Physics Guided Machine Learning: A New Paradigm for Modeling Dynamical Systems

Vipin Kumar

University of Minnesota

kumar001@umn.edu
www.cs.umn.edu/~kumar
Physics-based Models of Dynamical Systems

- Relationships b/w input & output variables governed by physics-based partial differential equations (PDEs)

Examples from Hydrology, Limnology, Fluid Dynamics, ...

<table>
<thead>
<tr>
<th>Input</th>
<th>Output</th>
<th>Parameters</th>
</tr>
</thead>
<tbody>
<tr>
<td>Rainfall, topography, land use, river width</td>
<td>River discharge</td>
<td>Soil conductivity, channel flow</td>
</tr>
<tr>
<td>Solar radiation, air temp, wind speed</td>
<td>Lake quality</td>
<td>Lake bathymetry, water clarity</td>
</tr>
<tr>
<td>Pressure, strain rate tensor, kinetic energy</td>
<td>Velocity field, lift, drag</td>
<td>Reynolds stress, flow geometry</td>
</tr>
</tbody>
</table>
Limitations of Physics-based Models

- Unknown parameters ($\theta$) need to be “calibrated”
  - Computationally Expensive
  - Easy to overfit: large number of parameter choices, small number of samples

For every grid cell

$\theta_1$, % vegetation
$\theta_2$, % soil porosity
$\theta_3$ to $\theta_n$

Errors
Limitations of Physics-based Models

- Unknown parameters ($\theta$) need to be “calibrated”
  - Computationally Expensive
  - Easy to overfit: large number of parameter choices, small number of samples

- Incomplete or missing physics ($F, G$)
  - Physics-based models often use approximate forms to meet “scale-accuracy” trade-off
  - Results in *inherent model bias*
“Black-box” Data Science Models

An alternative to modeling dynamical systems?

- Hugely successful in commercial applications
- But disappointing results in scientific domains!
  - Require lots of data
  - Unable to provide valuable physical insights

- Choice of model family not governed by physics

Support Vector Machine

Deep Learning

LSTM & Gates, Attention, ...

Choice of model family not governed by physics

$x_t$ → $c_t$ → $y_t$ → $DS$
Hybrid-Physics-Data (HPD) Modeling: A Paradigm Shift in Data Science

PHY \rightarrow Z_t \rightarrow DS \rightarrow y_t

PHYS \rightarrow F, G, \theta

DS \rightarrow SVMs \rightarrow ANNs \rightarrow ...

y_t

HPD Models

Overcome complementary weaknesses of both by combining PHY and DS in novel ways

Physics-based Models

Contain knowledge gaps in describing certain processes

Data Science Models

Require large number of representative samples

Hybrid-Physics-Data (HPD) Modeling: A Paradigm Shift in Data Science

Physics-based Models

- Contain knowledge gaps in describing certain processes

Data Science Models

- Require large number of representative samples

HPD Models

- Overcome complementary weaknesses of both by combining PHY and DS in novel ways

Illustrating Physics Guided Machine Learning (PGML) for Modeling Lake Water Temperature
Illustrating Physics Guided Machine Learning (PGML) for Modeling Lake Water Temperature

**Input Drivers:**
- Solar Radiation,
- Air Temperature,
- Relative Humidity,
- Wind Speed, ...

**PHY (GLM)**

**$Y_{PHY}$**

**Black-Box Model**
A Generic Framework for Hybrid-Physics-Data (HPD) Modeling:

1. If $Y_{\text{PHY}}$ is accurate (closely resembles $Y$):
   - $Y_{\text{pred}}$ learns to match $Y_{\text{PHY}}$
A Generic Framework for Hybrid-Physics-Data (HPD) Modeling:

1. If \( Y_{\text{PHY}} \) is accurate (closely resembles \( Y \)):
   - \( Y_{\text{pred}} \) learns to match \( Y_{\text{PHY}} \)

2. If \( Y_{\text{PHY}} \) has systematic biases
   - \( Y_{\text{pred}} \) learns the bias using drivers & \( Y_{\text{PHY}} \)
Training HPD Models

Labeled Data

Drivers + \( Y_{PHY} \)

\[ \begin{array}{c}
W_0 \\
W_1 \\
\vdots \\
W_N
\end{array} \]

\( Y_{pred} \)

\( Y_{true} \)

\text{input layer}

\text{hidden layer 1}

\text{hidden layer N}

\text{output layer}

Objective := Training Loss\( (Y_{true}, Y_{pred}) \) + \( \lambda \) R(\( W \))

Regularization (e.g., L1/L2-norm)

Challenges:

1. Labels \( (Y_{true}) \) are scarce
   – Difficult to train models with sufficient complexity
   – Standard methods for assessing generalization performance break down

2. \( Y_{pred} \) may violate \textbf{physical relationships} b/w \( Y \) and other variables
Can we learn from unlabeled data?

Labeled Data

Drivers + $Y_{PHY}$

Unlabeled Data

Drivers + $Y_{PHY}$

Diagram:

**Physical Constraint:**
Denser water is at higher depth

$Y_{pred}$

$Y_{true}, Y_{pred}$

Training Loss

$Y_{pred}$

Physics-based Loss ($Y_{pred}$)

---

Physics-guided Neural Network (PGNN)\textsuperscript{1}

Objective Function :=
Training Loss \((Y_{true}, Y_{pred}) + \lambda R(W) +\) 
Physics-based Loss \((Y_{pred})\)

Experimental Results

Lake Mille Lacs, MN

- **PHY**
- **NN**
- **PGNN**
- **PGNN0**
Experimental Results

Lake Mille Lacs, MN

Lake Mendota, Wisconsin

PGNN ensures Generalizability + Physical Consistency
Analyzing Physical Inconsistency

Lake Mille Lacs, MN

Test RMSE vs. Physical Inconsistency

02-Oct-2012

Obs
PHY

Depth vs. Density

Density

Lake Mille Lacs, MN

0.6
0.8
1
1.2
1.4
1.6
1.8
2

0 0.2 0.4 0.6 0.8 1

PHY

NN

PGNN

PGNN0

0.6 998.6 998.7 998.8 998.9 999 999.1 999.2 999.3 999.4
Analyzing Physical Inconsistency

Lake Mille Lacs, MN

Test RMSE vs. Physical Inconsistency

Density vs. Depth

02–Oct–2012
Analyzing Physical Inconsistency

Lake Mille Lacs, MN

Test RMSE

Physical Inconsistency

Depth

02–Oct–2012

Obs

PHY

NN

PGNN

PGNN0
Analyzing Physical Inconsistency

Lake Mille Lacs, MN

Test RMSE

Physical Inconsistency

Depth

Density

02–Oct–2012
Include **physical consistency** as another evaluation criterion, going beyond standard metrics for test error.
PGML using Recurrent Neural Networks (RNN)

- The performance on Lake Mendota and Lake Mille lacs
  - PHY: the state-of-the-art physics-based general lake model (GLM).
  - RNN: a pure RNN structure along the time.
  - PGRNN0: a hybrid recurrent model without using depth-density relationship

<table>
<thead>
<tr>
<th></th>
<th>Mendota</th>
<th>Mille lacs</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>RMSE</td>
<td>Phy-inconsistency</td>
</tr>
<tr>
<td>PHY</td>
<td>2.6544</td>
<td>0.0051</td>
</tr>
<tr>
<td>ANN</td>
<td>1.8830</td>
<td>0.1920</td>
</tr>
<tr>
<td>RNN</td>
<td>1.6042</td>
<td>0.2024</td>
</tr>
<tr>
<td>PGRNN0</td>
<td>1.6068</td>
<td>0.1798</td>
</tr>
<tr>
<td>PGRNN</td>
<td>1.4791</td>
<td>0.0732</td>
</tr>
</tbody>
</table>
Performance

- RMSE at different depths from 0-25m by 0.5m.

![GLM vs RNN-based models graph]
Performance

- RMSE at different depths from 0-25m by 0.5m.

GLM

RNN-based models

05-Apr-1993 to 22-Oct-1993
Monitoring Phosphorus Using PGML

- Monitoring phosphorus concentration at the surface of Lake Mendota.
- A mass balance-based physical model captures the exchange process.

\[
\begin{align*}
\frac{dP_{\text{epi}}}{dt} &= (1 - \alpha) \times \text{Load} + \text{Entrainment} - \text{Sedimentation} - \text{Export} \\
\frac{dP_{\text{hypo}}}{dt} &= \text{Recycling} - \text{Entrainment} \\
\frac{dP_{\text{sed}}}{dt} &= \alpha \times \text{Load} + \text{Sedimentation} - \text{Recycling} - \text{Burial}
\end{align*}
\]
Monitoring Phosphorus

- Monitoring phosphorus concentration at the surface of Lake Mendota.
- A mass balance-based physical model captures the exchange process.

5/9/1995 to 1/23/2015

- RMSE: PHY 0.0266  RNN 0.0243  PGRNN 0.0242
- Winter 0.0306 0.0285 0.0279
- Summer 0.0237 0.0205 0.0188
Incorporating Energy Conservation

- **Lake energy budget** - a balance between incoming energy fluxes and heat losses from the lake.
- A mismatch in losses and gains results in a temperature change.
- Thermal energy change \( \frac{dU_t}{dt} = R_{SW} (1 - \alpha_{SW}) + R_{LWin} (1 - \alpha_{LW}) - R_{LWout} - E - H \)

The predictions by our physics-aware model should conform to the energy conservation over time.
Incorporating Energy Conservation

- Prediction by PGRNN with and without energy conservation.
Incorporating Energy Conservation

• Prediction by PGRNN with and without energy conservation.

- Detection of Thermocline
  - **Thermocline** - the layer in which temperature changes more rapidly.
  - Thermocline is critical to study lake stratification and energy propagation in large water body.

<table>
<thead>
<tr>
<th>Without EC</th>
<th>With EC</th>
</tr>
</thead>
<tbody>
<tr>
<td>March 5th 2008 to March 4th 2009</td>
<td>March 5th 2008 to March 4th 2009</td>
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</table>

**RMSE**

Graph showing RMSE vs depth for different conditions with and without energy conservation.
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USGS

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UMN

Jared Willard
UMN
Modeling Dynamical Systems

- Use recurrent network structure to capture the dependencies among data.
  - Energy transfer
  - Volume change
  - Nutrient accumulation

Physics-guided Recurrent Neural Networks

- A hybrid model with outputs from physical model $Y_{PHY}$.

- Fill in the missing observations with $Y_{PHY}$.

- Additional constraints / hybrid structure along time dimension and depth dimension.
  - depth-density constraint, energy conservation, mass conservation.