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Uncertainty Quantification for E3SM Land Component using Low-Rank Surrogate Models

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https://climatemodeling.science.energy.gov/projects/optimization-sensor-networks-improving-climate-model-predictions

Goal

Deploy surrogates that exploit structure in parameter to output map - seek low-rank functional tensor-train representation to reveal couplings in high-dimensional models.

Surrogate Models via Low-Rank Functional Tensor-Train Decomposition

Employ an approach analoguous to low-rank tensor decompositions:

$$f(\lambda_1,\lambda_2,\dots\lambda_d)=\sum_{i_0=1}^{r_0}\sum_{i_1=1}^{r_1}\cdots\sum_{i_d=1}^{r_d}f_1^{(i_0i_1)}(\lambda_1)f_2^{(i_1i_2)}(\lambda_2)\cdots f_d^{(i_{d-1}i_d)}(\lambda_d)$$

A compact expression can be assembled using a set of products of matrix-valued functions

$$f(\lambda_1,\lambda_2,\dots\lambda_d)=\mathcal{F}_1(\lambda_1)\mathcal{F}_2(\lambda_2)\cdots\mathcal{F}_d(\lambda_d),\quad \mathcal{F}_i(\lambda_i)=\begin{bmatrix} f_k^{(11)}(\lambda_k) & f_k^{(12)}(\lambda_k) & \dots & f_k^{(1r_k)}(\lambda_k)\\ f_k^{(21)}(\lambda_k) & f_k^{(22)}(\lambda_k) & \dots & f_k^{(2r_k)}(\lambda_k)\\ \vdots & \vdots & \ddots & \vdots\\ f_k^{(r_{i-1}1)}(\lambda_k) & f_k^{(r_{i-1}2)}(\lambda_k) & \dots & f_k^{(r_{i-1}r_k)}(\lambda_k)\end{bmatrix}$$

Each matrix-valued function $\mathcal{F}_k(\lambda_k)$ is a collection of univariate functions indexed by two indices (i,j) where i spans the range of rank r_{k-1} and j spans the range of rank r_k.

Univarite Functions Represented via Polynomial Chaos Approximations

- The input parameter set $\boldsymbol{\lambda}$ is in general viewed as a jointly distributed random vector, but for surrogate construction over ranges $\lambda_k\in[\lambda_{k,\min},\lambda_{k,\max}]$, for $k=1,2,\dots,d$, can be written component-wise as

$$\lambda_k=0.5\left(\lambda_{k,\min}+\lambda_{k,\max}+(\lambda_{k,\max}-\lambda_{k,\min})\,\xi_k\right)$$

- $\boldsymbol{\xi}\in[-1,1]^d$ - vector of d independent and identically distributed (*i.i.d.*) uniform random variables

The univariate function $f_k^{(ij)}(\lambda_k)$ can be viewed as a random variable induced by the uniform random input ξ_k,

$$\xi_k\to\lambda_k\to f_k^{(ij)}(\lambda_k(\xi_k))$$

and can written as a Polynomial Chaos Expansion [1] with respect to standard polynomials $\Psi_\alpha(\xi_k)$,

$$f_k^{(ij)}(\lambda_k(\xi_k))\approx\sum_{l=0}^{p_k}\theta_{ijkl}\Psi_l^{(ijk)}(\xi_k),$$

where p_k is the number of basis terms chosen to approximate $f_k^{(ij)}(x_k(\xi_k))$.

- Legendre polynomials are orthogonal with respect to uniform measure of ξ_k, $\pi(\xi_k)=1/2$ in $[-1,1]$

$$\langle\Psi_\alpha(\xi_k)\Psi_{\alpha'}(\xi_k)\rangle\equiv\int_{-1}^{1}\Psi_\alpha(\xi_k)\Psi_{\alpha'}(\xi_k)\pi(\xi_k)d\xi_k=0\quad\text{if}\quad\alpha\neq\alpha',$$

- Other polynomials are available depending on the expected behavior of the QoIs.

Fitting Low-Rank Models Through Sparse Data

Consider a number of simulation results $\mathbf{y}$ corresponding to a set of choices λ for the model inputs. The coefficients for the low-rank functional representation are determined through optimization

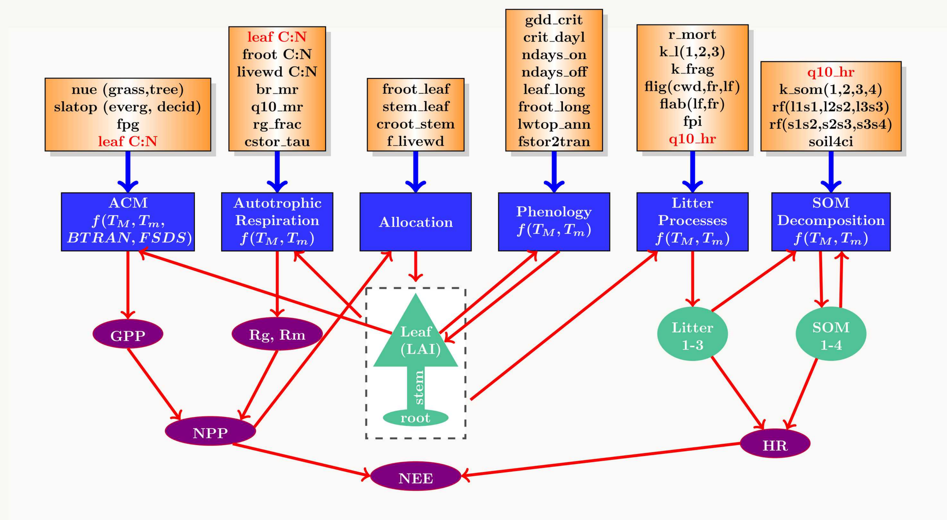
$$\text{argmin}_{\boldsymbol{\theta}}||\boldsymbol{y}-\boldsymbol{f}||_2^2+\Omega[\boldsymbol{f}]$$

A regularization term is added to minimize the number of non-zero functions in the matrix-valued $\mathcal{F}_k(\lambda_k)$

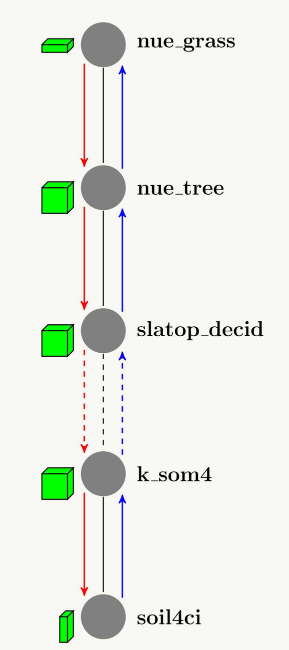
$$\Omega[\boldsymbol{f}]=\gamma\sum_{k=1}^{d}\sum_{i=1}^{r_{k-1}}\sum_{j=1}^{r_k}||f_k^{ij}||^2$$

- employ multi-way k-fold cross-validation to determine optimal knob values for the tensor-train approximation
  - regularization parameter γ
  - set of ranks $r_1,r_2,\dots,r_d$
  - polynomial order p
- Quasi-Newton method using L-BBFGS

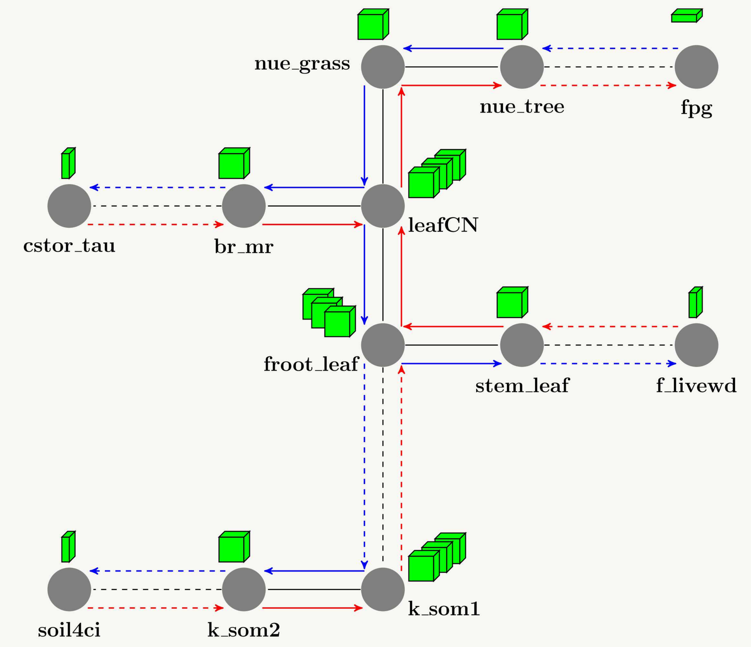
ASCR-BER Partnership: Optimization of Sensor Networks for Improving Climate Model Predictions (OSCM)



Tensor-Train Model



Tensor-Network Model



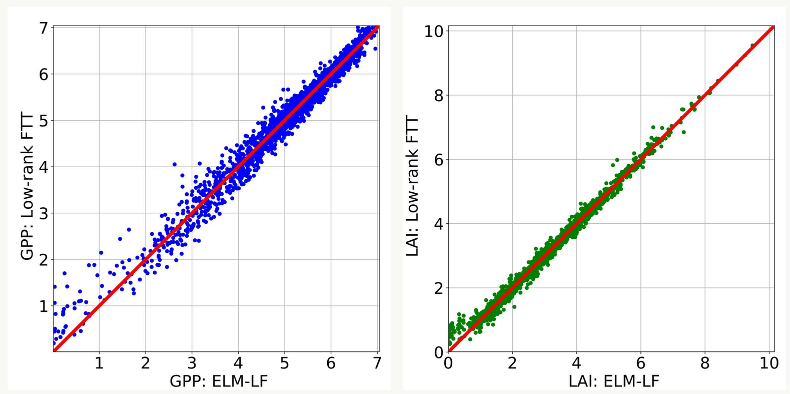
- sELM is a lower-fidelity, python version of the land model component of E3SM
- Processes are shown with blue boxes with dependencies on environmental data.
- Parameter inputs associated with each process are listed in orange rectangles.
  - 47-dimensional input space
- **Tensor-Train** and **Tensor Network** Models follow the structure of sELM componennts.
  - Tensor-Train models employ a collection of 2D/3D univariate tensors associated with input parameters
  - Tensor Network models offer more flexibility to replicate the complex model structure; employs 2D/3D/4D univariate tensors

Optimal Low-Rank Functional Tensor Train Solutions

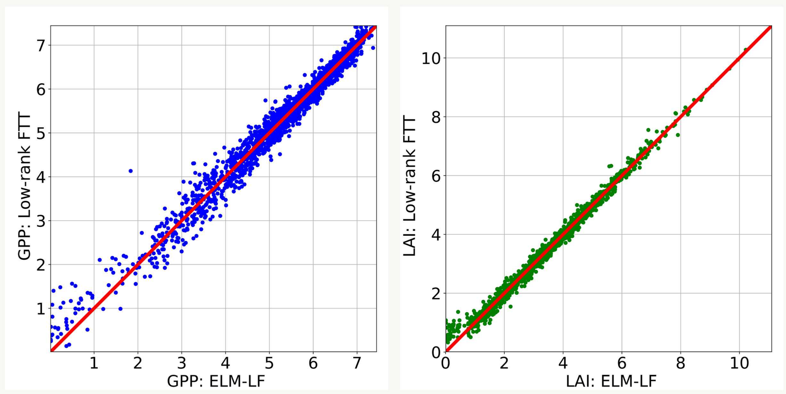
Typical cross-validation errors **5-10%** for both Quantities of Interest targeted in this study, Gross Primary Production (GPP) and Leaf Area Index (LAI)

- 5-fold cross validation
- 2-nd order univariate Legendre polynomials & univariate ranks between 2 and 4

Harvard Forest Site



near Harvard Forest Site



Combine Stochastic and Physical Spaces into a Joint Representation

Embed parametric (space and/or time) dependencies into a generalized low-rank functional tensor-train decomposition

A) Concatenate the stochastic $\boldsymbol{\lambda}$ and spatial $\mathbf{x}$ coordinates

$$f(\mathbf{x},\boldsymbol{\lambda})=\mathcal{F}_1(\lambda_1)\mathcal{F}_2(\lambda_2)\cdots\mathcal{F}_j(\lambda_j)\mathcal{F}_{\mathbf{x}}(\mathbf{x})\mathcal{F}_{j+1}(\lambda_{j+1})\cdots\mathcal{F}_d(\lambda_d)$$

B) Augment the rank of select cores in the representation to generate a multi-output surrogate corresponding to several spatial coordinates

$$f(\mathbf{x},\boldsymbol{\lambda})=\mathcal{F}_1(\lambda_1)\mathcal{F}_2(\lambda_2)\cdots\mathcal{F}_{j-1}(\lambda_{j-1})\begin{Bmatrix}\mathcal{F}_j^{(1)}(\lambda_j)\\ \vdots\\ \mathcal{F}_j^{(n)}(\lambda_j)\end{Bmatrix}\mathcal{F}_{j+1}(\lambda_{j+1})\cdots\mathcal{F}_d(\lambda_d)$$

C) Augment the representation of select tensor-train cores with spatial dependencies

$$f(\mathbf{x},\boldsymbol{\lambda})=\mathcal{F}_1(\lambda_1)\mathcal{F}_2(\lambda_2)\cdots\mathcal{F}_{j-1}(\lambda_{j-1})\mathcal{F}_j(\mathbf{x},\lambda_j)\mathcal{F}_{j+1}(\lambda_{j+1})\cdots\mathcal{F}_d(\lambda_d)$$

Next Steps

- Construct surrogate models that adapt simultanously to stochastic space/physical space dependencies
- Adaptive sampling of the mixed stochastic/physical spaces to target regions of high-probability and/or non-linear behavior in the joint space

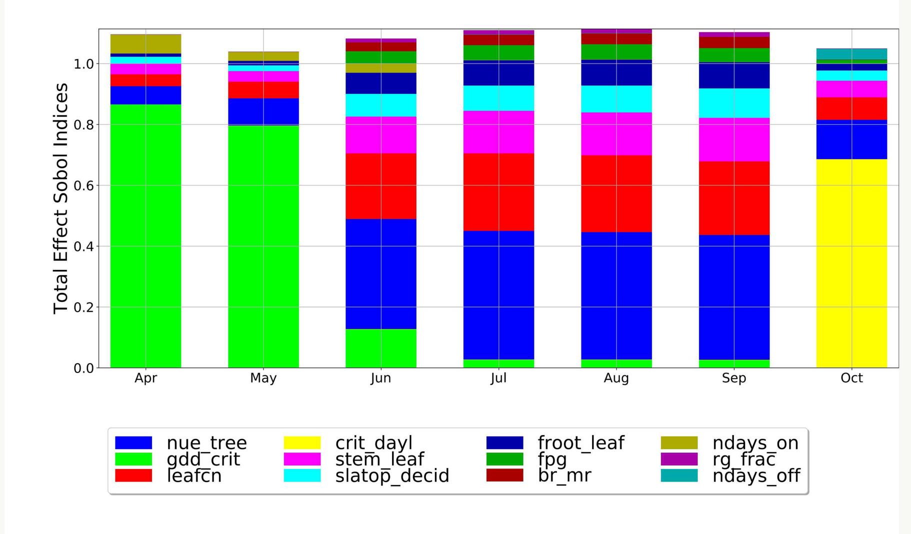
[1] Ghanem, R., and P. Spanos (1991), *Stochastic Finite Elements: A Spectral Approach*, Springer Verlag, New York.

[2] Gorodetsky, A. A. and Jakeman, J. D. (2018), Gradient-based optimization for regression in the functional tensor-train format, *Journal of Computational Physics, 374*, 1219 - 1238.

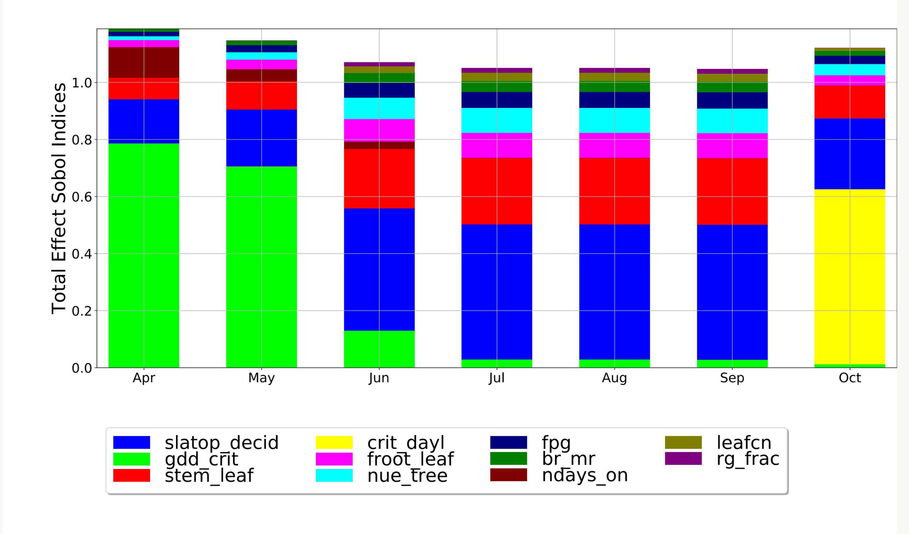
Global Sensitivity Analysis - Temporal and Spatial Similarities

Total Effect Sobol Indices for Model Parameters Relevant at Harvard Forest

Gross Primary Production (GPP)

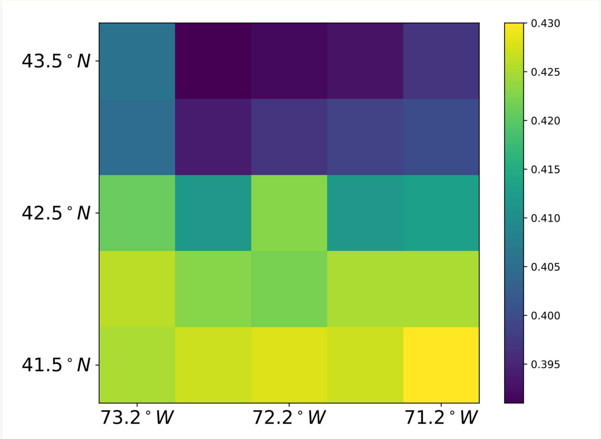


Leaf Area Index(LAI)

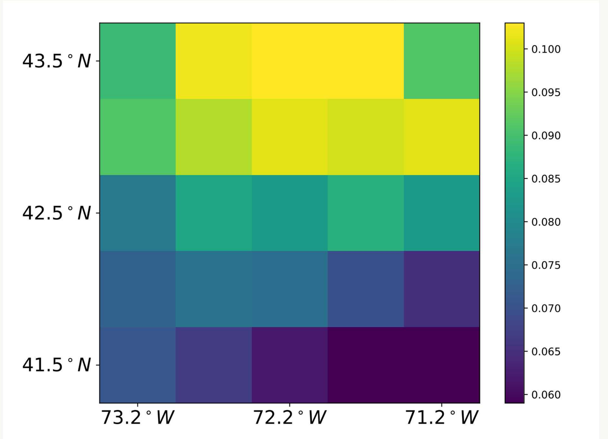


Total Effect Sobol Indices for Select Model Parameters around Harvard Forest Average July Results

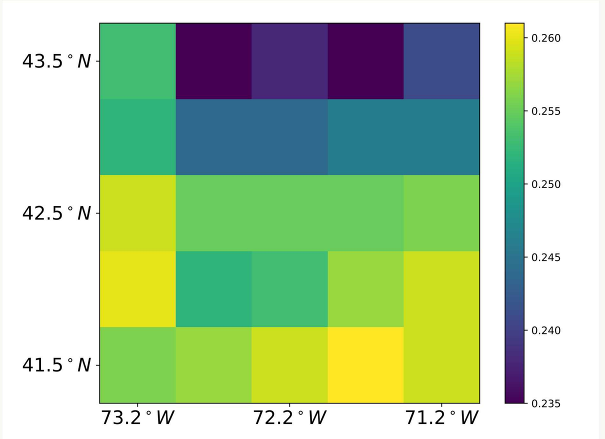
Parameter: nue tree



Parameter: slatop decid



Parameter: leafcn



Findings pertaining to the approximation model

- Low-rank Functional Tensor-Train models are within 5-10% of ELM-LF model results for the range of conditions investigated.
  - improved performance compared to total-order Polynomial Chaos representations

Findings pertaining to the ELM-LF application

- Identified a set of 8-12 parameters (out of 47) that control model outputs of interest.
  - Parameter contributions to the total variance is consistent with intuition based on the physics of the problem.
  - Expected similarities in space and time recovered via tensor-train models.

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