proposed hierarchical deep learning architecture. Each of the intermediate task uses its own LSTM to model the intermediate flux/state. This enables the architecture to model variables that change at different temporal scales using different LSTMs. Another benefit of this formulation is that we can impose physical constraints across these different tasks. For example, mass conservation budget constraint can be used to ensure that outputs from different tasks/modules adhere to water budget equation. Furthermore, memory states (Soil Water and Snowpack) behave very differently than the traditional notion of memory in natural language processing applications (e.g. gender of the subject). In case of Soil Water, it does not reset but gradually accumulates and dissipates. For example, Figure 2 shows the variation of Soil Water for a period of 10 years in the simulation dataset (described later). Similarly, for Snowpack, while it accumulates and dissipates during winter, it resets during summer. Hence, new innovations will be required to capture these states more effectively.

In this paper, we present the results and analysis of an initial version of this framework where we don’t introduce the physics based loss function, and only focus on Soil Water and Snowpack as intermediate variables to aid the estimation of streamflow from weather inputs. Furthermore, the intermediate tasks were learned separately instead of being learned simultaneously with the main task of streamflow prediction. For modeling Soil Water, we introduced a variation to improve the prediction performance. Specifically, instead of using just weather variables during training, we provided the value of Soil Water at the starting day of the sample. This initial constant value (replicated for other timesteps in the sequence to maintain input dimensions) avoids cold start of hidden and cell states and thus improve the temporal modeling of Soil Water changes. During prediction phase, we use the predicted value from the previous sample to act as the initial value for the next sample. Note that this is one of the ways in which physical concepts can be used to aid the machine learning algorithms. As part of future work, we aim to develop new LSTM architecture that is more suitable for modeling these memory states in physical systems.

Dataset

In this paper, we demonstrate the utility of the proposed architecture using a simulation dataset generated by the SWAT model. Specifically, we created 200 years of simulation from SWAT which takes 6 weather variables as input (precipitation, minimum day temperature, maximum day temperature, solar radiation, relative humidity, and wind speed) and gen-
erates different fluxes and states as output. The model was set up for a watershed in Southwest Minnesota as show in Figure 4. The weather variables were generated for this region using the weather generated module which is part of the SWAT model. The main goal of the paper is to show the utility of the proposed architecture in emulating the SWAT model. The evaluation of the proposed framework using real-world streamflow data will be pursued in future work.

Figure 4: The geographical location of the watershed.

**Experimental Setup**

To evaluate the framework, we use first 120 years of the simulation data for training and test it on the last 80 years. To ensure robust evaluation, we also evaluate different algorithms on first 80 years while being trained on the last 120 years. All three different LSTMs in our framework (one each for Snowpack, Soil Water and Streamflow) were chosen to have 180 days has sequence length and 28 hidden features. The learning rate was chosen to be 0.001. These hyper-parameters were chosen because based on their performance. We calculate two different error metrics to evaluate the proposed framework, namely RMSE (Root Mean Squared Error) and NSE (Nash Sutcliffe Efficiency). NSE is a widely used metric in the hydrology community. It is defined as follows:

\[
NSE = 1 - \frac{\sum_{t=1}^{T} |Q - \hat{Q}|}{\sum_{t=1}^{T} |Q - \bar{Q}|}
\]  

where \(Q\) is the reference streamflow, \(\hat{Q}\) is the predicted streamflow, and \(\bar{Q}\) is the mean of the reference streamflow. We also compare the LSTM architecture with CNN based architecture that has been shown to perform well for streamflow monitoring task (Duan, Ullrich, and Shu 2020) (henceforth referred to as TCNN).

**Results**

Table 1 shows the RMSE and NSE values for three different model configurations. First, the model that uses the CNN architecture (TCNN) performs poorly than the model with the traditional LSTM architecture (LSTM-No Physics) which suggests that for this dataset, LSTM is able to better capture the temporal dependencies to predict streamflow. Among the different LSTM architectures, the configuration where no physics is used (i.e. a single LSTM is used to directly learn the mapping between weather inputs and streamflow) gives the lowest performance (RMSE = 0.78 and NSE = 0.57), whereas the configuration that uses both Snowpack and Soil Water modules (which are fed as input to the streamflow module) performs much better (RMSE = 0.45 and NSE = 0.76). Hence, it is evident that modeling of intermediate states explicitly helps in reducing the complexity to model streamflow directly, and thus improving the performance. Figure 5 shows the timeseries of one of the years in the test data (year 128). As we can see, the proposed architecture was able to improve the performance on peak values and also reduced the spurious low streamflow values.

**Physical Interpretation of LSTM Features**

In order to gain physical insights, we compared Snowpack and Soil Water with hidden features from an LSTM that was used to directly learn the mapping between weather in-
Figure 5: An illustrative example of prediction performance of different architecture configurations. The black diamonds represent streamflow values simulated by SWAT which is being used as reference in our experiments to emulate to SWAT. The green circles represent predictions from a traditional LSTM based RNN architecture. The red line represents predictions from our initial version of the proposed architecture that models both Snowpack and Soil Water as intermediate tasks.

puts and streamflow. In other words, this architecture did not have any knowledge about Snowpack and Soil Water. To this end, we calculated correlation between timeseries of different hidden features and soil water (and Snowpack). The hidden features that showed very high correlation were selected for visualization. As we can see from Figure 6 and Figure 7 the LSTM is automatically learning features that correspond to the memory states, which suggests that even a traditional LSTM architecture has the ability to automatically capture these physical states. However, the agreement between the hidden features is not very high which suggests that it would require much more training data to achieve more accurate modelling of these hidden states without any explicit modeling. Another possible reason could be that a traditional LSTM might not be suitable to capture these physical states. For example, in the case of Snowpack, the decay pattern of the hidden feature is much more gradual than Snowpack. Hence, new variations of LSTM might be required to effectively capture these physical states.

Figure 6: Comparison of Soil Water and hidden feature 24 for year 150 in our simulation dataset. The red line represents the Soil Water value (right Y-axis) and the blue line represents the hidden feature (left Y-axis).

Figure 7: Comparison of Snowpack and hidden feature 4 for year 150 in our simulation dataset. The red line represents the Snowpack value (right Y-axis) and the blue line represents the hidden feature (left Y-axis).

dicting streamflow from weather variables. The key idea is to model intermediate states and fluxes of the hydrological cycle explicitly in the model architecture. The hierarchical approach allows different processes that change at different temporal scales to be learned using different LSTMs, and thus improve their modeling. The results on the simulation data using a preliminary version of the proposed architecture demonstrate the utility of the hierarchical approach. The visual analysis of hidden features from a basic architecture suggests that even a purely data driven architecture is automatically trying to learn the memory states, which confirms their importance for improving performance. For future work, we will evaluate different versions of the proposed architecture. For example, in the current version, individual tasks were trained separately. We aim to train all tasks simultaneously so that the errors in higher level task can inform the training of a low level task. In order to introduce mass conservation based loss function, other relevant tasks would be added such that all the components of the equation are available during training. Finally, the efficacy of the proposed framework will be tested on real world streamflow observations.

**Summary and Future Work**

In this paper, we presented a physics guided deep learning architecture to improve the performance on the task of predicting streamflow from weather variables. The key idea is to model intermediate states and fluxes of the hydrological cycle explicitly in the model architecture. The hierarchical approach allows different processes that change at different temporal scales to be learned using different LSTMs, and thus improve their modeling. The results on the simulation data using a preliminary version of the proposed architecture demonstrate the utility of the hierarchical approach. The visual analysis of hidden features from a basic architecture suggests that even a purely data driven architecture is automatically trying to learn the memory states, which confirms their importance for improving performance. For future work, we will evaluate different versions of the proposed architecture. For example, in the current version, individual tasks were trained separately. We aim to train all tasks simultaneously so that the errors in higher level task can inform the training of a low level task. In order to introduce mass conservation based loss function, other relevant tasks would be added such that all the components of the equation are available during training. Finally, the efficacy of the proposed framework will be tested on real world streamflow observations.

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