R: High-Dimensional Surrogate Model for UQ

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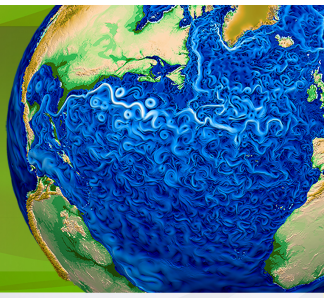


Objective

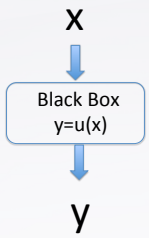
Surrogate Modeling:
- Build a surrogate model that approximates ACME output QoIs
- Explore a range of variability of parameters and operating conditions

Input Parameter Dependence:
- Account for correlated/dependent inputs

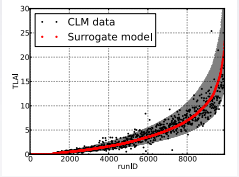
Strongly Nonlinear Input-Output Map:
- Capture failed-vegetation runs with classification

Output Uncertainty Attribution:
- Evaluate individual parameter contributions to output uncertainty

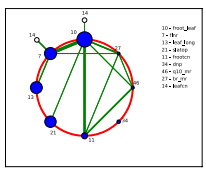
Curse of Dimensionality:
- Many parameters (50-100)
- Expensive simulations (single run in a few hours)
- Learn the model behavior with as few training simulations as possible



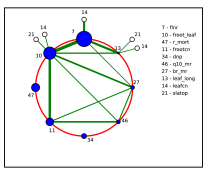
AmeriFlux site Niwot Ridge (#1)



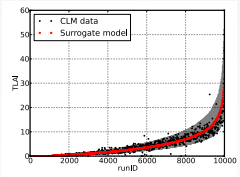
TLAI



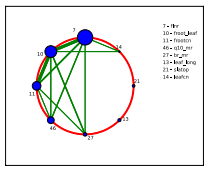
TOTVEGC



Evergreen Forest at Campbell river (#2)



TLAI Surrogate



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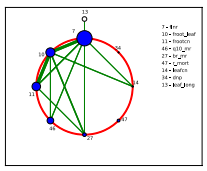
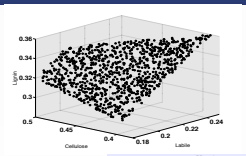


TOTVEGC

Approach

Rosenblatt Transformation:
- Create dependent input configurations
- High-D generalization of CDF transform
- Probability-preserving map



Polynomial Chaos Surrogate:
- Cast input/outputs as random variables
- Flexible representation for both forward and inverse UQ

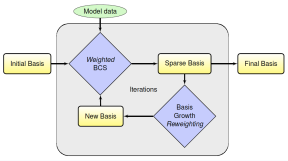
$$y = u(\boldsymbol{x}) \approx \sum_{k=0}^{K-1} c_k \Psi_k(\boldsymbol{x})$$

$$\Psi_k(x_1, x_2, ..., x_d) = \psi_{k_1}(x_1)\psi_{k_2}(x_2)\cdots\psi_{k_d}(x_d)$$

Bayesian Approach:
- Uses any number of model simulations
- Provides an uncertain surrogate with quantified error

$$\underbrace{P(c_k|u(\boldsymbol{x}_j))}_{\text{Posterior}} \propto \underbrace{P(u(\boldsymbol{x}_j)|c_k)}_{\text{Likelihood}} \underbrace{P(c_k)}_{\text{Prior}}$$

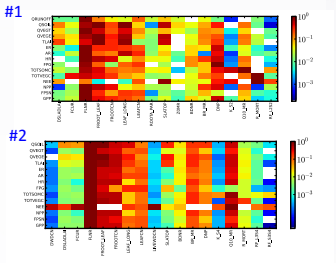
Weighted Iterative Bayesian Compressive Sensing:
- Iterative search for most relevant polynomial bases



Variance-based Decomposition:
- Sobol sensitivities attribute output uncertainties to input parameters

Impact

Parameter Ranking:
- Provides an efficient parameter ranking by their impact to each output QoI.



Dimensionality Reduction:
- Large set of input parameters (50-100) can easily be reduced to about 10 without much loss of information

Model Surrogate for Computationally Intensive Studies:
- Calibration and optimization can proceed using the uncertain model surrogate

Key Parameters:
- Leaf and fine root nitrogen
- Fine root allocation
- Leaf longevity, denitrification
- Temperature sensitivity of autotrophic respiration

ACME Accelerated Climate Modeling for Energy

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