Sparse Polynomial Chaos Surrogate for ACME Land Model via Iterative Bayesian Compressive Sensing

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Sponsored by DOE, Biological and Environmental Research,
under Accelerated Climate Modeling for Energy (ACME).

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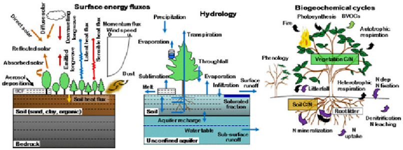
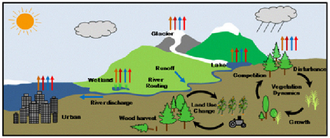
OUTLINE

- Surrogates needed for complex models
- Polynomial Chaos (PC) surrogates do well with uncertain inputs
- Bayesian regression provide results with uncertainty certificate
- Compressive sensing ideas deal with high-dimensionality

Application of Interest: ACME Land Model





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- A single-site, 1000-yr simulation takes ~ 10 hrs on 1 CPU
- Involves ~ 70 input parameters; some dependent
- Non-smooth input-output relationship

Surrogate construction: scope and challenges

Construct surrogate for a complex model $f(\boldsymbol{\lambda})$ to enable

- Global sensitivity analysis
- Optimization
- Forward uncertainty propagation
- Input parameter calibration
- $\cdots$

- Computationally expensive model simulations, data sparsity
  - Need to build accurate surrogates with as few training runs as possible
- High-dimensional input space
  - Too many samples needed to cover the space
  - Too many terms in the polynomial expansion

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Polynomial Chaos surrogate for $f(\boldsymbol{\lambda})$

- Scale the input parameters $\lambda_i \in [a_i, b_i]$

$$\lambda_i = \frac{a_i + b_i}{2} + \frac{b_i - a_i}{2}\, x_i$$

- Forward function $f(\cdot)$, output u

$$u(\boldsymbol{x}) = f(\boldsymbol{\lambda}(\boldsymbol{x})) \qquad \approx \qquad \sum_{k=0}^{K-1} c_k \Psi_k(\boldsymbol{x}) \equiv g(\boldsymbol{x})$$

- Global sensitivity information for free
  - Sobol indices, variance-based decomposition.

- Bayesian inference useful for finding c_k:

$$P(\boldsymbol{c}|\boldsymbol{u}) \propto P(\boldsymbol{u}|\boldsymbol{c})P(\boldsymbol{c})$$

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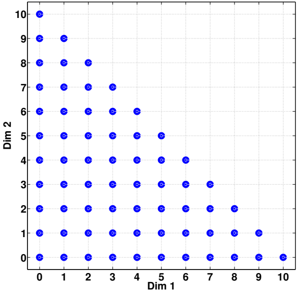
Bayesian inference of PC surrogate: high-d, low-data regime

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

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



- Issues:
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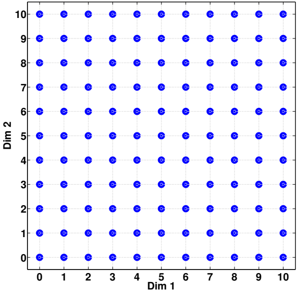

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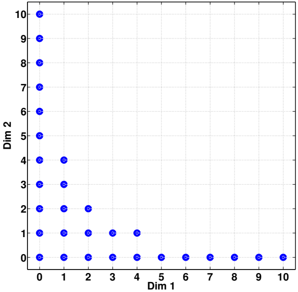

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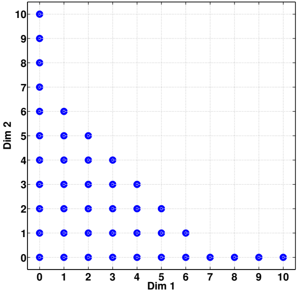

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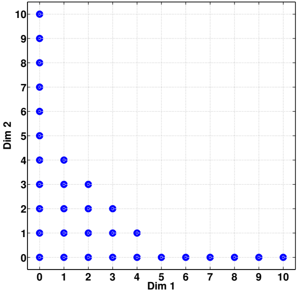

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In a different language....

- N training data points $(\boldsymbol{x}_n, u_n)$ and K basis terms $\Psi_k(\cdot)$
- Projection matrix $\boldsymbol{P}^{N\times K}$ with $\boldsymbol{P}_{nk} = \Psi_k(\boldsymbol{x}_n)$
- Find regression weights $\boldsymbol{c} = (c_0, \ldots, c_{K-1})$ so that

$$\boldsymbol{u} \approx \boldsymbol{P}\boldsymbol{c} \qquad \text{or} \qquad u_n \approx \sum_k c_k \Psi_k(\boldsymbol{x}_n)$$

- The number of polynomial basis terms grows fast; a p-th order, d-dimensional basis has a total of $K = (p+d)!/(p!d!)$ terms.
- For limited data and large basis set ($N < K$) this is a sparse signal recovery problem $\Rightarrow$ need some regularization/constraints.

- Least-squares $\quad$ *argmin*$_{\boldsymbol{c}}$ $\{||\boldsymbol{u} - \boldsymbol{P}\boldsymbol{c}||_2\}$
- The 'sparsest' $\quad$ *argmin*$_{\boldsymbol{c}}$ $\{||\boldsymbol{u} - \boldsymbol{P}\boldsymbol{c}||_2 + \alpha||\boldsymbol{c}||_0\}$
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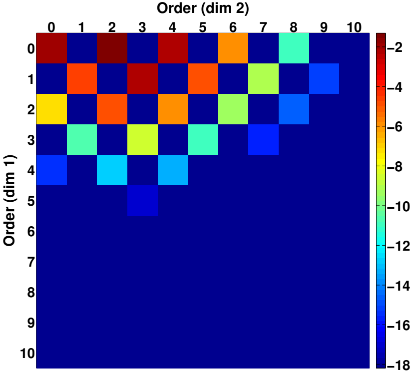
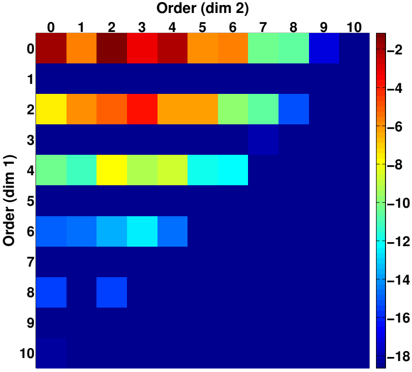
Bayesian $\qquad$ Likelihood $\qquad$ Prior

BCS removes unnecessary basis terms

$$f(x,y) = \cos(x + 4y)$$



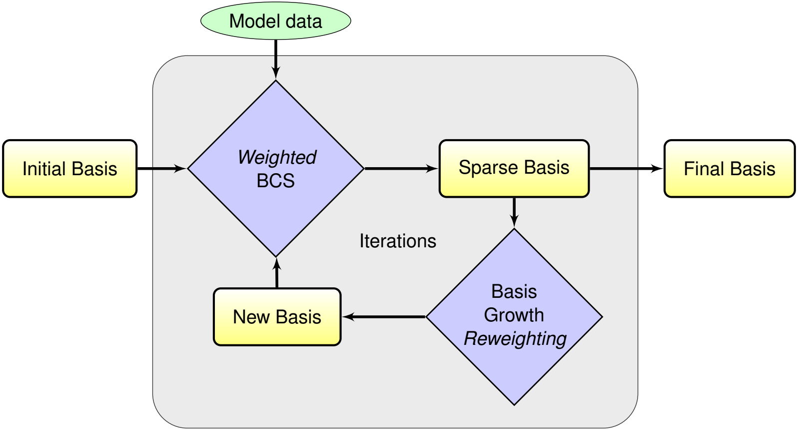
$$f(x,y) = \cos(x^2 + 4y)$$

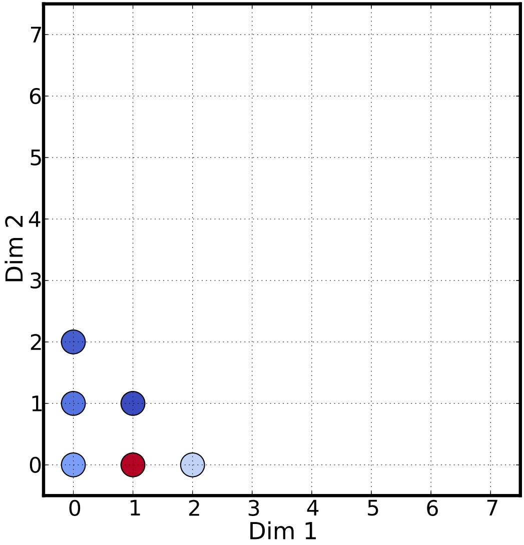


The square (i,j) represents the (log) spectral coefficient for the basis term $\psi_i(x)\psi_j(y)$.

Iterative Bayesian Compressive Sensing (iBCS)

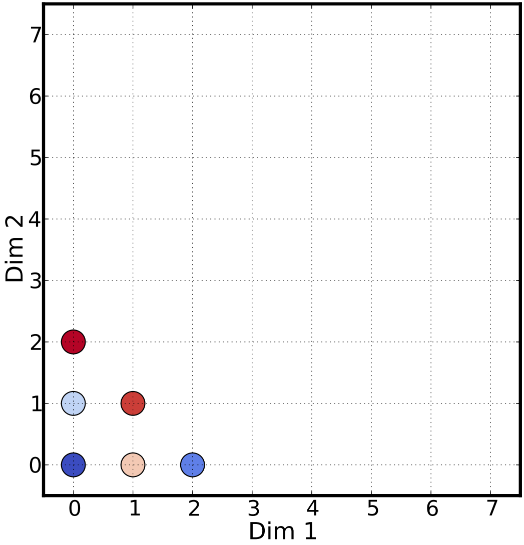
- *Iterative BCS*: We implement an iterative procedure that allows increasing the order for the relevant basis terms while maintaining the dimensionality reduction [Sargsyan *et al.* 2014], [Jakeman *et al.* 2015].
- Combine basis growth and reweighting!



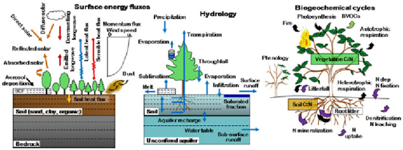


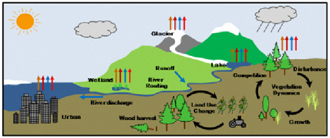
Dim 2
Dim 1
0
1
2
3
4
5
6
7

Basis set growth: ... added outlier term



Application of Interest: ACME Land Model





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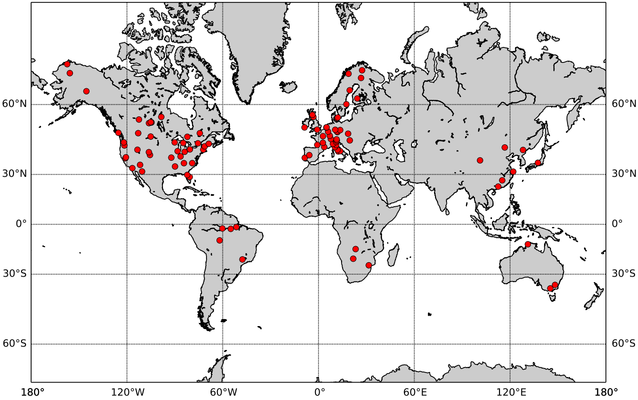
FLUXNET experiment

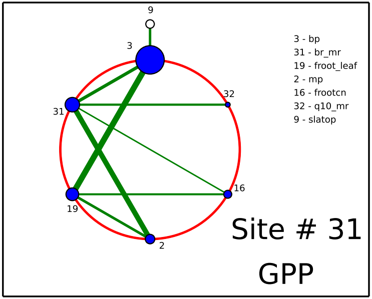


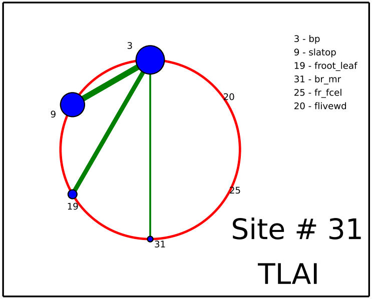
FLUXNET sites

- 96 FLUXNET sites covering major biomes and plant functional types
- Varying 68 input parameters over given ranges; 5 steady state outputs
- Ensemble of 3000 runs on Titan, DoE Leadership Computing Facility at Oak Ridge National Lab

Sparse PC surrogate and uncertainty decomposition for the ACME Land Model

- Main effect sensitivities : rank input parameters
- Joint sensitivities : most influential input couplings
- About 200 polynomial basis terms in the 68-dimensional space
- Sparse PC will further be used for
  - sampling in a reduced space
  - parameter calibration against experimental data





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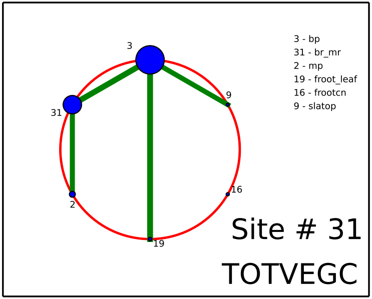

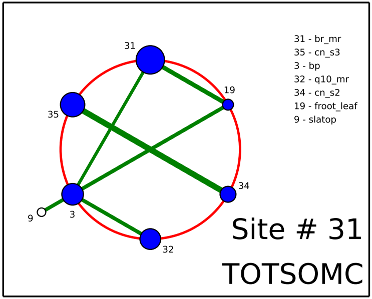

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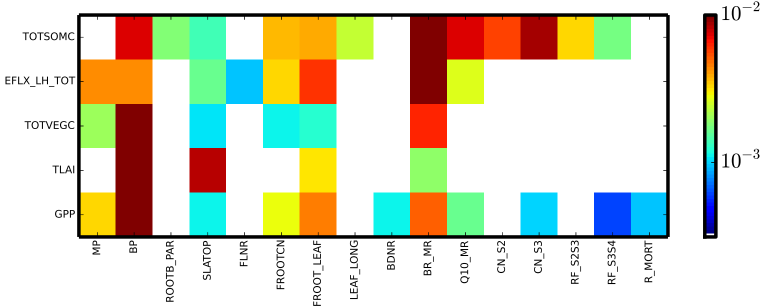

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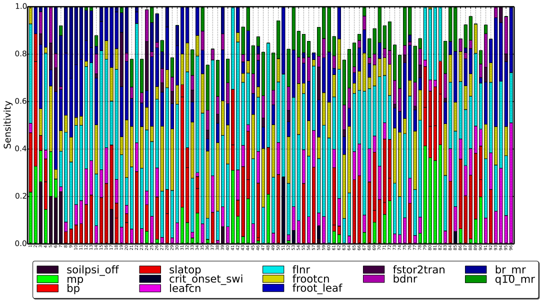
- GPP
  gross primary
  productivity



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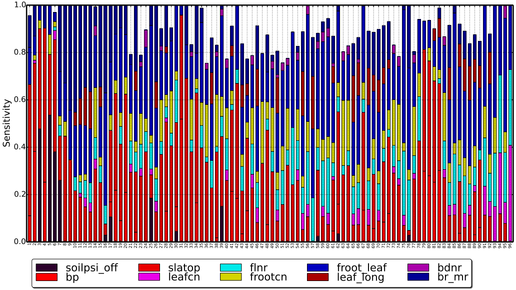
- TLAI
  leaf area index



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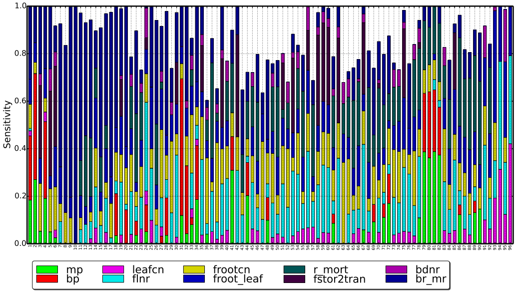
- TOTVEGC
  vegetation carbon



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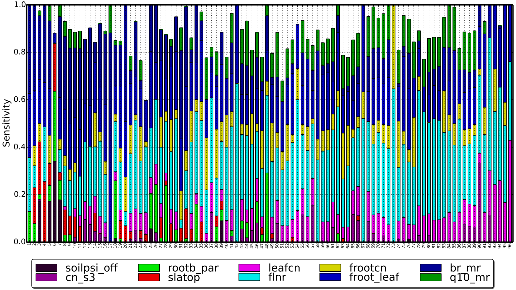
- EFLX_LH_TOT
  latent heat flux



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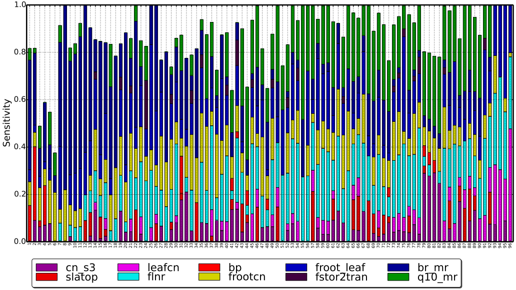
- TOTSOMC soil organic matter carbon



Summary

- Surrogate models are necessary for complex models
  - Replace the full model for both forward and inverse UQ
- Uncertain inputs
  - Polynomial Chaos surrogates well-suited
- Limited training dataset
  - Bayesian methods handle limited information well
- Curse of dimensionality
  - The hope is that not too many dimensions matter
  - Compressive sensing (CS) ideas ported from machine learning
  - We implemented *iteratively* reweighting Bayesian CS algorithm that reduces dimensionality and increases order on-the-fly.

- Open issues
  - Computational design. What is the best sampling strategy?
  - Overfitting still present. Cross-validation techniques help.

- Software: employed SNL-CA UQ library UQTk (www.sandia.gov/uqtoolkit)

Literature

- M. Tipping, “Sparse Bayesian learning and the relevance vector machine”, *J Machine Learning Research*, 1, pp. 211-244, 2001.
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- K. Sargsyan, C. Safta, H. Najm, B. Debusschere, D. Ricciuto and P. Thornton, “Dimensionality reduction for complex models via Bayesian compressive sensing”, *Int J for Uncertainty Quantification*, 4(1), pp. 63-93, 2014.

- J. Jakeman, M. Eldred and K. Sargsyan, “Enhancing ℓ_1-minimization estimates of polynomial chaos expansions using basis selection”, *J Comp Phys*, 289, pp. 18-34, 2015.

Random variables represented by Polynomial Chaos

$$X \simeq \sum_{k=0}^{K-1} c_k \Psi_k(\boldsymbol{\eta})$$

- $\boldsymbol{\eta} = (\eta_1, \cdots, \eta_d)$ standard i.i.d. r.v.
  Ψ_k standard polynomials, orthogonal w.r.t. $\pi(\boldsymbol{\eta})$.

$$\Psi_k(\eta_1, \eta_2, \ldots, \eta_d) = \psi_{k_1}(\eta_1)\psi_{k_2}(\eta_2)\cdots\psi_{k_d}(\eta_d)$$

- Typical truncation rule: total-order p, $k_1 + k_2 + \ldots k_d \leq p$.
  Number of terms is $K = \frac{(d+p)!}{d!p!}$.
- Essentially, a parameterization of a r.v. by deterministic spectral modes c_k .
- Most common standard Polynomial-Variable pairs:
  (continuous) Gauss-Hermite, Legendre-Uniform,
  (discrete) Poisson-Charlier.

[Wiener, 1938; Ghanem & Spanos, 1991; Xiu & Karniadakis, 2002; Le Maître & Knio, 2010]

Bayesian inference of PC surrogate

$$u \simeq \sum_{k=0}^{K-1} c_k \Psi_k(\boldsymbol{x}) \equiv g_{\boldsymbol{c}}(\boldsymbol{x}) \qquad \overbrace{P(\boldsymbol{c}|\mathcal{D})}^{\text{Posterior}} \propto \overbrace{P(\mathcal{D}|\boldsymbol{c})}^{\text{Likelihood}} \overbrace{P(\boldsymbol{c})}^{\text{Prior}}$$

- Data consists of *training runs*

$$\mathcal{D} \equiv \{(\boldsymbol{x}_i, u_i)\}_{i=1}^{N}$$

- Likelihood with a gaussian noise model with σ^2 fixed or inferred,

$$L(\boldsymbol{c}) = P(\mathcal{D}|\boldsymbol{c}) = \left(\frac{1}{\sigma\sqrt{2\pi}}\right)^N \prod_{i=1}^{N} \exp\left(-\frac{(u_i - g_{\boldsymbol{c}}(\boldsymbol{x}))^2}{2\sigma^2}\right)$$

- Prior on $\boldsymbol{c}$ is chosen to be conjugate, uniform or gaussian.
- Posterior is a *multivariate normal*

$$\boldsymbol{c} \quad \in \quad \mathcal{MVN}(\boldsymbol{\mu}, \boldsymbol{\Sigma})$$

- The (uncertain) surrogate is *a gaussian process*

$$\sum_{k=0}^{K-1} c_k \Psi_k(\boldsymbol{x}) = \boldsymbol{\Psi}(\boldsymbol{x})^T \boldsymbol{c} \quad \in \quad \mathcal{GP}(\boldsymbol{\Psi}(\boldsymbol{x})^T \boldsymbol{\mu}, \boldsymbol{\Psi}(\boldsymbol{x}) \boldsymbol{\Sigma} \boldsymbol{\Psi}(\boldsymbol{x}')^T)$$

Sensitivity information comes free with PC surrogate,

$$g(x_1, \ldots, x_d) = \sum_{k=0}^{K-1} c_k \Psi_k(\boldsymbol{x})$$

- Main effect sensitivity indices

$$S_i = \frac{Var[\mathbb{E}(g(\boldsymbol{x}|x_i)]}{Var[g(\boldsymbol{x})]} = \frac{\sum_{k \in \mathbb{I}_i} c_k^2 ||\Psi_k||^2}{\sum_{k>0} c_k^2 ||\Psi_k||^2}$$

$\mathbb{I}_i$ is the set of bases with only x_i involved

Sensitivity information comes free with PC surrogate,

$$g(x_1, \ldots, x_d) = \sum_{k=0}^{K-1} c_k \Psi_k(\boldsymbol{x})$$

- Main effect sensitivity indices

$$S_i = \frac{Var[\mathbb{E}(g(\boldsymbol{x}|x_i)]}{Var[g(\boldsymbol{x})]} = \frac{\sum_{k \in \mathbb{I}_i} c_k^2 ||\Psi_k||^2}{\sum_{k>0} c_k^2 ||\Psi_k||^2}$$

- Joint sensitivity indices

$$S_{ij} = \frac{Var[\mathbb{E}(g(\boldsymbol{x}|x_i, x_j)]}{Var[g(\boldsymbol{x})]} - S_i - S_j = \frac{\sum_{k \in \mathbb{I}_{ij}} c_k^2 ||\Psi_k||^2}{\sum_{k>0} c_k^2 ||\Psi_k||^2}$$

$\mathbb{I}_{ij}$ is the set of bases with only x_i and x_j involved

Sensitivity information comes free with PC surrogate,

but not with piecewise PC

$$g(x_1, \ldots, x_d) = \sum_{k=0}^{K-1} c_k \Psi_k(\boldsymbol{x})$$

- Main effect sensitivity indices

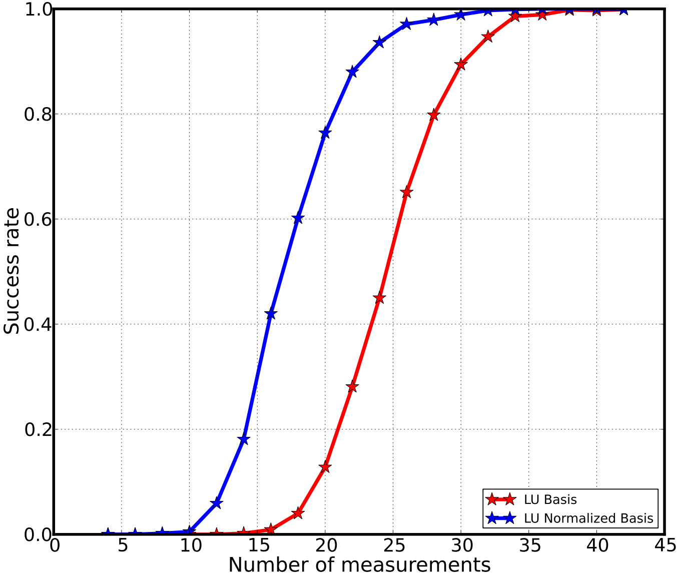
$$S_i = \frac{Var[\mathbb{E}(g(\boldsymbol{x}|x_i)]}{Var[g(\boldsymbol{x})]} = \frac{\sum_{k\in\mathbb{I}_i} c_k^2 ||\Psi_k||^2}{\sum_{k>0} c_k^2 ||\Psi_k||^2}$$

- Joint sensitivity indices

$$S_{ij} = \frac{Var[\mathbb{E}(g(\boldsymbol{x}|x_i, x_j)]}{Var[g(\boldsymbol{x})]} - S_i - S_j = \frac{\sum_{k\in\mathbb{I}_{ij}} c_k^2 ||\Psi_k||^2}{\sum_{k>0} c_k^2 ||\Psi_k||^2}$$

- For piecewise PC, need to resort to Monte-Carlo estimation [Saltelli, 2002].

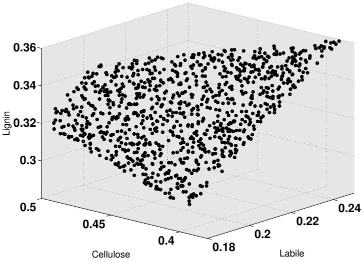
Basis normalization helps the success rate



Input correlations: Rosenblatt transformation

- Rosenblatt transformation maps any (not necessarily independent) set of random variables $\boldsymbol{\lambda} = (\lambda_1, \ldots, \lambda_d)$ to uniform i.i.d.'s $\{x_i\}_{i=1}^d$ [Rosenblatt, 1952].

$$\begin{aligned}
x_1 &= F_1(\lambda_1) \\
x_2 &= F_{2|1}(\lambda_2|\lambda_1) \\
x_3 &= F_{3|2,1}(\lambda_3|\lambda_2, \lambda_1) \\
&\vdots \\
x_d &= F_{d|d-1,\ldots,1}(\lambda_d|\lambda_{d-1}, \ldots, \lambda_1)
\end{aligned}$$



- Inverse Rosenblatt transformation $\boldsymbol{\lambda} = R^{-1}(\boldsymbol{x})$ ensures a well-defined input PC construction

$$\lambda_i = \sum_{k=0}^{K-1} \lambda_{ik} \Psi_k(\boldsymbol{x})$$

- Caveat: the conditional distributions are often hard to evaluate accurately.

Strong discontinuities/nonlinearities challenge global polynomial expansions

- Basis enrichment [Ghosh & Ghanem, 2005]
- Stochastic domain decomposition
  - Wiener-Haar expansions,
    Multiblock expansions,
    Multiwavelets, [Le Maître *et al*, 2004,2007]
  - also known as Multielement PC [Wan & Karniadakis, 2009]
- Smart splitting, discontinuity detection
  [Archibald *et al*, 2009; Chantrasmi, 2011; Sargsyan *et al*, 2011; Jakeman *et al*, 2012]
- Data domain decomposition,
  - Mixture PC expansions [Sargsyan *et al*, 2010]
- Data clustering, classification,
  - Piecewise PC expansions

Piecewise PC expansion with classification

- Cluster the training dataset into non-overlapping subsets $\mathcal{D}_1$ and $\mathcal{D}_2$, where the behavior of function is smoother
- Construct global PC expansions $g_i(\boldsymbol{x}) = \sum_k c_{ik}\Psi_k(\boldsymbol{x})$ using each dataset individually ($i = 1, 2$)
- Declare a surrogate

$$g_s(\boldsymbol{x}) = \begin{cases} g_1(\boldsymbol{x}) & \text{if } \boldsymbol{x} \in^* \mathcal{D}_1 \\ g_2(\boldsymbol{x}) & \text{if } \boldsymbol{x} \in^* \mathcal{D}_2 \end{cases}$$

* Requires a classification step to find out which cluster $\boldsymbol{x}$ belongs to. We applied Random Decision Forests (RDF).

- Caveat: the sensitivity information is harder to obtain.