Physics Informed Neural Network Surrogate for E3SM Land Model

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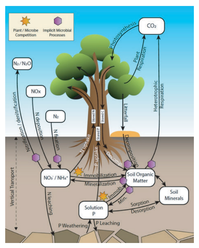
Application

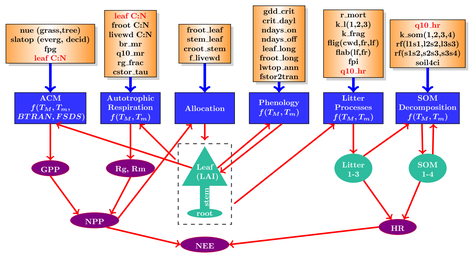
- Complex climate models typically include large number of input parameters and are computationally expensive.
- Need many evaluations of climate models for calibration and sensitivities
- Need accurate and efficient surrogates for UQ
- Use of Recurrent Neural Network with structure



- Use Recurrent Neural Networks (RNN) to tackle temporal dependencies.
- RNN has shown promising results for time series
- **Tree-LSTM RNN** allows for model hierarchy within ML framework
- Able to train daily and get more accurate surrogates compared to PCE and LSTM-RNN

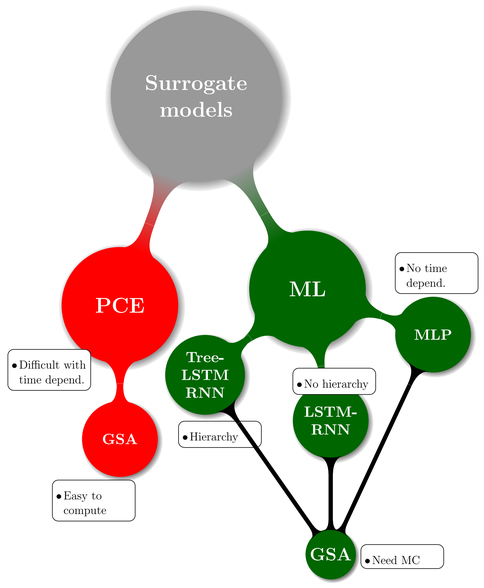
Hierarchical Structure of E3SM Land Model

- Land Model composed of **Daily Forcings** and **47D Stochastic Parameters**
- Each land cell has different *plant functional types*
- Daily Forcings:
  - Minimum/Maximum Temperature
  - Radiation



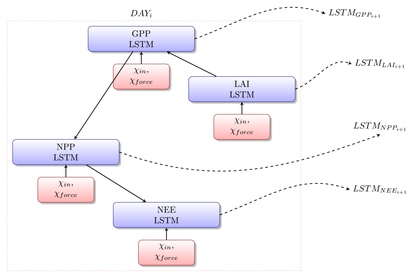
Hierarchical Structure of E3SM Land Model

Surrogate Construction Methods



Physics Informed Machine Learning Methodology

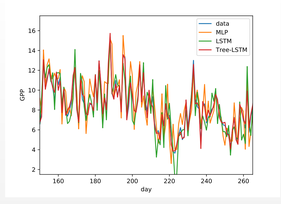
- Capture hierarchical nature of E3SM Land model
- Account for temporal aspects of QoIs
- Incorporate hierarchical structure into LSTM-Gate
- Flexibility to train on daily or monthly QoIs



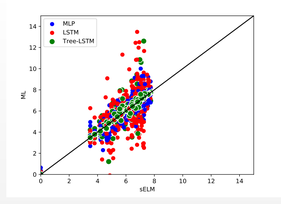
Tree-LSTM RNN example for E3SM Land Model

Surrogate Construction Results

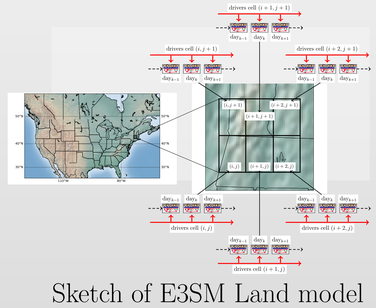
- Trained on simulations at University of Michigan Biological Station site
- Dropout Regularization
- 500 training samples
- 500 validation samples
- Varied Number of Layers: 1 or 2
- Neurons Per Layer: 150



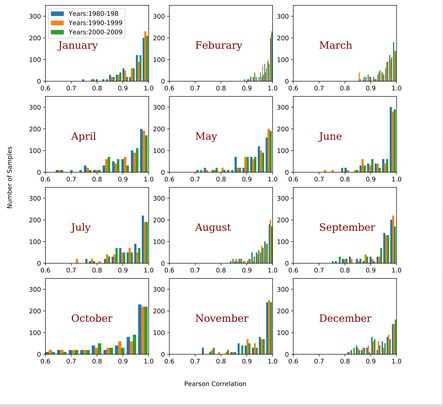
Daily training Snapshot



Parity Plot for March



Sketch of E3SM Land model (simplified version, python)



Pearson Correlation per month for Tree-LSTM

RMSE Error Summary

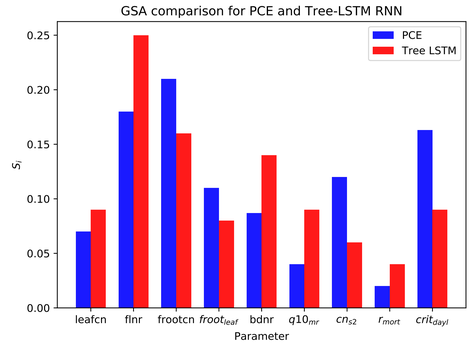
- PCE: Polynomial Chaos Expansion
- MLP: Multilayer (feed forward) Perceptron
- LSTM: Long Short-Term Memory recurrent NN
- Tree-LSTM: Hierarchical LSTM

Method	Train	Val
PCE	35%	46%
MLP	19%	32%
LSTM	14%	21%
Tree-LSTM	6%	9%

- Compared Average MSE for each surrogate
- Tree-LSTM is the most accurate compared to PCE, MLP and LSTM

GSA Results

- Global Sensitivity Analysis (GSA): computed Sobol indices for Tree-LSTM RNN and PCE
- Tree-LSTM relies on Monte-Carlo sampling, while PCE provides Sobol indices analytically



GSA comparison for PCE and Tree-LSTM

Summary

- Tree-LSTM is informed by the physics
- Tree-LSTM outperforms LSTM, MLP and PCE
- The advantage is stronger for daily data training

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