Dimensionality Reduction and Physics-Informed Neural Networks for Climate Land Models

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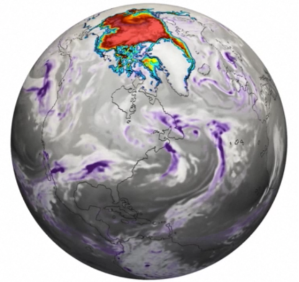
Outline

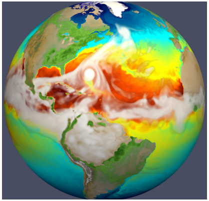
- Motivation
  - Energy Exascale Earth System Model (E3SM): Land component
- Need for Surrogate Models
  - Polynomial Chaos Surrogate
  - **Karhunen-Loève expansions for field quantities**
  - Neural Network Surrogates
    - Multilayer Perceptron (MLP)
    - Long short term memory (LSTM)
    - **Physics-based LSTM**
- Global Sensitivity Analysis (GSA)
- Preliminary Results

E3SM Model Overview

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

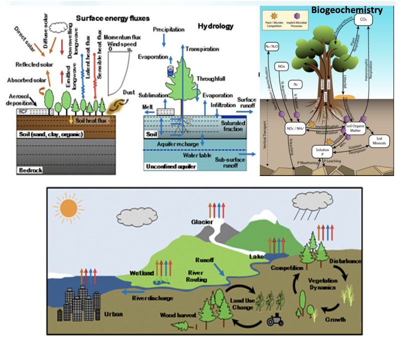
- US Department of Energy (DOE) sponsored Earth system model https://e3sm.org
- Ocean, Atmosphere, Sea ice and **Land** Components
- Computationally expensive to run the coupled mode (including ocean and atmosphere)
- Can only do a few global simulations of coupled E3SM models $\rightarrow$ hard to get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

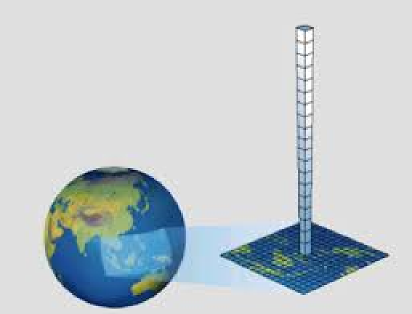




Land model incorporates a set of biogeophysical processes:

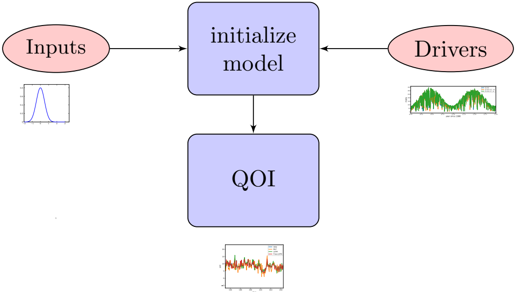
- Cheapest component, can run in single column mode
- Simplified python model available (sELM)
- Can evaluate model many times for various input parameters

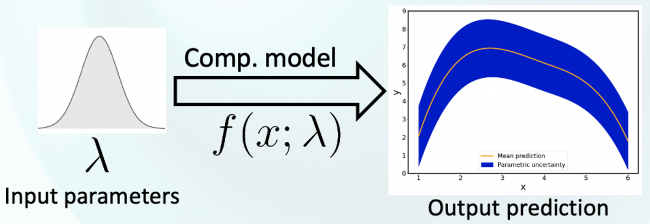




ELM Produces Time Series given Input Parameters and Forcing Drivers

- $\mathcal{O}(10) - \mathcal{O}(100)$ uncertain inputs
- Daily Forcings/Drivers
  1. Min/Max Temperature
  2. Day of Year
  3. Solar radiation
  4. Water Availability





Surrogates are necessary for **expensive** computational models

- ... otherwise called supervised ML, metamodel, emulator, proxy, response surface.

$$f(x; \lambda) \approx f_s(x; \lambda)$$

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

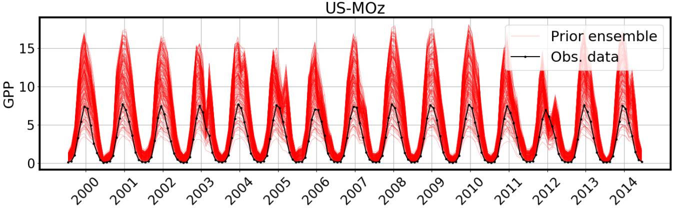
This talk

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

Curse of dimensionality hits twice

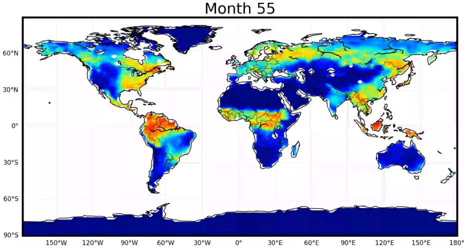
$$f(x; \boldsymbol{\lambda}) \approx f_s(x; \boldsymbol{\lambda})$$

- Input : large number of input parameters



$$f(\boldsymbol{x}; \lambda) \approx f_s(\boldsymbol{x}; \lambda)$$

- Output : spatio-temporal resolution



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

- Represent QOIs as orthogonal expansion of random variables

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

- Germ: $\xi = (\xi_1, \xi_2, ..., \xi_d)$, e.g. uniform: $\boldsymbol{\lambda}(\boldsymbol{\xi})$ is a linear scaling
- Multi-index $\alpha = \{\alpha_1, \ldots, \alpha_d\}$
- Orthogonal polynomials wrt $p(\boldsymbol{\xi})$, $\Psi_\alpha(\boldsymbol{\xi}) = \prod_{i=1}^d \psi_{\alpha_i}(\xi_i)$
- Typical construction approach: regression to find PC modes c_α
- **Advantages of PC**
  - moment estimation, uncertainty propagation, global sensitivity
- **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

$$f(\boldsymbol{\lambda}(\boldsymbol{\xi})) \simeq \sum_{\alpha\in\mathcal{I}} c_\alpha \Psi_\alpha(\boldsymbol{\xi})$$

- Main effect sensitivity indices

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

  - $\mathcal{I}_i$ 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

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

  - $\mathcal{I}_i^T$ 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]

Spatio-temporal surrogate model via Karhunen-Loève expansions

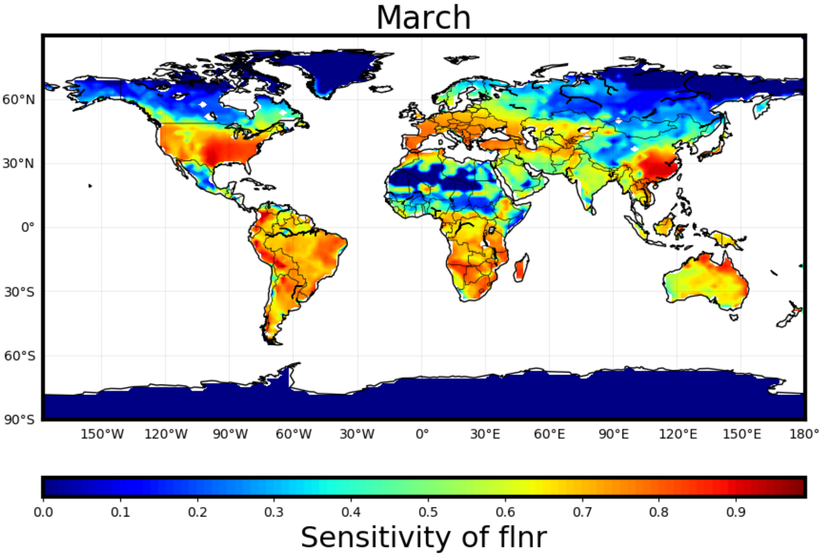
- 3183 active land cells over 180 months is $> 500,000$ outputs
- Karhunen-Loève expansions help reduce dimensionality due to strong spatio-temporal correlations

$$f(x;\lambda) = \bar{f}(\lambda) + \sum_{j=1}^{J} f_j(\lambda)\sqrt{\mu_j}\phi_j(x)$$

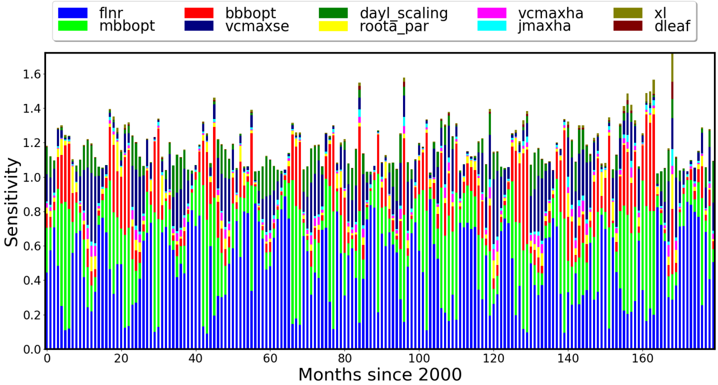
- Instead of 500,000 surrogates, we build about $J = 2,000$ surrogates, one for each coefficient $f_j(\lambda)$

$$\begin{aligned} f(x;\lambda) &= \sum_{j=0}^{J}\sum_{k=0}^{K} f_{jk}\Psi_k(\lambda)\sqrt{\mu_j}\phi_j(x) \\ &= \sum_{k=0}^{K}\left(\sum_{j=0}^{J} f_{jk}\sqrt{\mu_j}\phi_j(x)\right)\Psi_k(\lambda) \end{aligned}$$

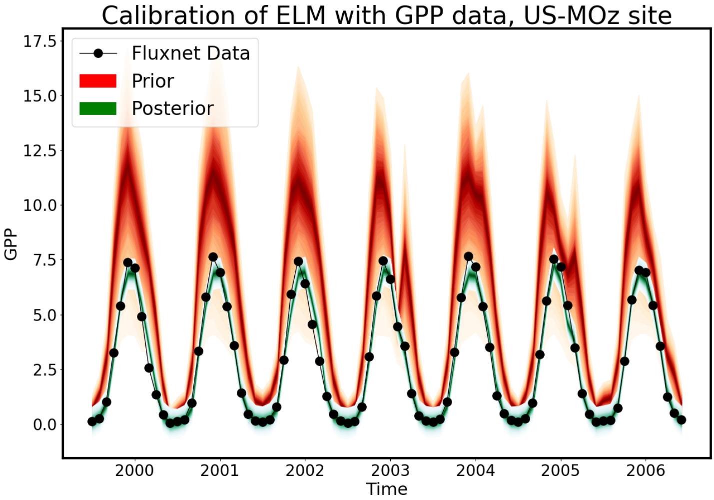
Spatially resolved GSA



Time-resolved GSA

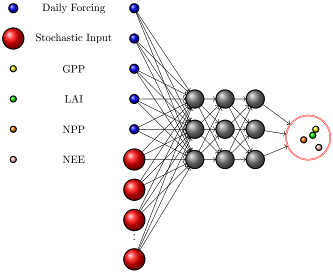


Bayesian inference and prediction with surrogate



Transitioning from UQ technologies to ML

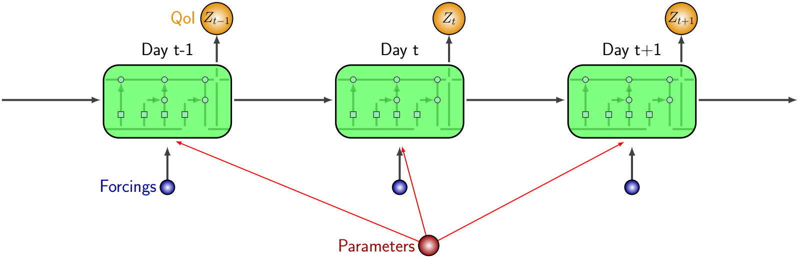
- Polynomial chaos requires smooth QoIs
- Exploring transient behavior and daily dynamics requires more accurate surrogates
- Benign MLP, feed-forward network did not do too well



- Does not account for temporal aspect of model
- Cannot propagate information of QOIs day to day (or month to month)

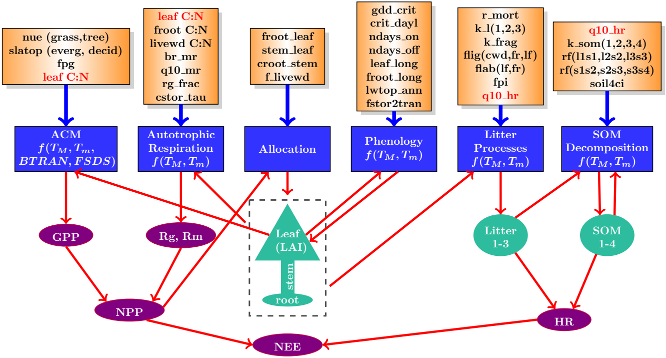
Long short term memory (LSTM) accounts for temporal evolution

- Vanilla LSTM Recurrent NN architecture
- One network per QoI
- Much better than PC, better than MLP

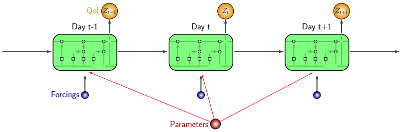


Graph Structure of ELM Land Model

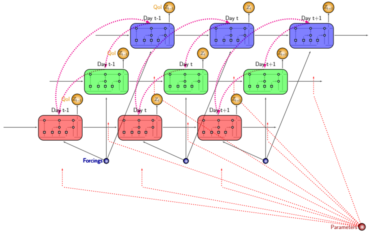
Looking under the hood helps build physics-informed architecture



Physics-driven architecture incorporates known connections into LSTM

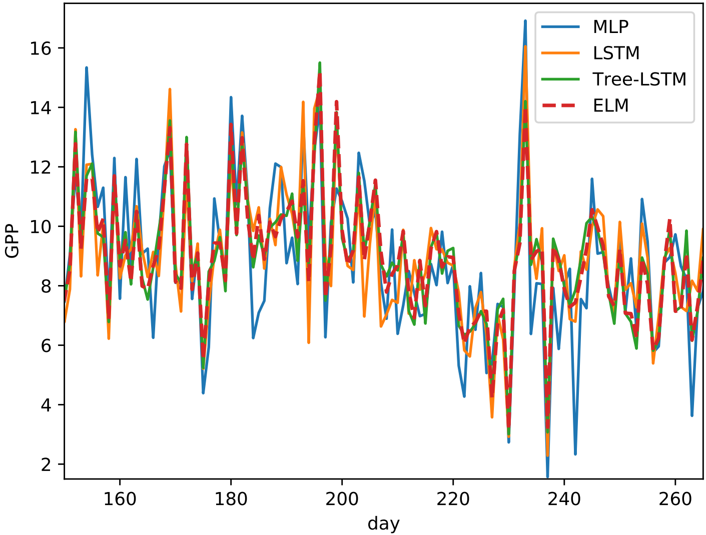


Vanilla LSTM



Physics-informed LSTM

NN fits to ELM



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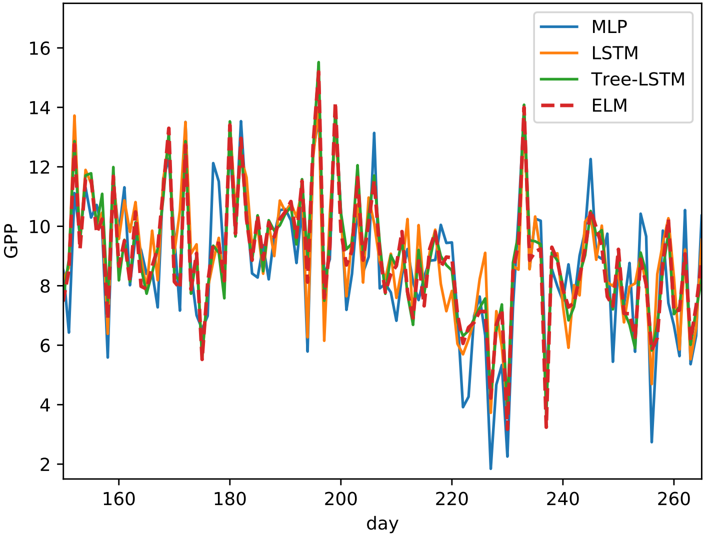

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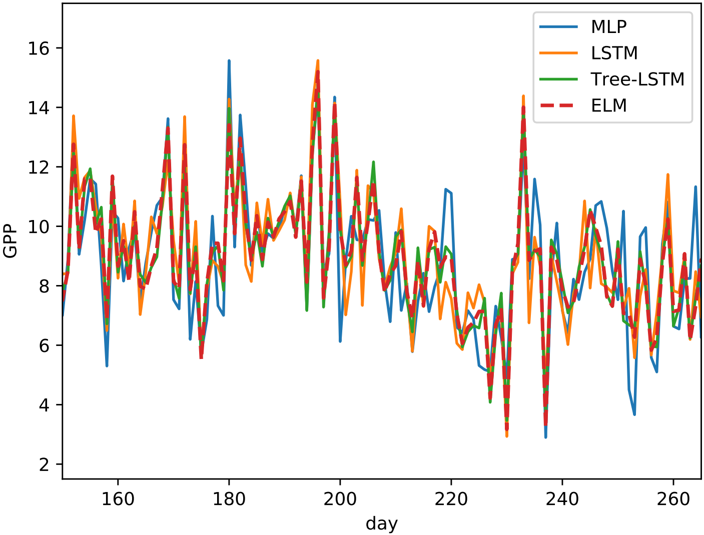

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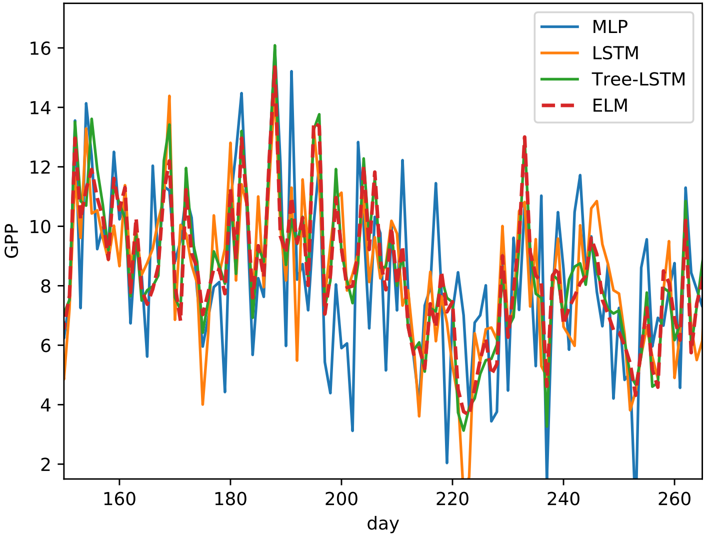

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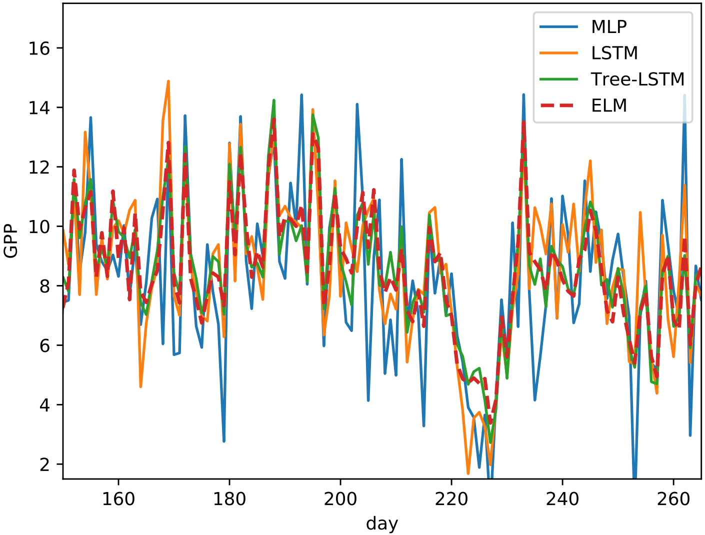

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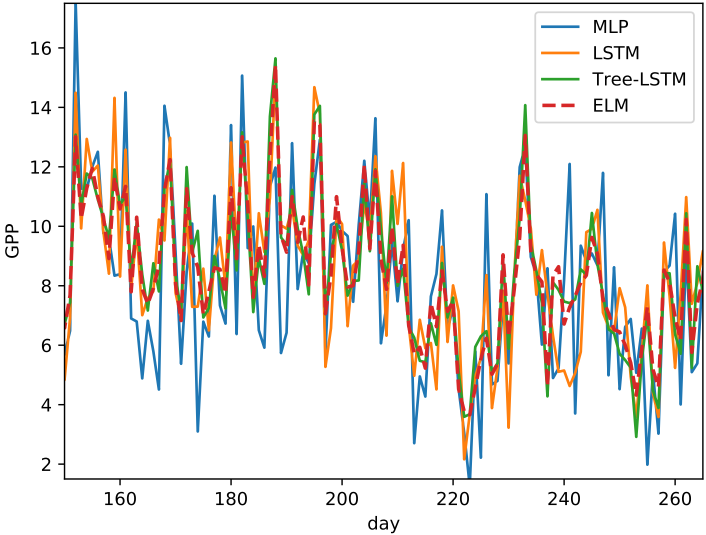

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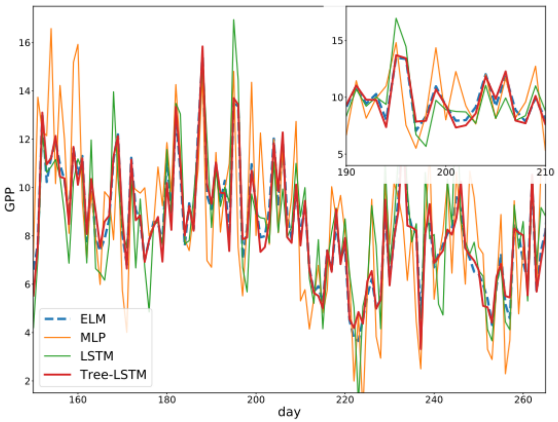

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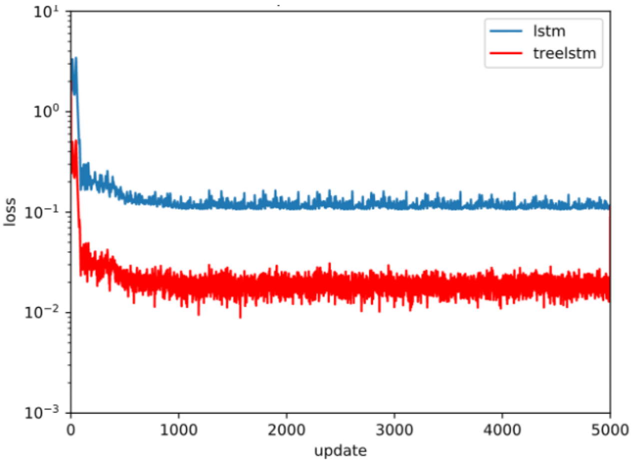


Price to pay: for NN surrogates, GSA should be carried out with Monte-Carlo

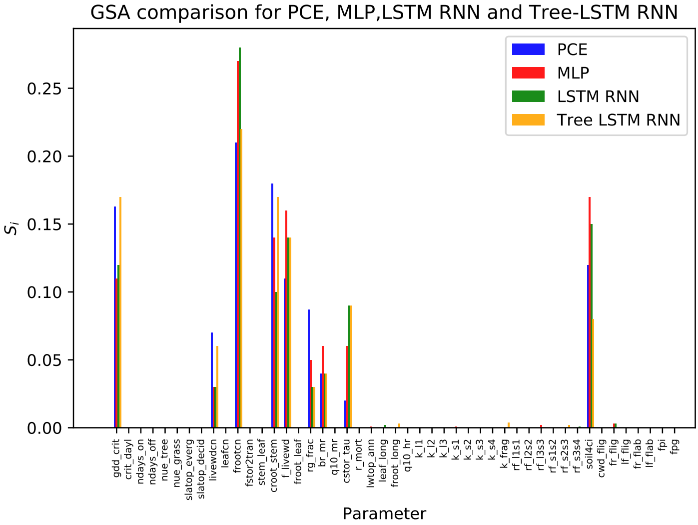
- Mean estimate: $E[f(\boldsymbol{\lambda})] \approx \frac{1}{N}\sum_{n=1}^{N} f(\boldsymbol{\lambda}^{(n)})$
- Variance estimate: $Var[f(\boldsymbol{\lambda})] \approx \frac{1}{N}\sum_{n=1}^{N} f(\boldsymbol{\lambda}^{(n)})^2 - E[f(\boldsymbol{\lambda})]^2$
- Main sensitivity:

$$S_i = \frac{Var[\mathbb{E}(f(\boldsymbol{\lambda}|\lambda_i)]}{Var[f(\boldsymbol{\lambda})]} \approx \frac{1}{Var[f(\boldsymbol{\lambda})]} \left(\frac{1}{N}\sum_{n=1}^{N} f(\boldsymbol{\lambda}^{(n)}) f(\boldsymbol{\lambda}_{-i}^{'(n)} \cup \boldsymbol{\lambda}_i^{(n)}) - E[f(\boldsymbol{\lambda})]^2\right.$$

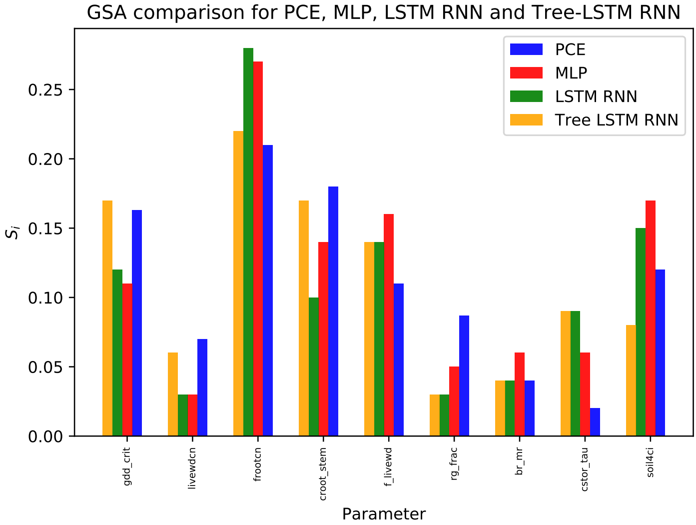
  where $\boldsymbol{\lambda}_{-i}^{'(n)} \cup \boldsymbol{\lambda}_i^{(n)}$ is a single-column swap sample given two sampling schemes $\boldsymbol{\lambda}^{(n)}$ and $\boldsymbol{\lambda}^{'(n)}$
- ... similar estimators for total sensitivity
- Inherits all the challenges of Monte-Carlo

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

Global Sensitivity Analysis Comparison



Global Sensitivity Analysis Comparison



Summary **Thank you!**

Overview

- Key UQ step, surrogate construction $==$ supervised ML
- Dimensionality reduction via Karhunen-Loève expansions (aka autoencoder)
- Physics-based LSTM architecture outperforms traditional NN methods (MLP) and traditional UQ methods (PCEs)
- Qualitatively similar sensitivity results compared to PCE

Current:

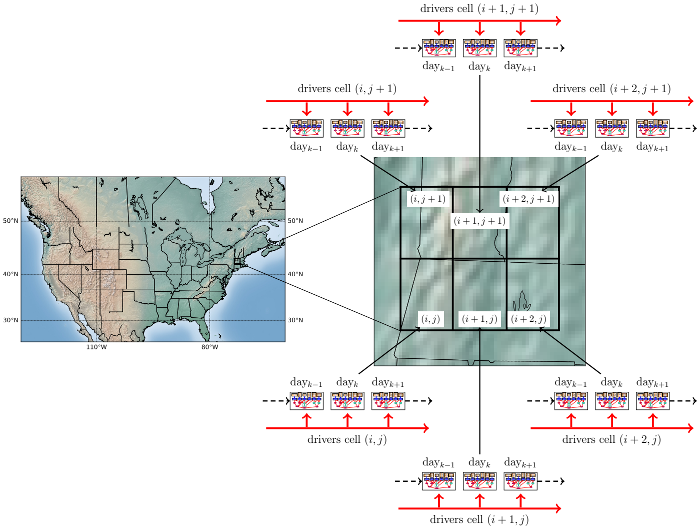
- Employing the reduced-dimensional spatio-temporal surrogate for calibration and optimal experimental design

Shameless Plug:

- Postdoc position(s) available at SNL-California at the intersection of UQ/ML
- www.sandia.gov/careers $\rightarrow$ 'View All Openings', e.g. job id 675390
- ... or email me at ksargsy@sandia.gov

Additional Material

ELM Simulation Details



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

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

$S_i = \frac{\text{Var}_{X_i}(E(Y|X_i))}{Var(Y)}$ 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

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