Functional Tensor Network Approximations for E3SM Land Model

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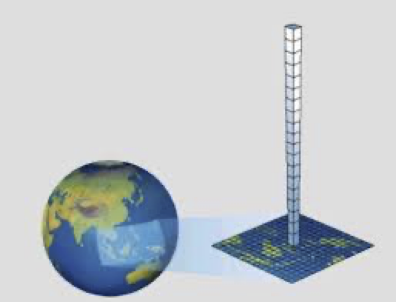
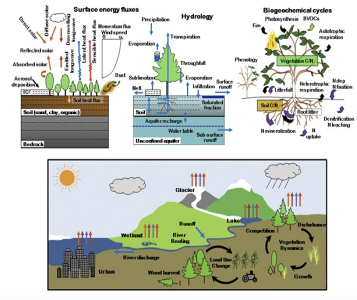
Outline

Energy Exascale Earth System Model (E3SM) – Land Component





- The Land Model (ELM) Component of the Energy Exascale Earth System Model (E3SM) is increasingly complex with many processes
  - Large ensembles are needed for uncertainty quantification... but computationally infeasible
  - Focus on surrogate models based on small ensembles to increase the efficiency of sensitivity analysis and model calibration studies

Cheaper Surrogates are Necessary to Replace Expensive Computational Models for UQ Assessments

Model Approximations:

- functional approximations
- non-parametric models, e.g. Gaussian processes
- neural networks and other supervised learning techniques

Requirements:

- expressivity with a limited number of parameters
- cheap – analyses often requiring $O(10^6)$ evaluations with limited computational resources

Functional Approximations

Tensor-product basis approximations:

$$f(\boldsymbol{\lambda}) = \sum_{i_1}^{N_1} \sum_{i_2}^{N_2} \dots \sum_{i_d}^{N_d} \phi_1^{i_1}(\lambda_1; \boldsymbol{\theta}) \phi_2^{i_2}(\lambda_2; \boldsymbol{\theta}) \dots \phi_d^{i_d}(\lambda_d; \boldsymbol{\theta})$$

- use orthogonal polynomials, radial basis functions, ...
- the curse of dimensionality $O(N^d)$ typically limits the polynomial order/no. of functions
  - this places limits on the surrogate model capacity to adapt to non-linear behavior

Functional Tensor-Train Models

Analogous to tensor-train models [Oseledets, 2013]: approximate multivariate functions instead of multidimensional arrays

$$\begin{aligned} f(\boldsymbol{\lambda}) &= \sum_{i_0=1}^{r_0} \sum_{i_1=1}^{r_1} \cdots \sum_{i_d=1}^{r_d} f_1^{(i_0 i_1)}(\lambda_1;\boldsymbol{\theta}_1) f_2^{(i_1 i_2)}(\lambda_2;\boldsymbol{\theta}_2) \cdots f_d^{(i_{d-1} i_d)}(\lambda_d;\boldsymbol{\theta}_d) \\ &= \mathcal{F}_1(\lambda_1;\boldsymbol{\theta}_1)\mathcal{F}_2(\lambda_2;\boldsymbol{\theta}_2)\cdots\mathcal{F}_d(\lambda_d;\boldsymbol{\theta}_d) \end{aligned}$$

$$\mathcal{F}_k(\lambda_k;\boldsymbol{\theta}_k) = \begin{bmatrix} f_k^{(11)}(\lambda_k;\boldsymbol{\theta}_k^{(11)}) & f_k^{(12)}(\lambda_k;\boldsymbol{\theta}_k^{(12)}) & \cdots & f_k^{(1 r_k)}(\lambda_k;\boldsymbol{\theta}_k^{(1 r_k)}) \\ f_k^{(21)}(\lambda_k;\boldsymbol{\theta}_k^{(21)}) & f_k^{(22)}(\lambda_k;\boldsymbol{\theta}_k^{(22)}) & \cdots & f_k^{(2 r_k)}(\lambda_k;\boldsymbol{\theta}_k^{(2 r_k)}) \\ \vdots & \vdots & \ddots & \vdots \\ f_k^{(r_{i-1} 1)}(\lambda_k;\boldsymbol{\theta}_k^{(r_{k-1} 1)}) & f_k^{(r_{i-1} 2)}(\lambda_k;\boldsymbol{\theta}_k^{(r_{k-1} 2)}) & \cdots & f_k^{(r_{i-1} r_k)}(\lambda_k;\boldsymbol{\theta}_k^{(r_{k-1} r_k)}) \end{bmatrix}$$

- Model evaluation/gradient computation consists of a sequence of matrix-vector multiplications [Gorodetsky & Jakeman, 2018]

Functional Representations – Univariate Functions

Linear Representations (e.g. polynomial chaos expansions)

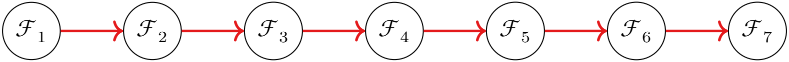
$$f_k^{(ij)}(\lambda_k(\xi_k);\boldsymbol{\theta}_k^{(ij)}) = \sum_{l=0}^{p_k} \theta_{k,l}^{(ij)} \Psi_l^{(ijk)}(\xi_k)$$

Non-Linear Representations (e.g. radial basis functions)

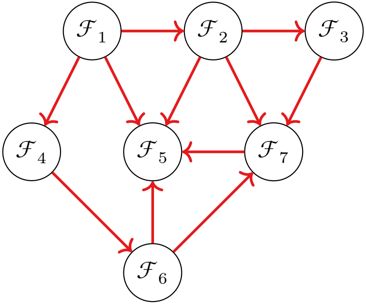
$$f_k^{(ij)}(\lambda_k;\boldsymbol{\theta}_k^{(ij)}) = \sum_{l=0}^{p_k} \theta_{k,l,1}^{(ij)} \exp(-\theta_{k,l,2}^{(ij)}(\lambda_k - \theta_{k,l,3}^{(ij)})^2)$$

Arbitrary Network Structure

Tensor train approximation

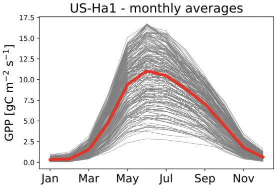


Tensor cores connected in an generic network - increased flexibility to represent model structure

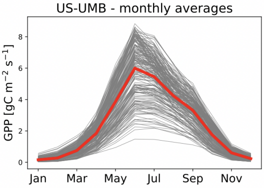


ELM Data – Simulations Corresponding to Select Observation sites

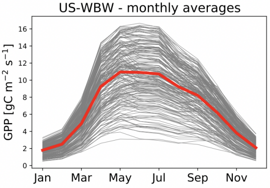
Harvard Forest EMS Tower



U. of Michigan Biological Station



Walker Branch Watershed



- *200 runs* corresponding to uniformly randomly sampled parameters over a *10D* parameter space
  - 160 training runs/40 validations runs
  - 8-fold cross validation over 160 training runs

Functional Tensor Network Models – Training

- Data split into 160 training runs / 40 validations runs
- Non-linear least squares with 8-fold cross validation over the training runs
- Univariate functions represented as polynomial expansions based on Legendre polynomials
  - Cross-validation to pick optimum regularization parameter, tensor rank, and polynomial order

$$\theta^* = \arg\min_{\theta} \left(\frac{1}{2} \sum_{i=1}^{N} \left(f(\lambda^{(i)}; \theta) - y^{(i)} \right)^2 + \alpha ||\theta||_2^2 \right)$$

  - Quality of fit assessed via mean-squared error (MSE)

$$MSE = \frac{1}{N} \sum_{i=1}^{N} \left(f(\lambda^{(i)}; \theta^*) - y^{(i)} \right)^2$$

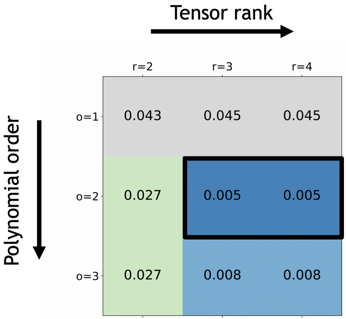
ELM Fit Results – FTN Models (in Hierarchical Tucker Format)

Hierarchical Tucker Format

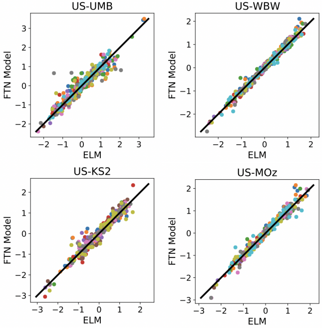
Tensor Train Format

Site US-Ha1/June: Validation MSE

ELM Fit Results – FTN Models (in Hierarchical Tucker Format)



Site US-Ha1/June: Validation MSE



Validation data centered and normalized by the monthly standard deviation

ELM Results: Variance-based GSA

Main Effect Sobol Index

$$S_i = \frac{Var[\mathbb{E}(f(\boldsymbol{\lambda}|\lambda_i)]}{Var[f(\boldsymbol{\lambda})]}$$

Total Effect Sobol Index

$$S_i^T = 1 - \frac{Var[\mathbb{E}(f(\boldsymbol{\lambda}|\lambda_{-i})]}{Var[f(\boldsymbol{\lambda})]}$$

Parameter	March		June		September		October	
	S_i	S_i^T	S_i	S_i^T	S_i	S_i^T	S_i	S_i^T
flnr	0.70	0.72	0.80	0.83	0.84	0.86	0.76	0.77
mbbopt	0.01	0.02	0.09	0.13	0.04	0.06	0.02	0.02
vcmaxse	0.13	0.15	0.02	0.02	0	0	0.02	0.02
dayl_scaling	0.06	0.07	0	0	0.04	0.05	0.14	0.14

- fnlr (fraction of N in RuBisCO – CO2 conversion process)
- mbbopt (stomatal conductance slope – net CO2 flux)
- vcmaxse (entropy for photosynthetic parameters)
- dayl_scaling (day length scaling parameter)

Closure

- Extended functional tensor train models to accommodate generic tensor network configurations
  - Expanded flexibility in capturing the structure of the original model
  - Efficient gradient computations through tensor network contractions
  - Alex Gorodetsky, CS, John Jakeman (2021) https://tinyurl.com/2p92thbn
- Functional tensor network models constructed via ridge regression are in good agreement with validation data for the driver application
  - Global Sensitivity Analysis results match subject matter expertise given the training runs available for this study