National Laboratories

Expressive Surrogate Models via Functional Tensor Networks

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Presented by:

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Sandia National Laboratories

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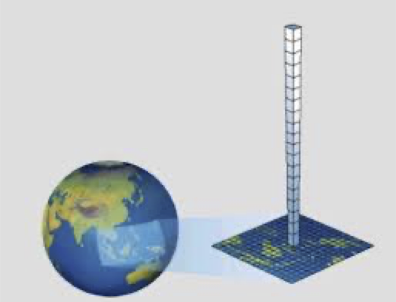
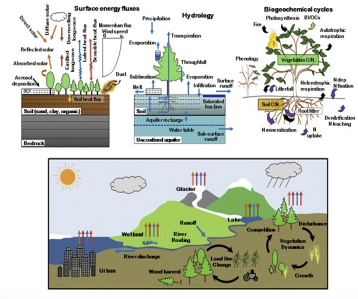
Outline

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 are not computationally infeasible
  - Focus on surrogate models that exploit model structure to increase the efficiency of sensitivity analysis and model calibration studies

Cheaper Surrogates are Necessary for UQ Assessments

Requirements:

- expressivity with a limited number of parameters
- once constructed surrogate models need to be computationaly cheap analyses often requiring $O(10^6)$ evaluations with limited computational resources

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Functional Approximations:

- tensor-product basis approximations

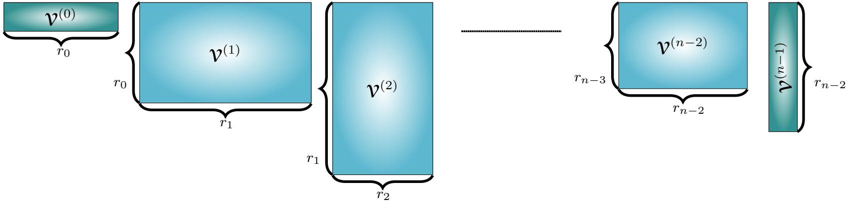
$$f(\boldsymbol{\lambda}) = \sum_{i_1}^{N_1} \sum_{i_2}^{N_2} \cdots \sum_{i_d}^{N_d} \phi_1^{(i_1)}(\lambda_1; \boldsymbol{\theta}) \phi_2^{(i_2)}(\lambda_2; \boldsymbol{\theta}) \ldots \phi_d^{(i_d)}(\lambda_d; \boldsymbol{\theta})$$

  - 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

- Instead focus on *low-rank functional tensor network* models

Functional Tensor-Train Models

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

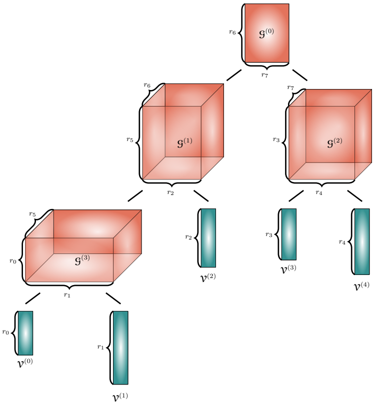


$$\mathcal{V}^{(k)}(\lambda_k;\boldsymbol{\theta}_k) = \begin{bmatrix} f_{11}^{(k)}(\lambda_k;\boldsymbol{\theta}_{11}^{(k)}) & f_{12}^{(k)}(\lambda_k;\boldsymbol{\theta}_{12}^{(k)}) & \cdots & f_{1r_k}^{(k)}(\lambda_k;\boldsymbol{\theta}_{1\,r_k}^{(k)}) \\ f_{21}^{(k)}(\lambda_k;\boldsymbol{\theta}_{21}^{(k)})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

- Model evaluation/gradient computation consists of a sequence of matrix-vector multiplications
  - A.A. Gorodetsky, J.D. Jakeman, doi:10.1016/j.jcp.2018.08.010 (2018)

Tensor Models can have Arbitrary Network Structure

- Increased flexibility to represent model structure
- Example: a hierarchical Tucker format for a 5-dimensional model



- $\mathcal{V}^{(k)}$ represent tensor cores constructed with univariate functions in λ_k.
- $\mathcal{G}^{(i)}$ represent tensor cores with scalar elements (constant functions).

Functional Tensor Networks – Definitions

A tensor contraction is a binary operation on two tensors $\mathcal{A} \in \mathbb{R}^{I_1 \times \ldots \times I_{d_A}}$ and $\mathcal{B} \in \mathbb{R}^{J_1 \times \ldots \times J_{d_B}}$ yielding a tensor $\mathcal{C}$.

$$\mathcal{C} = \mathcal{A} \;{}_{\Gamma}\!\times_{\Upsilon}\; \mathcal{B}$$

- The operation is parameterized by two index sets, $\Gamma = \{\gamma_1, \ldots, \gamma_\ell\}$ and $\Upsilon = \{\eta_1, \ldots, \eta_\ell\}$, satisfying certain conditions; after permuting the modes so that the contracting dimensions are first

$$c_{j_1,\ldots,j_{d_A-\ell},k_1,\ldots,k_{d_B-\ell}} = \sum_{\gamma_1=1}^{I_{\gamma_1}} \cdots \sum_{\gamma_\ell=1}^{I_{\gamma_\ell}} \tilde{a}_{\gamma_1,\ldots,\gamma_\ell,j_1,\ldots,j_{d_A-\ell}} \tilde{b}_{\gamma_1,\ldots,\gamma_\ell,k_1,\ldots,k_{d_B-\ell}},$$

with $\mathcal{C}$ having order $d_A + d_B - 2\ell$.

Example: Matrix-Matrix multiplication

$$c_{j,k} = \sum_{\gamma_1=1}^{I_\gamma} \tilde{a}_{\gamma,j} b_{\gamma,k}$$

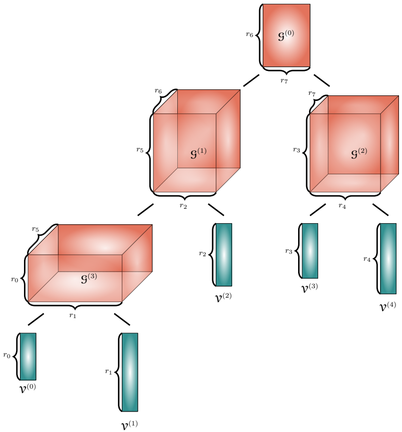
Functional Tensor Networks – Definitions

A tensor network is a connected graph

$$\mathcal{TN} = (V, E)$$

- each vertex $\mathcal{V}^{(i)} \in V$ is a tensor of order $d^{(i)}$
- the set of edges E denote contractions
  - An edge $E^{(ij)}$ from vertex $\mathcal{V}^{(i)}$ to vertex $\mathcal{V}^{(j)}$ is a pair of multi-indices $E^{(ij)} = \{\vec{i}, \vec{j}\}$ and denotes the contraction

$$\mathcal{V}^{(i)} \;{}_{\vec{i}}\!\times_{\vec{j}}\; \mathcal{V}^{(j)}.$$



Here, $V = \{\mathcal{V}^{(0)}, \mathcal{V}^{(1)}, \ldots, \mathcal{G}^{(0)}, \mathcal{G}^{(1)}, \ldots\}$

Full tensor network contraction consists of a set of recursive pairwise contractions until all edges are exhausted.

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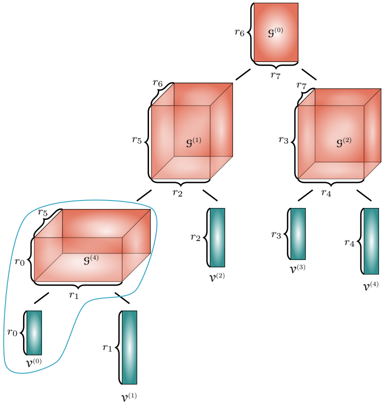

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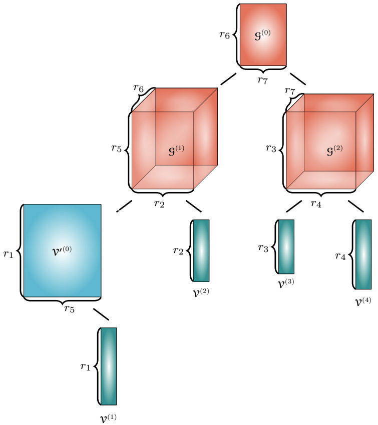

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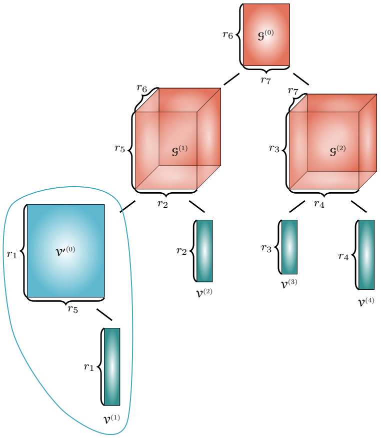

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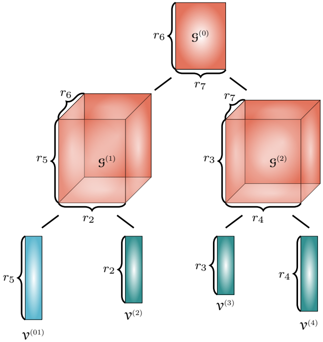

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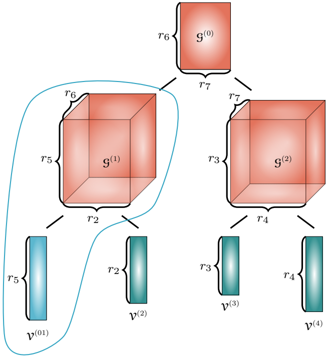

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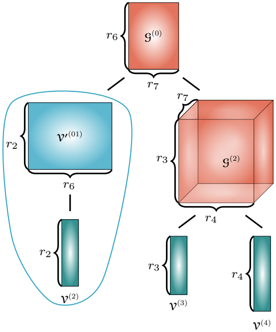

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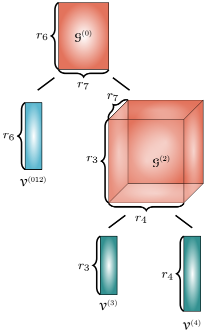

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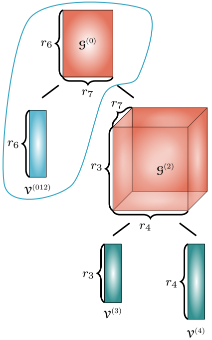

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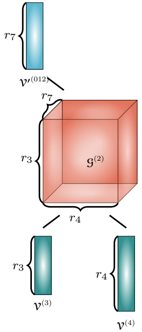

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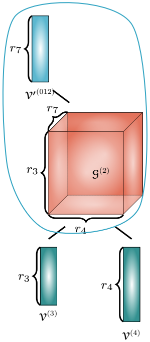

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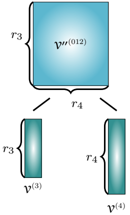

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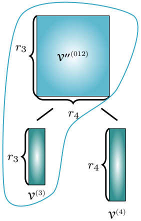

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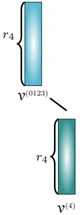

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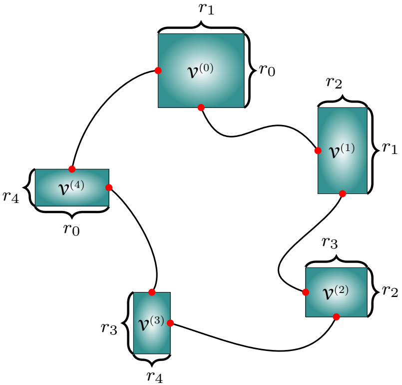

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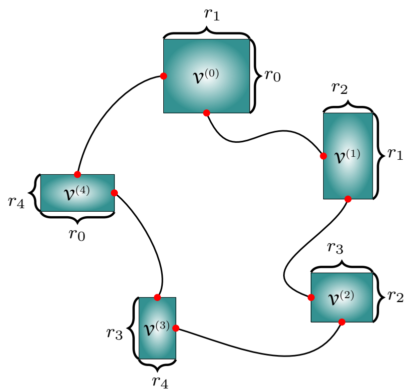

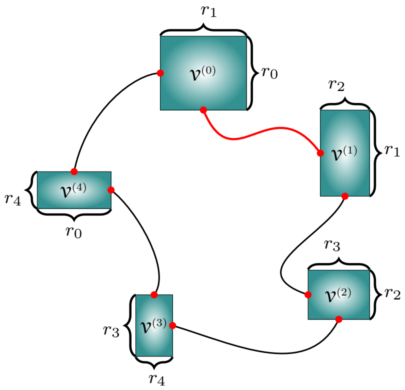

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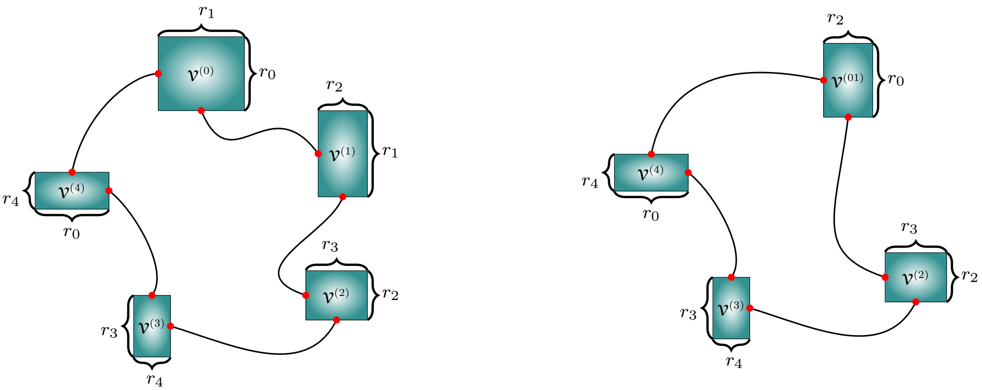

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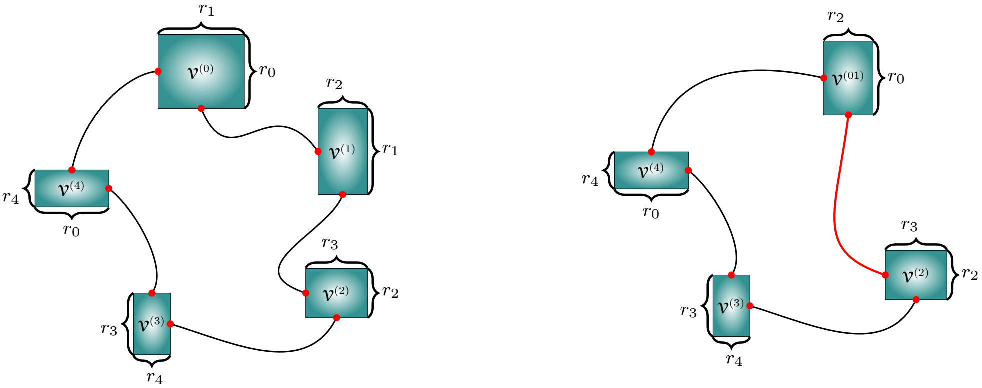

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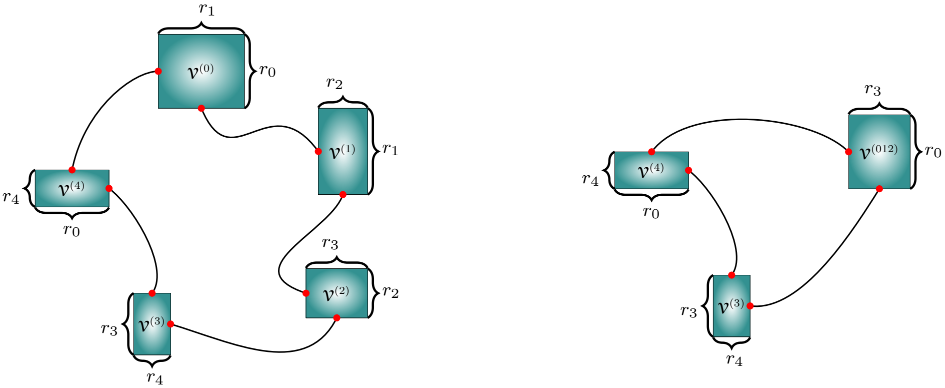

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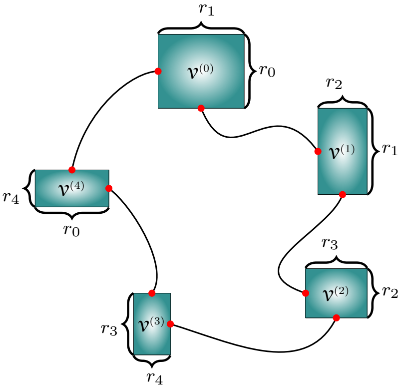

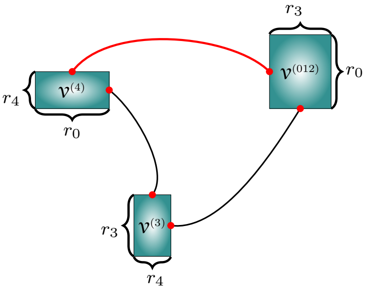

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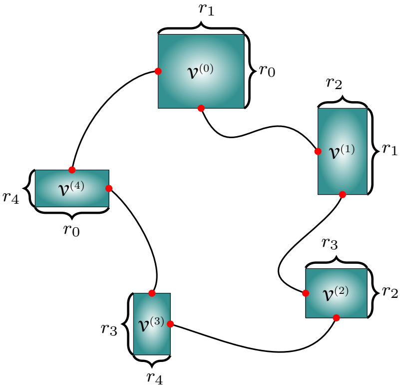

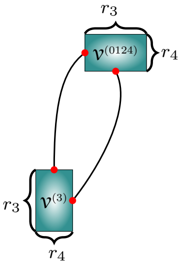

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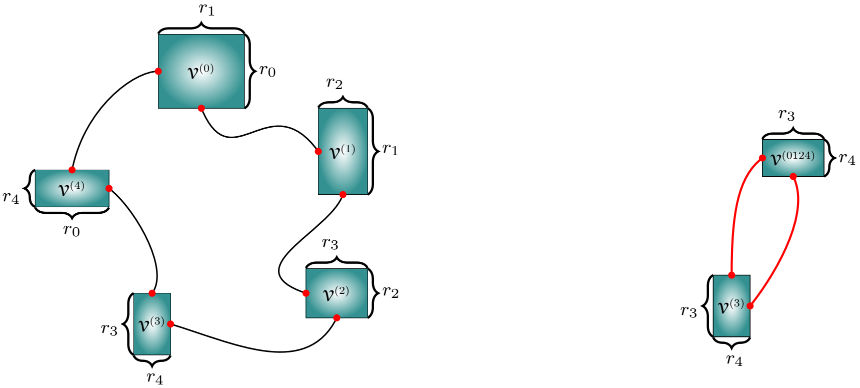

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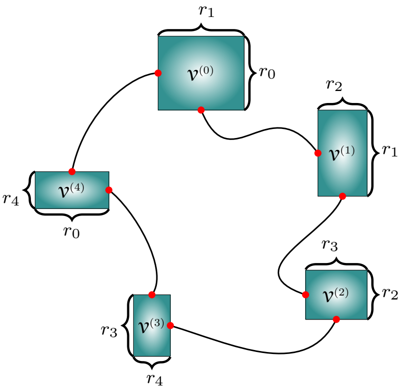

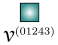

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Functional Representations – Univariate Functions

Linear Representations (e.g. polynomial chaos expansions)

$$f_{ij}^{(k)}(\lambda_k(\xi_k);\boldsymbol{\theta}_{ij}^{(k)}) = \sum_{l=0}^{p_k} \theta_{ijl}^{(k)} \Psi_l^{(k)}(\xi_k)$$

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

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

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Functional Tensor Networks – Evaluate (Conditional) Statistics

Each tensor core consists of scalars or univariate functions therefore contractions and integrals commute

Expectation

$$\mathbb{E}[\mathcal{TN}] = (\mathbb{E}[\mathcal{V}], E)$$

where $\mathbb{E}[\mathcal{V}] \triangleq \{\mathbb{E}_{\lambda_0}[\mathcal{V}^{(0)}], \mathbb{E}_{\lambda_1}[\mathcal{V}^{(1)}], \ldots\}$

- For univariate functions given by polynomial chaos expansions, the elements of a 2D tensor $\mathbb{E}_{\lambda_k}[\mathcal{V}^{(k)}]$ are given by

$$\mathbb{E}_{\lambda_k}[\mathcal{V}^{(k)}(\lambda_k; \boldsymbol{\theta}_k)] = \begin{bmatrix} \theta^{(k)}_{110} & \theta^{(k)}_{120} & \cdots & \theta^{(k)}_{1\,r_k0} \\ \theta^{(k)}_{210} & \theta^{(k)}_{220} & \cdots & \theta^{(k)}_{2\,r_k0} \\ \vdots & \vdots & \ddots & \vdots \\ \theta^{(k)}_{r_{k-1}10} & \theta^{(k)}_{r_{k-1}20} & \cdots & \theta^{(k)}_{r_{k-1}\,r_k0} \end{bmatrix}$$

- Conditional expectations $\mathbb{E}_i[\mathcal{TN}]$ require marginalization over subset i of the set of tensor cores, e.g.

$$\mathbb{E}_1[\mathcal{V}] \triangleq \{\mathcal{V}^{(0)}, \mathbb{E}_{\lambda_1}[\mathcal{V}^{(1)}], \mathcal{V}^{(2)}, \ldots\}$$

Functional Tensor Networks – Evaluate (Conditional) Statistics

Variance

$$\mathbb{V}[\mathcal{TN}] = \mathbb{E}[(\mathcal{TN})^2] - \mathbb{E}[\mathcal{TN}]^2$$

The first term can be written as

$$\mathbb{E}[(\mathcal{TN})^2] = \left(\mathbb{E}[\tilde{\mathcal{V}}], E\right)$$

where $\mathbb{E}[\tilde{\mathcal{V}}] \triangleq \{\mathbb{E}_{\lambda_0}[\mathcal{V}^{(0)} \otimes \mathcal{V}^{(0)}], \mathbb{E}_{\lambda_1}[\mathcal{V}^{(1)} \otimes \mathcal{V}^{(1)}], \ldots\}$

- For univariate functions given by polynomial chaos expansions, the elements of a 2D tensor $\mathbb{E}_{\lambda_k}[\mathcal{V}^{(k)} \otimes \mathcal{V}^{(k)}]$ are given by

$$\sum_{l=0}^{p_k} \theta^{(k)}_{i_1 j_1 l} \theta^{(k)}_{i_2 j_2 l} \langle \Psi^{(k)}_l (\xi_k)^2 \rangle$$

Functional Tensor Networks – Sobol Indices

Law of Total Variance

$$\mathbb{V}[\mathcal{TN}] = \mathbb{V}_i[\mathbb{E}_{\setminus i}[\mathcal{TN}]] + \mathbb{E}_i[\mathbb{V}_{\setminus i}[\mathcal{TN}]]$$

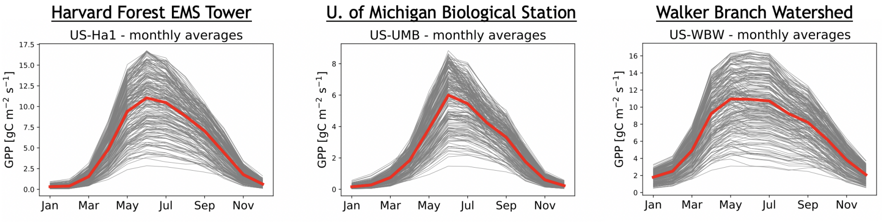
after normalization

$$1 = \underbrace{\frac{\mathbb{V}_i[\mathbb{E}_{\setminus i}[\mathcal{TN}]]}{\mathbb{V}[\mathcal{TN}]}}_{S_i} + \underbrace{\frac{\mathbb{E}_i[\mathbb{V}_{\setminus i}[\mathcal{TN}]]}{\mathbb{V}[\mathcal{TN}]}}_{S^T_{\setminus i}}$$

- First order S_i and total order $S_i^T = 1 - S_{\setminus i}$ are computed using tensor network algebra described on previous slides.
- Joint sensitivity indices are evaluated through a similar approach

$$S_{ij} = \frac{\mathbb{V}_{i,j}[\mathbb{E}_{\setminus i,j}[\mathcal{TN}]]}{\mathbb{V}[\mathcal{TN}]} - S_i - S_j$$

ELM Data Simulations Corresponding to Select Observation sites



- *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

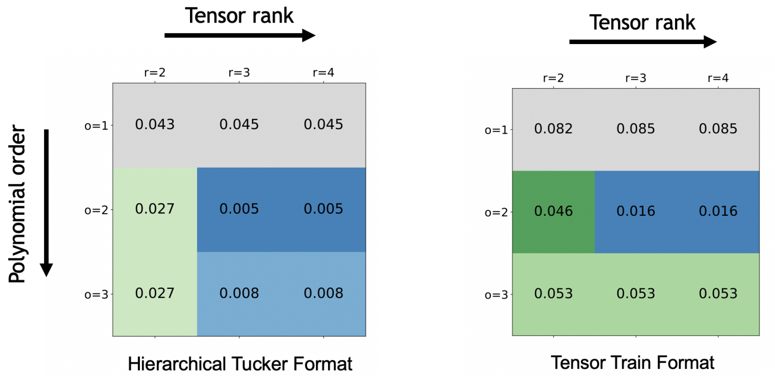
- Data split into 160 training runs / 40 validations runs
- Non-linear least squares with 8-fold cross validation over the training runs
- Univariate functions represented as polynomial expansions based on Legendre polynomials
  - Cross-validation to pick optimum regularization parameter, tensor rank,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

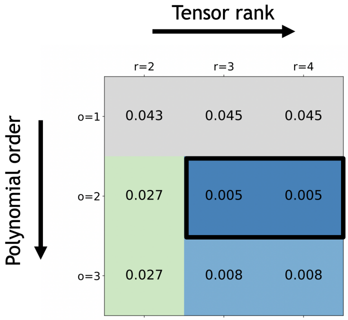
$$MSE = \frac{1}{N}\sum_{i=1}^{N}\left(f(\lambda^{(i)};\theta^*) - y^{(i)}\right)^2$$

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

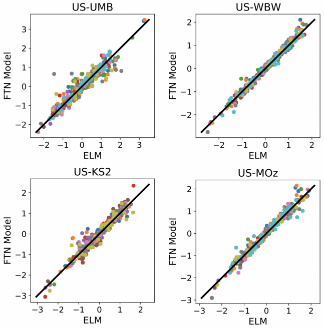


Site US-Ha1/June: Validation mean-squared error for Hierarchical Tucker models compared to Tensor Train models

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)

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
- Next steps: account for spatio-temporal dependencies and model calibration in a Bayesian setting.