Physics-Informed Recurrent Neural Networks for Land Model Surrogate Construction

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Outline

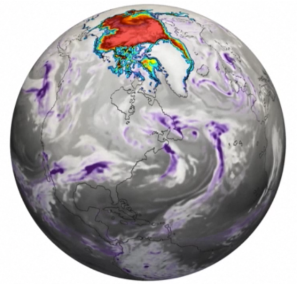
- Motivation
  - Energy Exascale Earth System Model (E3SM): Land component
- Need for Surrogate Models
  - Polynomial Chaos Surrogate
  - Neural Network Surrogates
    - Multilayer Perceptron
    - LSTM RNN
    - **Tree-LSTM RNN**
- Global Sensitivity Analysis (GSA)
- Preliminary Results

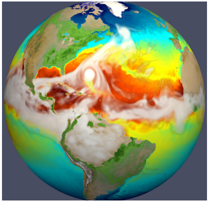
E3SM Model Overview

Energy Exascale Earth System Model (E3SM) is a coupled earth model

- US Department of Energy (DOE) sponsored Earth system model https://e3sm.org
- Ocean, Atmosphere, Sea ice and **Land** Components
- Computationally expensive to run the coupled mode (including ocean and atmosphere)
- Can only do a few global simulations of coupled E3SM models → hard to get training data

E3SM
Energy Exascale
Earth System Model

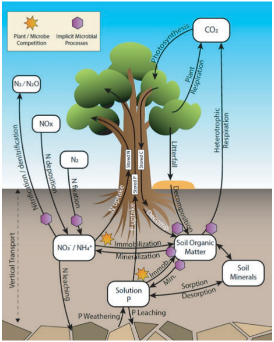


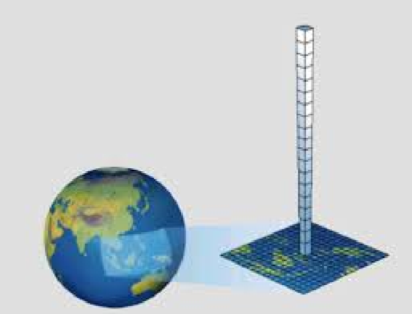


E3SM Land Model (ELM) Overview

Land model incorporates a set of biogeophysical processes:

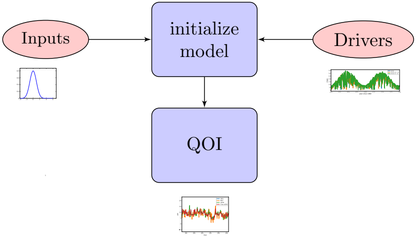
- Cheapest component, can run in single column mode
- Simplified python model available (sELM)
- Can evaluate model many times for various input parameters





ELM Produces Time Series given Input Parameters and Forcing Drivers

- Daily Forcings (site dependent)
  1. Min/Max Temperature
  2. Day of Year
  3. Solar radiation
  4. Water Availability
- Thirty year record (1980-2009) of forcings
- 47D Stochastic Space
- QOIs dependent on previous day's output



Surrogates are necessary for **expensive** computational models

- ... otherwise called supervised ML
- Surrogates are required for ensemble-intensive studies, such as
  - parameter estimation
  - uncertainty propagation
  - global sensitivity analysis
  - optimal experimental design

This talk

Investigating surrogate construction approaches for ELM to enable all of the above

Polynomial chaos (PC) surrogate for black-box $f(\lambda)$

- Represent QOIs as orthogonal expansion of random variables

$$f(\lambda) \approx f_c(\lambda(\xi)) = \sum_{\alpha \in \mathcal{I}} c_\alpha \Psi_\alpha(\xi)$$

- Germ: $\xi = (\xi_1, \xi_2, ..., \xi_d)$, e.g. uniform: $\lambda(\xi)$ is a linear scaling
- Multi-index $\alpha = \{\alpha_1, \ldots, \alpha_d\}$
- Orthogonal polynomials wrt $p(\xi)$, $\Psi_\alpha(\xi) = \prod_{i=1}^{d} \psi_{\alpha_i}(\xi_i)$
- Typical construction approach: regression to find PC modes c_α
- **Advantages of PC**
  - moment estimation, uncertainty propagation, global sensitivity analysis
- **Expensive model challenge**
  - Use Bayesian regression, helps to quantify lack of simulation data
- **High-d challenge** $d \gg 1$
  - Number of terms in expansion of order p and dimension d : $|\mathcal{I}| = \frac{(d+p)!}{d!p!}$
  - Use sparse regression
- We employ Bayesian compressed sensing (BCS): iterative algorithm for Bayesian sparse learning [Babacan, 2010; Sargsyan, 2014; Ricciuto, 2018]

'Free' Global Sensitivity Analysis with PC $f(\lambda(\xi)) \simeq \sum_{\alpha \in \mathcal{I}} c_\alpha \Psi_\alpha(\xi)$

- Main effect sensitivity indices

$$S_i = \frac{Var[\mathbb{E}(f(\lambda|\lambda_i)]}{Var[f(\lambda)]} = \frac{\sum_{\alpha \in \mathcal{I}_i} c_\alpha^2 ||\Psi_\alpha||^2}{\sum_{\alpha \in \mathcal{I} \setminus \{0\}} c_\alpha^2 ||\Psi_\alpha||^2}$$

  - $\mathcal{I}_i$ is the set of bases with only ξ_i involved
  - S_i is the uncertainty contribution that is due to i-th parameter only

- Total effect sensitivity indices

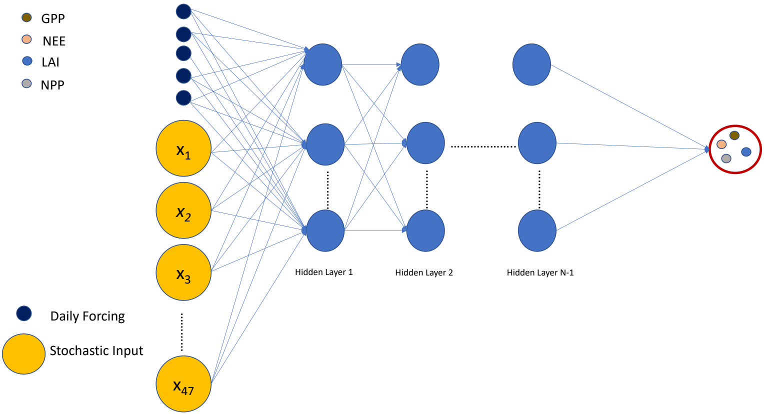
$$T_i = 1 - \frac{Var[\mathbb{E}(f(\lambda|\lambda_{-i})]}{Var[f(\lambda)]} = \frac{\sum_{\alpha \in \mathcal{I}_i^T} c_\alpha^2 ||\Psi_\alpha||^2}{\sum_{\alpha \in \mathcal{I} \setminus \{0\}} c_\alpha^2 ||\Psi_\alpha||^2}$$

  - $\mathcal{I}_i^T$ is the set of bases with ξ_i involved, including all its interactions.
  - T_i is the total uncertainty contribution due to i-th parameter

[Sudret, 2008; Crestaux, 2009; Sargsyan, 2017]

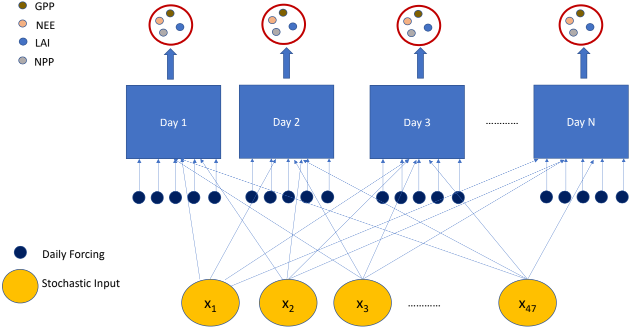
Surrogate Modeling: MLP Approach

- Benign feed-forward network
- Does not account for temporal aspect of model
  - Cannot propagate information of QOIs day to day (or month to month)
- Model dealt with as a black box



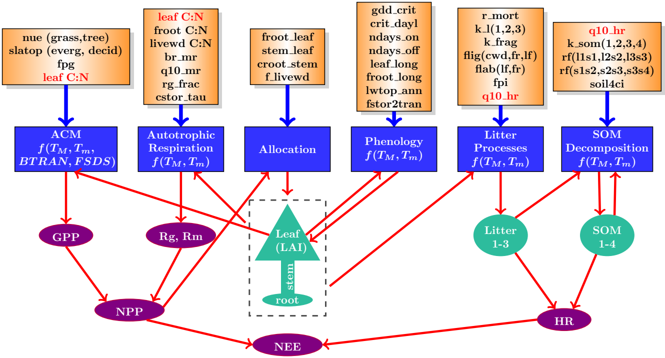
Surrogate Modeling: LSTM-RNN

- Vanilla LSTM Recurrent NN architecture
- Accounts for temporal aspect of model
- Model dealt with as a black box



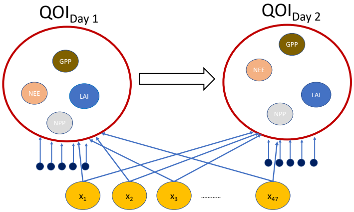
Graph Structure of ELM Land Model

Looking under the hood helps build physics-informed architecture

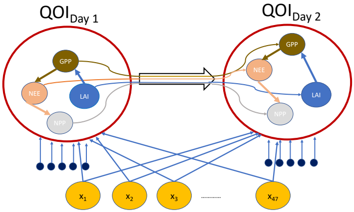


Surrogate Modeling: Tree LSTM RNN

- Retain similar structure to Gated RNN ([Tai, 2015])
- Incorporate physical connections into LSTM
- Each QOI has a LSTM gate



LSTM RNN
Vanilla



Tree-LSTM RNN
Physics-informed

For NN surrogates, GSA can be carried out with Monte-Carlo

- Mean estimate: $E[f(\lambda)] \approx \frac{1}{N}\sum_{n=1}^{N} f(\lambda^{(n)})$
- Variance estimate: $Var[f(\lambda)] \approx \frac{1}{N}\sum_{n=1}^{N} f(\lambda^{(n)})^2 - E[f(\lambda)]^2$
- Main sensitivity:

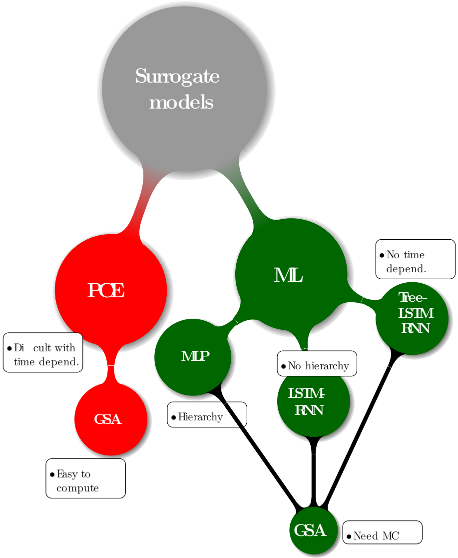
$$S_i = \frac{Var[\mathbb{E}(f(\lambda|\lambda_i)]}{Var[f(\lambda)]} \approx \frac{1}{Var[f(\lambda)]}\left(\frac{1}{N}\sum_{n=1}^{N} f(\lambda^{(n)}) f(\lambda_{-i}^{\prime(n)} \cup \lambda_i^{(n)}) - E[f(\lambda)]^2\right),$$

  where $\lambda_{-i}^{\prime(n)} \cup \lambda_i^{(n)}$ is a single-column swap sample given two sampling schemes $\lambda^{(n)}$ and $\lambda^{\prime(n)}$

- ... similar estimators for total sensitivity
- Inherits all the challenges of Monte-Carlo

[Jansen, 1999; Sobol, 2001; Saltelli, 2002]

Overview of Surrogate Models Implemented



Summary of Case Study

Training Details

- Generate samples from sELM model: 30 years (1980-2009)
- Each training set (time history) has $10,950$ data points (daily)
- Simulation at University of Michigan Biological Station site
- 500 training samples, 500 validation samples

NN Details

- Train on daily QoIs
- 500 Epochs of SGD
- 2 layers, 150 neurons
- L_2 loss, dropout regularization

MLP

- No time dynamics
- No physics

LSTM

- Time dynamics
- No physics

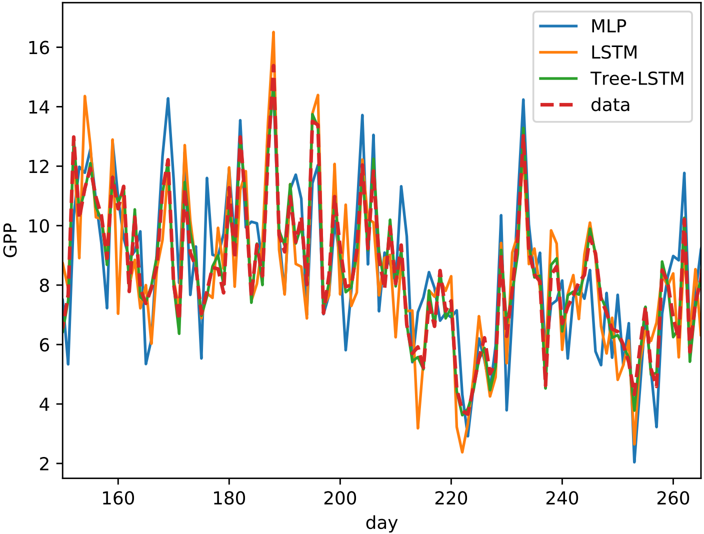
Tree-LSTM

- Time dynamics
- Physics

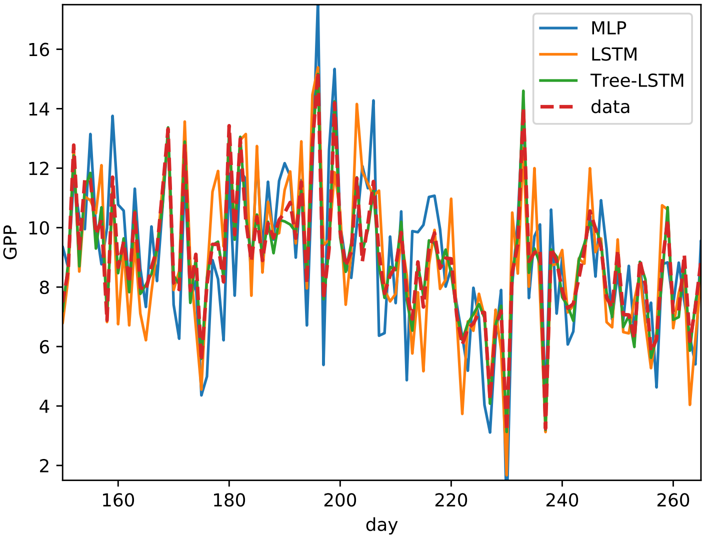
PC Details

- Hard to train on daily averages (noisy)
- Train on monthly averages
- Use Bayesian compressive sensing to compute coefficients
- Build surrogate for each average month, i.e. 30×12 surrogates

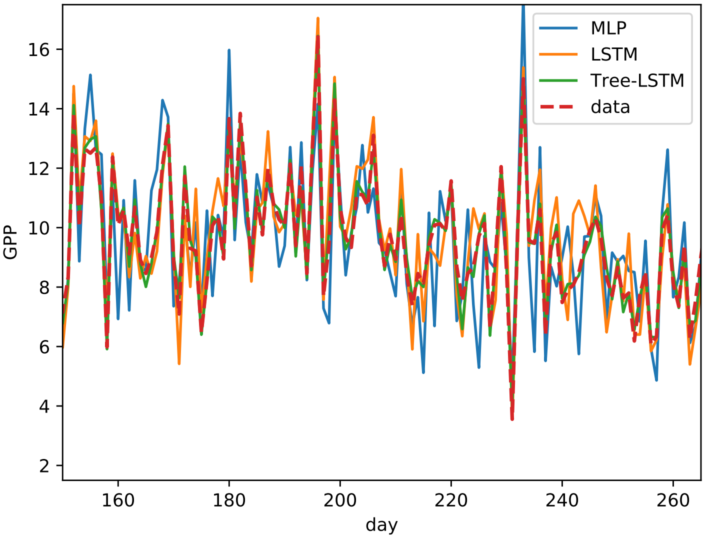
Snapshot of training sample 1



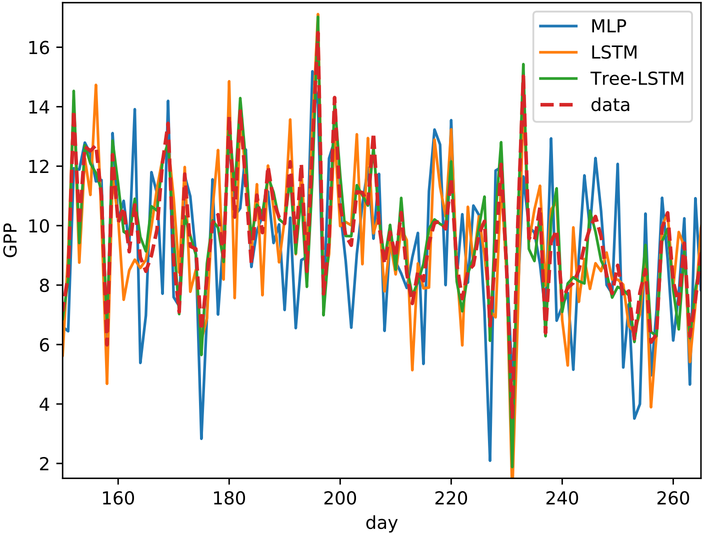
Snapshot of GPP training sample 2



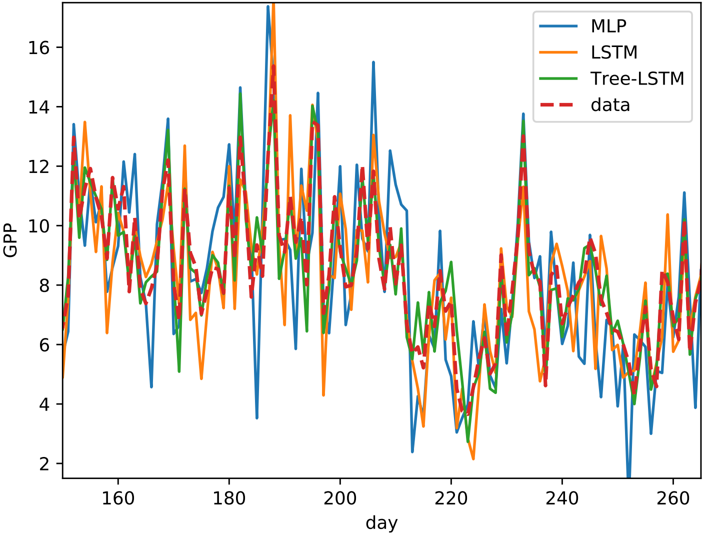
Snapshot of GPP training sample 3



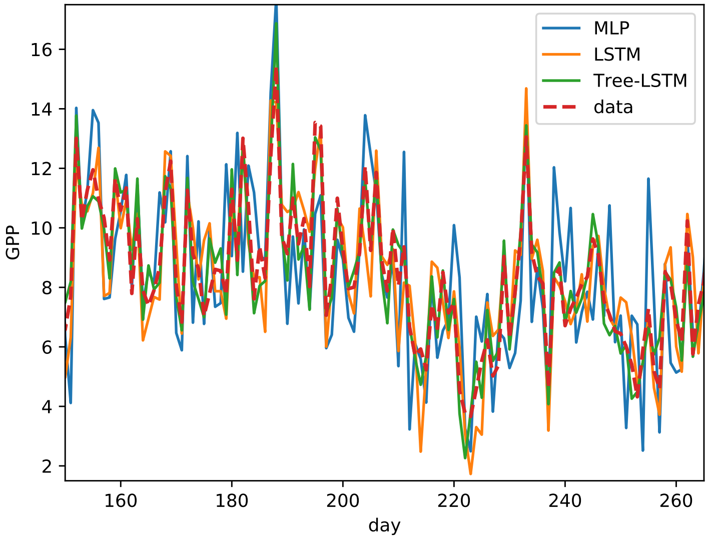
Snapshot of GPP validation sample 1



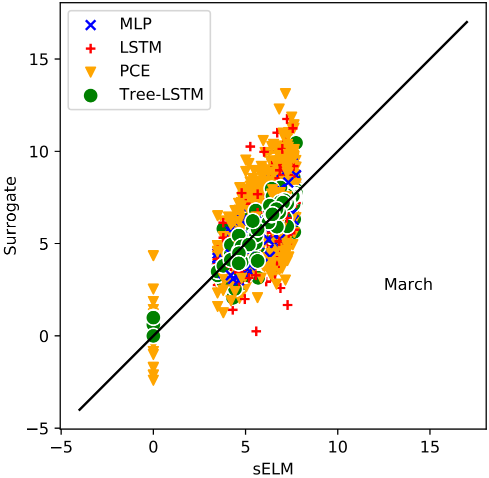
Snapshot of GPP validation sample 2



Snapshot of GPP validation sample 3



GPP Parity Plot comparisons for various months



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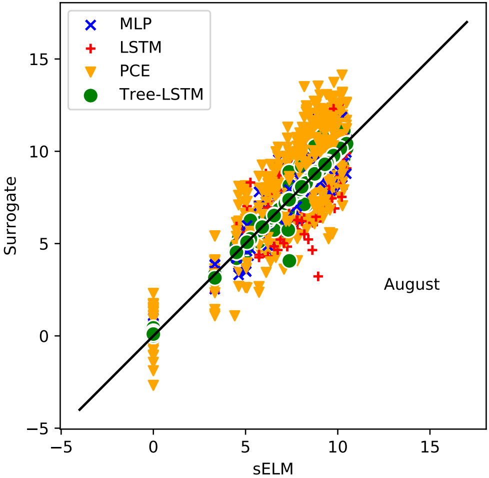
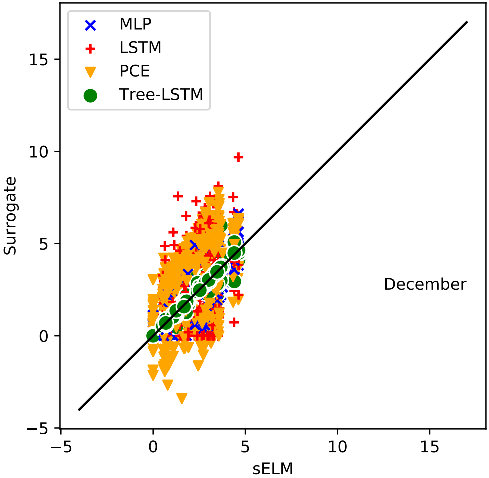
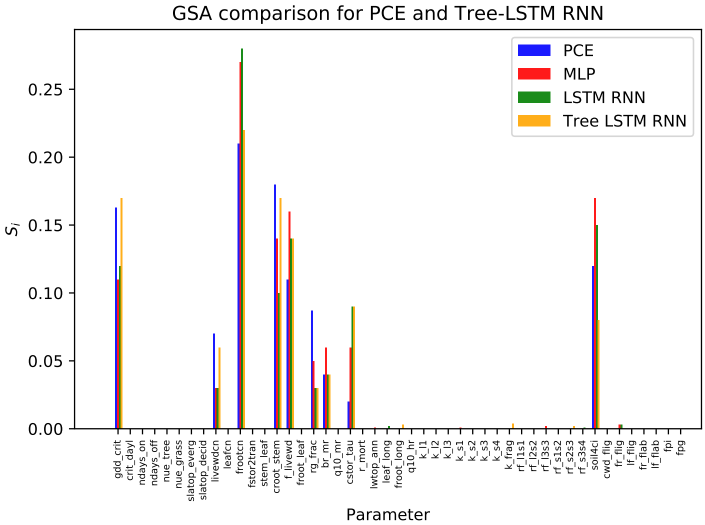


GPP Parity Plot comparisons for various months



Global Sensitivity Analysis Comparison



Tree RNN more accurate than PCE and traditional ML methods

- Computed Mean RMS for each Surrogate

Method	**Train (Daily/Month)**	**Val (Daily/Month)**
PCE	$(N/A)/35\%$	$(N/A)/46\%$
MLP	$19/14\%$	$32/20\%$
LSTM	$14/10\%$	$21/16\%$
Tree-LSTM	$6/2\%$	$9/5\%$

- Tree-LSTM outperforms PCE, MLP and LSTM-RNN

Conclusions and Future Work **Thank you!**

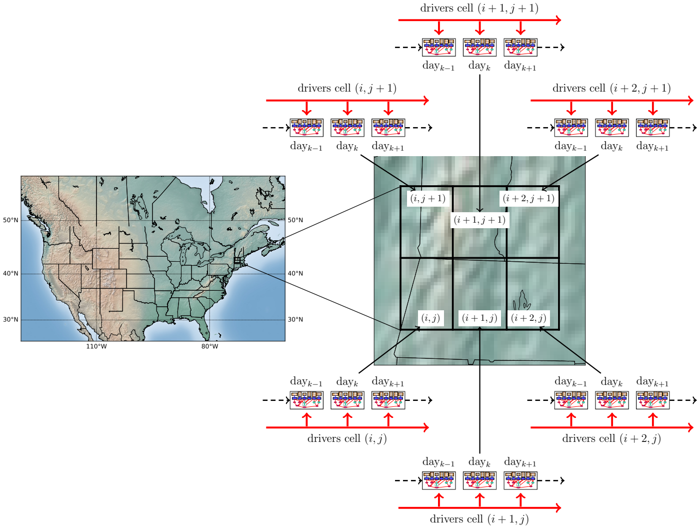
Conclusions

- Physics-based NN architecture outperforms traditional NN methods and PCE
- Using Tree-Structure LSTM gate can train on the noisy daily data
- Qualitatively similar sensitivity results compared to PCE

Future Work

- Employ the surrogate for calibration and optimal experimental design
- Analyze multiple sites
- Spatio-temporal physics-based RNN
- Incorporate low-rank tensor structure into RNN

ELM Simulation Details



Global Sensitivity Analysis

- $Y = f(X_1, X_2, X_3, ..., X_N)$
- Total Variance decomposition (normalized)

$$Var(Y) = E[Var(Y|X)] + Var(E[Y|X])$$

- If X_i are independent: $V(Y) = \sum_{i=1}^{N} V_i + \sum_{1 \leq i \leq j \leq N} V_{ij} + .. + V_{1,..,p}$
- Use Sobol indices $\rightarrow$ QOI's variance to be decomposed based on variances of inputs

Sobol Indices

$S_i = \frac{\mathrm{Var}_{X_i}(E(Y|X_i))}{Var(Y)}$ First Sobol Indices

$S_{ij} = \frac{Var_{ij}}{Var(Y)}$ Second Order Sobol Indices

Method

- PCE allows for analytical computation of S_i
- ML needs Monte Carlo Integration to compute S_i

Surrogate Modeling:Tree LSTM

LSTM Equations

$$
\begin{aligned}
f_{jk} &= \sigma(W_f x_j + \sum U_{kl} h_{jl}) \\
i_j &= \sigma(W_i x_j + \sum U_l h_{jl}) \\
o_j &= \sigma(W_o x_j + U_l h_{jl}) \\
u_j &= \tanh(W_c x_j + U_l h_{jl}) \\
c_j &= \sum f_{jl} \odot c_{jl} + i_j \odot u_j \\
h_j &= \sigma_j \odot \tanh(c_j)
\end{aligned}
\tag{1}
$$