A Mass-Conserving-Perceptron for Machine-Learning-Based Modeling of Hydrologic Systems

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Abstract

Decades of effort have been devoted to building models of catchment-scale precipitation-runoff dynamics of hydrological systems. Recently, Wang & Gupta (2023) proposed the machine-learning-based physically-interpretable Mass-Conserving Perceptron (MCP) as a way to bridge the gap between physics-based and ML-based modeling approaches, thereby addressing the "*accuracy-interpretability*" dilemma incurred when applying only one of the modeling representations. The physically-interpretable MCP computational unit has been developed to exploit the inherent isomorphism between Gated Recurrent Neural Network (GRNN) structures and dynamical physical systems explicitly represent the mass/energy-conserving nature of hydrological process. We show how and why MCP-based modeling can more effectively facilitate hypothesis testing.

We develop a MCP unit/node/cell that represents a generic bucket model, where the "*input/bypass gate*" controls how much of the water input enters the cell and how much bypasses the cell on its way to the output, a newly introduced "*loss gate*" that accounts for external losses (such as evaporative) of water from the system, and impose a constraint on the "*output*", "*loss*" and "*forget/remember*" gating functions to ensure conservation of mass. An energy conservation constraint is applied to regularize the flux produced by the "*loss gate*". Further, the "*input bias-correction gate"* is introduced to account for precipitation under/over-catch. A "*mass-relaxation gate*" is incorporated to model the interception storage/loss effect.

Our methodology is demonstrated using the 40-year Leaf River catchment daily rainfall-runoff data set. Particular attention is devoted to exploiting ML technologies that ensure robust training to achieve good generalization performance. Overall, the MCP paves the way for exploiting inferential methods that use neural network architecture search, and the information theoretic notion of minimum description length to identify '*optimal'* model hypotheses.