Physics Guided RNNs for Modeling Dynamical Systems: A Case Study in Simulating Lake Temperature Profiles

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This paper proposes a physics-guided recurrent neural network model (PGRNN) that combines RNNs and physics-based models to leverage their complementary strengths and improve the modeling of physical processes. Specifically, we show that a PGRNN can improve prediction accuracy over that of physical models, while generating outputs consistent with physical laws, and
https://arxiv.org/abs/1810.13075

Abstract

- Physics Guided Recurrent Neural Networks (PGRNN): combine RNNs and physics based models
- improved prediction accuracy over physical models
- generating outputs which are consistent with physical laws
- good generalizability
- pre-training: use simulated data since no or few observed data is available

Introduction

- challenges when directly applying black-box ML models to scientific problems
    1. require a lot of training data
    2. identify statistical relations between inputs and outputs which are not consistent with physical laws
    3. relationships can only be valid on present training data, generalization to unseen scenarios is bad
- PGRNN
    - serves as a general framework for modeling physical phenomena
    - by generalizing the loss function to include physical laws
    - application: lake water temperatures
    - two parallel recurrent structures
        - **standard RNN flow**
            - models temporal dependencies that better fit observed data

    - **energy flow**
        - regularize the temporal progression of the model in a physically consistent fashion
- **pre-training**
    - use simulated data generated by physics-based models
    - produces better initialized status for the learning model and requires less observed data to fine-tune model parameters
- flexible to incorporate additional physical constraints that are involved in specific applications

Problem Formulation

→ simulating the temperature of water at each depth d and on each date t

- set of input drivers X = {x_d,t}
    - physical variables governing the dynamics of lake temperature at every depth
    - including meteorological recordings at the surface such as: solar radiation, wind speed, air temperature, etc.
- predict water temperature Y = {y_d,t}

Preliminaries

General Lake Model (GLM)

- choice of physics-based model for lake temperature modeling
- includes a number of parameters: vertical mixing, wind sheltering, water clarity,…
- need to be calibrated specifically to the individual lake
- calibration method
    - run the model of combinations of parameter values and select the parameter set that minimizes model error

  → labor and computationally intensive

  → limited by simplifications and rigid formulations of parameters

Long-Short Term Memory Networks

- defines a transition relationship for hidden representations through an LSTM cell
- combines input features at each time step and the inherited information from previous time steps
- LSTM cell

- cell state c_t: is the memory and allows reserving information from the past
- candidate cell state ~c_t
- forget gate f_t: filter information from c_t-1
- input gate g_t: filter candidate cell state at t
- output gate o_t

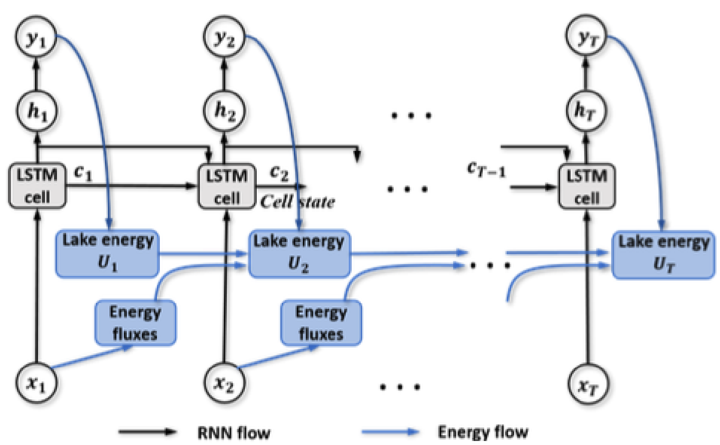
→ compute new cell state c_t and hidden representations h_t

- predicted temperature yhat_t

- Loss
  - apply LSTM for each depth separately

$$\mathcal{L}_{\text{RNN}} = \frac{1}{N_d T} \sum_t \sum_d (y_{d,t} - \hat{y}_{d,t})^2$$

  - N_d: total number of different depths
  - T: number of time steps
  - y_d,t: true observation



Methods

Energy conservation over time

- recurrent flow (standard RNN): captures data dependencies across time

  → implicitly encode useful information at each time step and pass it to the next time step

- modeling of energy flow: change of lake environment and predicted temperature conforms to the law of energy conservation

→ explicitly captures the key factor that leads to temperature change in dynamical systems

- PGRNN predicts what causes the temporal variation in dynamic systems
  - all lakes are different but they all follow the same universal law of energy conservation
  - better generalizability opportunity
- lake energy
  - incoming fluxes
    - terrestrial long-wave radiation
    - incoming short-wave radiation
  - outgoing fluxes
    - back radiation
    - sensible head fluxes
    - latent evaporative heat fluxes
  - the balance of these components results in a change on the thermal energy (U_t)
    - the lake will gain energy if the incoming heat fluxes are more than outgoing heat fluxes
    - the lake will lose energy if there are more outgoing heat fluxes than incoming heat fluxes
- combined loss

$$\mathcal{L} = \mathcal{L}_{\mathrm{RNN}} + \lambda_{\mathrm{EC}}\mathcal{L}_{\mathrm{EC}},$$
$$\mathcal{L}_{\mathrm{EC}} = \frac{1}{T_{\text{ice-free}}} \sum_{t \in \text{ice-free}} \mathrm{ReLU}(|\Delta U_t - \mathcal{F}| - \tau_{\mathrm{EC}})$$

  - F: sum of heat fluxes
  - tau_EC: threshold for the loss of energy conservation
    - physical processes can be affected by unknown factors like errors in the meterological data
  - ReLU: is adopted such that only the difference larger than the threshold is counted towards the penalty
  - Lambda_EC: controls the balance between the standard RNN loss and the energy conservation loss

Estimation of Heat Fluxes and Lake Thermal Energy

- see paper for details

- does not require any input of true labels, only based on input drivers and predicted temperature

Pre-training using Physical Simulations

- observed data is limited → training should be effective on small dataset
- pre-train PGRNN using the simulated data produced by GLM → physically consistent initialized model

Density-depth Constraint

- density of water monotonically increases with depth and thus can be used as constraints on the outputs of PGRNN
- loss including violation for density-depth relationship

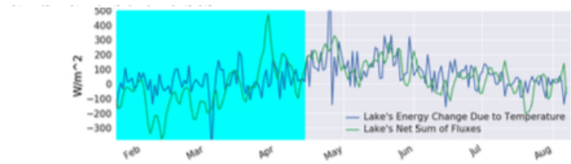
$$\Delta\rho_{d,t} = \rho_{d,t} - \rho_{d+1,t},$$
$$\mathcal{L}_{\mathrm{DC}} = \frac{1}{T(N_d - 1)} \sum_t \sum_d \mathrm{ReLU}(\Delta\rho_{d,t})$$

  - on any pair of consecutive depths d and d+1, if p_d,t is larger than p_d+1,t then this is considered as a violation
  - ReLU ensures that only pairs with inverse density values are counted towards the penalty

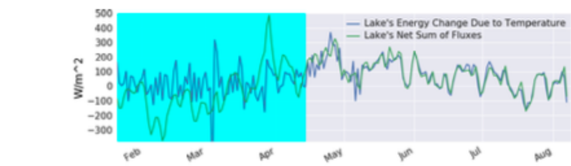
$$\mathcal{L} = \mathcal{L}_{\mathrm{RNN}} + \lambda_{\mathrm{EC}}\mathcal{L}_{\mathrm{EC}} + \lambda_{\mathrm{DC}}\mathcal{L}_{\mathrm{DC}}$$

Experiment

- see paper for details



(a)



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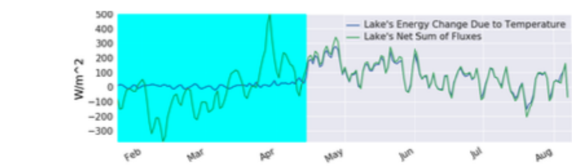

(c)

Figure 4: The sum of heat fluxes and the lake energy change genereated by (a) RNN, (b) PGRNN, and (c) the generic GLM, from January 21, 1989 to August 09, 1989. The blue part on the left indicates the frozen period (where we do not apply energy conservation).