A Mass-Conserving Perceptron for Modeling the Catchment-Scale Hydrologic System

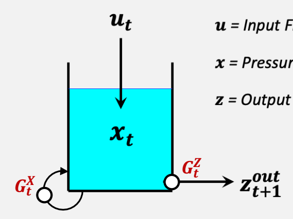
Yuan-Heng Wang & Hoshin V. Gupta

Department of Hydrology and Atmospheric Sciences, University of Arizona, Tucson, AZ, USA

Contact Info: yhwang0730@arizona.edu & hoshin@arizona.edu

1. Isomorphism Between GRN and PBM

Basic Unit of a Physical-Conceptual Model
(Mass Conserving Unit)



u = Input Flux

x = Pressure Head (State)

z = Output Flux

$0 \le K^Z(x_t|\theta) \le 1$ is a time-varying "Conductivity"

$G_t^X + G_t^Z = 1$ to enforce Mass Conservation

Flux Equation

$$z_{t+1}^{out} = f(x_t|\theta) = \left(\frac{f(x_t|\theta)}{x_t}\right) \circ x_t = K^Z(x_t|\theta) \circ x_t = G_t^Z \circ x_t$$

Conservation Equation

$$\frac{dx(t)}{dt} = u(t) - z(t)$$

$$x_{t+1} = x_t - z_{t+1}^{out} + u_t = x_t - G_t^Z \circ x_t + u_t = (1 - G_t^Z) \circ x_t + \mathrm{I} \circ u_t = G_t^X \circ x_t + G_t^U \circ u_t$$

Figure 1 (left):

Isomorphism between a generic Gated Recurrent Neuron and a simple physics-based two-parameter hydrological model unit.

$u[t]$: system input;
$z[t]$: system output;
$x[t]$: system internal state;
$K^Z(x_t|\theta)$: Conductivity Function;

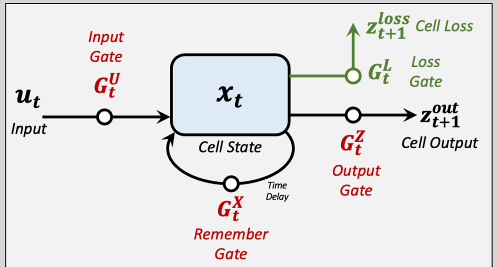
G_t^U: Input gate
G_t^Z: output gate;
G_t^X: Remember gate;

Figure 2 (right):

The proposed Physically-Interpretable mass-conserving perceptron node (MCPN) for modeling rainfall-runoff processes.

All the notations are kept the same as listed in Figure 1 and with a newly introduced loss gate that is denoted as G_t^L so as to properly account for the unobserved loss in the hydrological system (catchment).

2. Mass-Conserving Perceptron (MCP)



$$z_{t+1}^{out} = G_t^Z \circ x_t$$

$$z_{t+1}^{loss} = G_t^L \circ x_t$$

$$x_{t+1} = (1 - G_t^Z - G_t^L) \circ x_t + \mathrm{I} \circ u_t = G_t^X \circ x_t + G_t^U \circ u_t$$

To enforce Mass Conservation

$$G_t^X + G_t^Z + G_t^L = 1$$

3. Results for Leaf River: Single MCP Cases

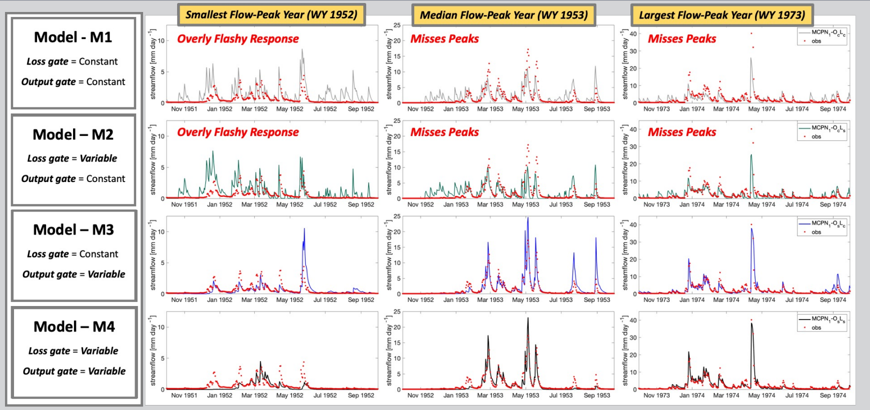


Figure 3: *Demonstration of the simulation results for different MCPN implementations applied to the Leaf River catchment. *Model-M1 is the case with constant conductivities at both the output and loss gates. Model-M2 is the case with a constant output gate and time variable (state-dependent) loss gate. Model-M3 is the case with a time variable (state-dependent) output gate and constant loss gate. Model-M4 is the case with both time variable output and loss gates. The time variable output/loss gates use internal cell state/potential evapotranspiration at the current time step as the only variables for learning the context-dependent gating responses.*

4. Results for Leaf River: Single MCPN Cases with PET constraint

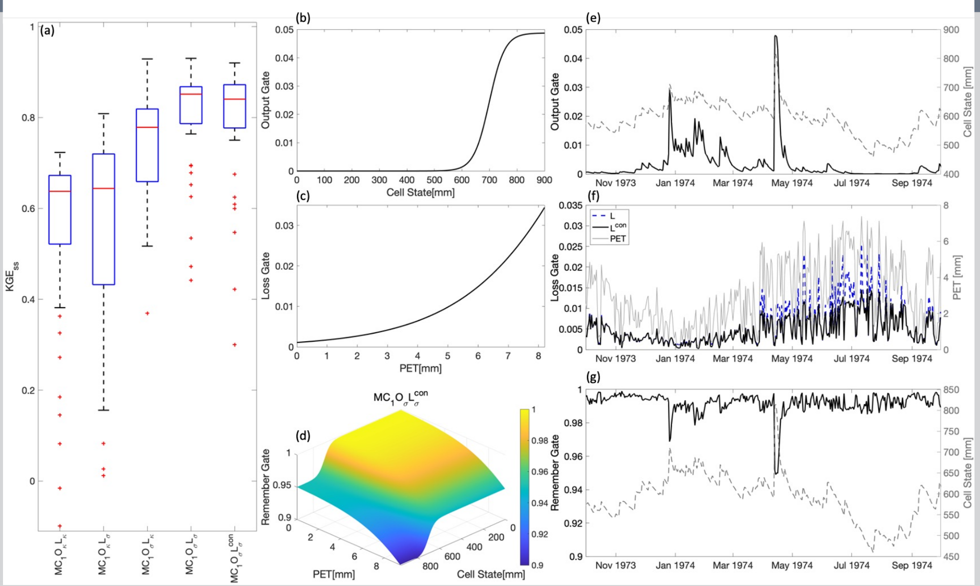


Figure 4 (left):

The results for a) Box and whisker plots of the distributions of annual KGE_{ss} values for various single-node (MC_1) architectures. The notation O and L represents the Output and Loss gates, respectively, and the subscripts "κ" and "σ" indicate Constant and Sigmoid (context-dependent) gating respectively. The notation L^{con} represents the case where the case where actual Loss L_t^1 is constrained to not exceed the value of the Potential Loss driver PL_t. The box corresponds to the 25th and 75th percentiles, the red line indicates the median value, the whiskers indicate the 5th and 95th percentiles, and the red crosses indicate the outlier years having relatively poor KGE_{ss} skill relative to other years in the distribution. Subplot (b) through (d) show the output, loss and remember gate, and subplot (e) to (g) presents the corresponding gate state for $MC_1 O_\sigma L_\sigma^{con}$ case

Figure 5 (right): The results of adding mass relaxation gate on the single node $\mathbf{MC_1\{O_\sigma L_\sigma^{con}\}}$ with a) Box and whisker plots of the distributions of annual KGE_{ss} values for single-node architectures with various mass relaxation including the cell-state-dependent $MC_1\{O_\sigma L_\sigma^{con} M_\sigma^R\}$, and cell-state-independent $MC_1\{O_\sigma L_\sigma^{con} M_I^R\}$as well as the case ($MC_1\{O_\sigma L_\sigma^{con} M_{\sigma r}^R\}$ & $MC_1\{O_\sigma L_\sigma^{con} M_{Ir}^R\}$) without constraining c_{1M_R} to be positive. Subplot (b) to (f) shows the analysis for $MC_1\{O_\sigma L_\sigma^{con} M_\sigma^R\}$ case with b) MR gate function, c) input precipitation & generated evaporative flux, d) internal cell state, e) flux generated through MR gate, and f) generated output streamflow.

References:

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Hochreiter, S. and Schmidhuber, J., 1997. Long short-term memory. *Neural computation*, *9*(8), pp.1735-1780.

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5. Results for Leaf River: Allowing Unobserved Mass Exchange with Environment