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Approximating Data with Stochastic and Physical Dependence using Functional Tensor Train Models

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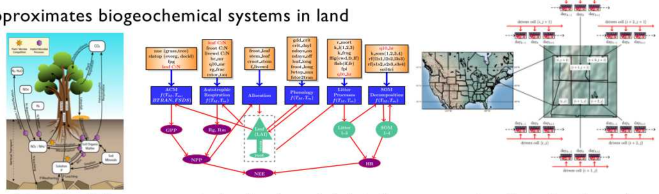
Motivation

- E3SM Land Model is land component of DOE Earth system model [3]
- Land Model has 47 stochastic inputs and is evaluated separately for each location and date
- Approximates biogeochemical systems in land



- Goal is using FT as surrogate for land model data for many sets of stochastic and physical inputs
- We need to incorporate physical dependence into the FT and develop optimization algorithms to fit this FT to the data.

Surrogate Modeling With Functional Tensor Train

- The Functional Tensor-Train (FT) approximates data, y, that depends on stochastic inputs, x, using the product of matrix valued functions called Tensor Cores [1]:

$$f(x) = \mathbf{F}^{(1)}(x_1)\mathbf{F}^{(2)}(x_2)\cdots\mathbf{F}^{(d)}(x_d)$$

- x has d dimensions, there is one tensor core for each dimension of x
- Dimensions of k^{th} tensor core are $r_k \times r_{k+1}$, called ranks of tensor core
- Tensor cores, $\mathbf{F}^{(k)}(x_k)$, are made of univariate functions
- Univariate functions are Polynomial Chaos Expansions (PCE) of the corresponding input [2]

$$f_{i,j}^{(k)} = \sum_{p=0}^{P_k} \theta_{k,i,l,j}\phi_p(x_k)$$

- $\theta_{k,i,l,j}$ is the coefficient and $\phi_p(x_k)$ is the degree p basis polynomial

Incorporating Physical Dependence in FT

- We want the FT to take physical and stochastic inputs separately
- Two ways to incorporate physical inputs:
  1. Treat physical input as another stochastic input
  2. Add physical dependence to coefficients in PCEs
- First method adds another tensor core for physical input p
- Second method replaces coefficients with polynomial expansions in terms of the physical input p:

$$\theta_{k,i,l,j}(p) := \sum_{s=1}^{S} \theta_{k,i,l,j,s}\psi_s(p)$$

- $\psi_s(p)$ is basis polynomial with corresponding coefficient $\theta_{k,i,l,j,s}$
- Not necessary to put physical dependence on all coefficients
- If physical dependence on all coefficients, PCE degree is $p_k = P$, and all ranks are equal to R, then there are dR^2SP coefficients to solve for

Determining Coefficients in FT

- To find the best coefficients we minimize the objective function

$$J(\theta) = \frac{1}{2}\sum_{u=1}^{V}\sum_{m=1}^{M}\sum_{n=1}^{N}\left(y_{m,n,u} - f(x^{(m)},p^{(n)})_u\right)^2$$

- Data is for V values at M instances of the stochastic input and N instances of the physical input
- Objective function is minimized using Alternating Least Squares or gradient based methods L-BFGS and Gradient Descent

Gradient

- Partial derivative of objective function used to compute gradient is

$$\frac{\partial J}{\partial \theta_{k,i,l,j,s,v}} = \sum_{u=1}^{V}\sum_{m=1}^{M}\sum_{n=1}^{N}\left(y_{m,n,u} - f(x^{(m)},p^{(n)})_u\right)\frac{\partial f(x^{(m)},p^{(n)})_u}{\partial \theta_{k,i,l,j,s,v}}$$

- Where

$$\frac{\partial f(x^{(m)},p^{(n)})_u}{\partial \theta_{k,i,l,j,s,v}} = \mathbf{F}^{(1)}\cdots\mathbf{F}^{(k-1)}\mathbf{G}\mathbf{F}^{(k+1)}\cdots\mathbf{F}^{(d)}$$

- And

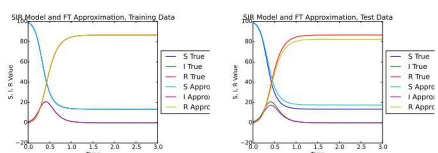
$$g_{w,z} = \begin{cases}\phi_l^{(k)}(x^{(m)})\psi_s(p^{(n)}) & (w,z)=(i,j)\\ 0 & (w,z)\neq(i,j)\end{cases}$$

Test Functions

- Test the FT by approximating the output of two types of test functions:
  1. Generating a random FT and using a different FT to approximate it
  2. Approximating system of ODEs (SIR Model and Lorenz System[4,5]) with parameters as stochastic input and time as physical input
- Stochastic inputs for ODE tests are sampled from a normal distribution centered at a nominal parameter value
- We fit the FT to data from the function and then test how well the FT approximates data with different stochastic and physical inputs

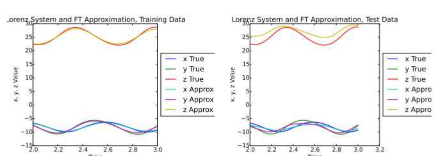
Approximating a Random FT
Trained and Tested with
100 Stochastic Samples, 100 Time Samples

	2 Norm Error
Training Data	9.30×10^{-4}
Test Data	3.41×10^{-3}



SIR Model
Trained and Tested with
25 Stochastic Samples, 100 Time Samples

	2 Norm Error
Training Data	3.12×10^{-3}
Test Data	7.56×10^{-2}



Lorenz System
Trained and Tested with
50 Stochastic Samples, 1000 Time Samples

	2 Norm Error
Training Data	1.90×10^{-2}
Test Data	1.51×10^{-1}

- Error on test data is higher than error on training data

Summary and Future Work

- FT can approximate a set of data dependent on stochastic and physical inputs
- Analytic derivative of objective function allows use of gradient based optimization
- We will apply the FT to approximate data from the E3SM Land Model
- Add more types of functions (radial basis functions, Fourier series) as options for univariate functions in tensor cores

Refrences

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[5] Lorenz, E. N. (1963). Deterministic nonperiodic flow. *Journal of the atmospheric sciences*, 20(2), 130-141. doi:0.1175/1520-0469(1963)020<0130:DNF>2.0.CO;2

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