

Sparse surrogate model construction via compressive sensing for high-dimensional complex models

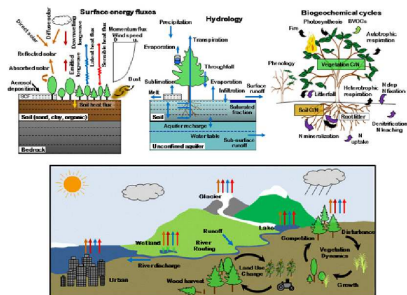
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under Climate Science for Sustainable Energy Future (CSSEF).*

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Application of Interest: Community Land Model



<http://www.cesm.ucar.edu/models/clm/>

- Nested computational grid hierarchy
- A single-site, 1000-yr simulation takes ~ 10 hrs on 1 CPU
- Involves ~ 70 input parameters; some dependent
- Non-smooth input-output relationship
- CLM simulations courtesy of Dan Ricciuto and Peter Thornton (ORNL)

Challenges we tackle

- Global sensitivity analysis
- Input parameter calibration
- Forward uncertainty propagation

- 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

- Input parameter correlations/dependencies

- Strongly non-smooth forward function

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Construct surrogate for a complex model

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Random variables represented by Polynomial Chaos

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

- $\boldsymbol{\eta} = (\eta_1, \dots, \eta_d)$ standard i.i.d. r.v.
 Ψ_k standard polynomials, orthogonal w.r.t. $\pi(\boldsymbol{\eta})$.
$$\Psi_k(\eta_1, \eta_2, \dots, \eta_d) = \psi_{k_1}(\eta_1) \psi_{k_2}(\eta_2) \cdots \psi_{k_d}(\eta_d)$$
- Typical truncation rule: total-order p , $k_1 + k_2 + \dots + k_d \leq p$.
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]

Polynomial Chaos surrogate construction

- Build/presume PC for input parameter λ

$$\lambda(\boldsymbol{\eta}) = \sum_{k=0}^{K-1} \mathbf{a}_k \Psi_k(\boldsymbol{\eta})$$

with respect to multivariate polynomials of choice.

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- e.g., gaussian with known moments, or uniform on an interval,

$$\lambda = \lambda_0 + \lambda_1 \eta$$

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- If input parameters are uniform $\lambda_i \sim \text{Uniform}[a_i, b_i]$, then

$$\lambda_i = \frac{a_i + b_i}{2} + \frac{b_i - a_i}{2} \eta_i.$$

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

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

- Global sensitivity information for free
 - Sobol indices, variance-based decomposition.
- Input dependencies/correlations \rightarrow Rosenblatt transformation

Estimation of PC coefficients

$$u \simeq \sum_{k=0}^{K-1} c_k \Psi_k(\boldsymbol{\eta}) \quad c_k = \frac{\langle u(\boldsymbol{\eta}) \Psi_k(\boldsymbol{\eta}) \rangle}{\langle \Psi_k^2(\boldsymbol{\eta}) \rangle}$$

The integral $\langle u(\boldsymbol{\eta}) \Psi_k(\boldsymbol{\eta}) \rangle = \int u(\boldsymbol{\eta}) \Psi_k(\boldsymbol{\eta}) \pi(\boldsymbol{\eta}) d\boldsymbol{\eta}$ can be estimated by

- Monte-Carlo

$$\frac{1}{N} \sum_{j=1}^N u(\boldsymbol{\eta}_j) \Psi_k(\boldsymbol{\eta}_j)$$



many samples from $\pi(\boldsymbol{\eta})$

- Quadrature

$$\sum_{j=1}^Q u(\boldsymbol{\eta}_j) \Psi_k(\boldsymbol{\eta}_j) w_j$$



samples at quadrature points

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samples at quadrature points

- *Bayesian inference*

$$P(c_k | u(\boldsymbol{\eta}_j)) \propto P(u(\boldsymbol{\eta}_j) | c_k) P(c_k)$$



any (number of) samples

Bayesian inference of PC surrogate

$$u \simeq \sum_{k=0}^{K-1} c_k \Psi_k(\boldsymbol{\eta}) \equiv g\mathbf{c}(\boldsymbol{\eta}) \quad \underbrace{P(\mathbf{c}|\mathcal{D})}_{\text{Posterior}} \propto \underbrace{P(\mathcal{D}|\mathbf{c})}_{\text{Likelihood}} \underbrace{P(\mathbf{c})}_{\text{Prior}}$$

- Data consists of *training runs*

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

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

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

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

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

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

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

In a different language....

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

$$\mathbf{u} \approx \mathbf{P}\mathbf{c}$$

- 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.
- Tikhonov regularization $\quad \operatorname{argmin}_{\mathbf{c}} \{ \|\mathbf{u} - \mathbf{P}\mathbf{c}\|_2 + \alpha \|\mathbf{c}\|_2 \}$
- Lasso regression $\quad \operatorname{argmin}_{\mathbf{c}} \{ \|\mathbf{u} - \mathbf{P}\mathbf{c}\|_2 \}$ subject to $\|\mathbf{c}\|_1 \leq \alpha$
- Compressive sensing $\quad \operatorname{argmin}_{\mathbf{c}} \{ \|\mathbf{u} - \mathbf{P}\mathbf{c}\|_2 + \alpha \|\mathbf{c}\|_1 \}$

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Bayesian Likelihood Prior

Bayesian Compressive Sensing (BCS)

- Dimensionality reduction by using hierarchical priors

$$p(c_k|\sigma_k^2) = \frac{1}{\sqrt{2\pi}\sigma_k} e^{-\frac{c_k^2}{2\sigma_k^2}} \quad p(\sigma_k^2|\alpha) = \frac{\alpha}{2} e^{-\frac{\alpha\sigma_k^2}{2}}$$

- Effectively, one obtains Laplace *sparsity* prior

$$p(\mathbf{c}|\alpha) = \int \prod_{k=0}^{K-1} p(c_k|\sigma_k^2)p(\sigma_k^2|\alpha)d\sigma_k^2 = \prod_{k=0}^{K-1} \frac{\sqrt{\alpha}}{2} e^{-\sqrt{\alpha}|c_k|}$$

- The parameter α can be further modeled hierarchically, or fixed.
- Evidence maximization dictates values for σ_k^2 , α , σ^2 and allows exact Bayesian solution

$$\mathbf{c} \sim \mathcal{MVN}(\boldsymbol{\mu}, \boldsymbol{\Sigma})$$

with

$$\boldsymbol{\mu} = \sigma^{-2}\boldsymbol{\Sigma}\mathbf{P}^T\mathbf{u} \quad \boldsymbol{\Sigma} = \sigma^2(\mathbf{P}^T\mathbf{P} + \text{diag}(\sigma^2/\sigma_k^2))^{-1}$$

[Ji *et al.*, 2008; Babacan *et al.*, 2010]

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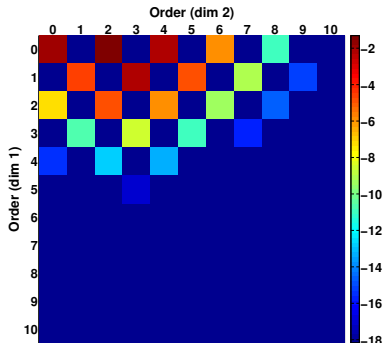
$$\boldsymbol{\mu} = \sigma^{-2}\boldsymbol{\Sigma}\mathbf{P}^T\mathbf{u} \quad \boldsymbol{\Sigma} = \sigma^2(\mathbf{P}^T\mathbf{P} + \text{diag}(\sigma^2/\sigma_k^2))^{-1}$$

- KEY: Some $\sigma_k^2 \rightarrow 0$, hence the corresponding basis terms are dropped.

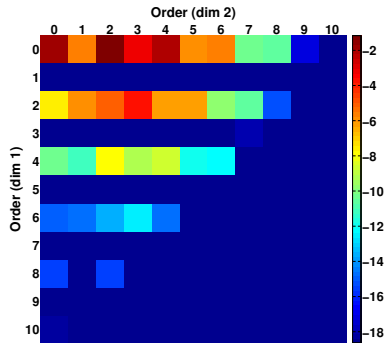
[Ji *et al.*, 2008; Babacan *et al.*, 2010]

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 $\psi_i(x)\psi_j(y)$.

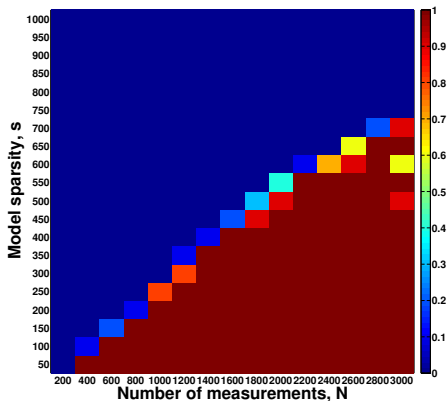
Success rate grows with more data and 'sparser' model

Consider test function

$$f(\mathbf{x}) = \sum_{k=0}^{K-1} c_k \Psi_k(\mathbf{x})$$

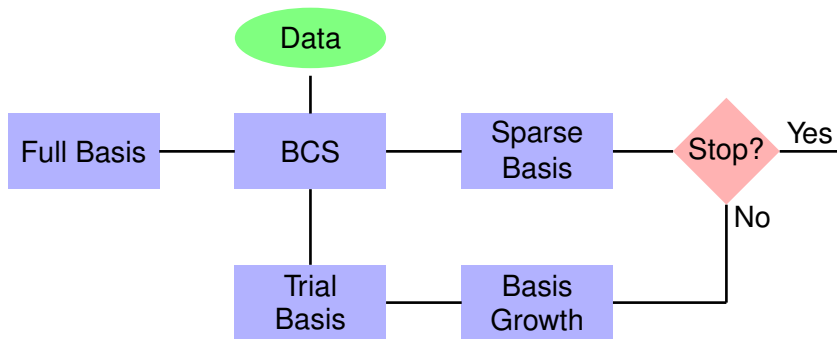
where only S coefficients c_k are non-zero. Typical setting is

$$S < N < K$$



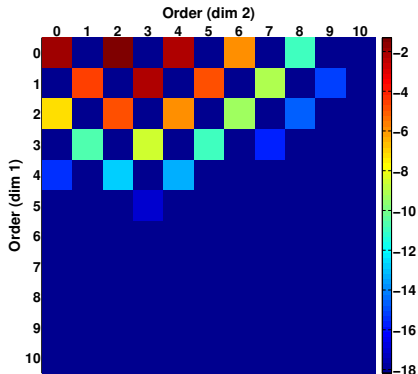
Iterative Bayesian Compressive Sensing (iBCS)

- *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.* 2013].



Basis set growth

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



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 $g_i(\mathbf{x}) = \sum_k c_{ik} \Psi_k(\mathbf{x})$ using each dataset individually ($i = 1, 2$)
- Declare a surrogate

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

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

- Caveat: the sensitivity information is harder to obtain.

Illustration of piecewise PC construction

Global 5-th order surrogate fails

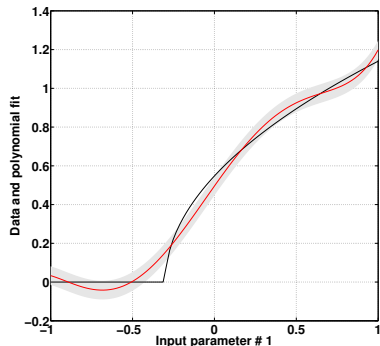
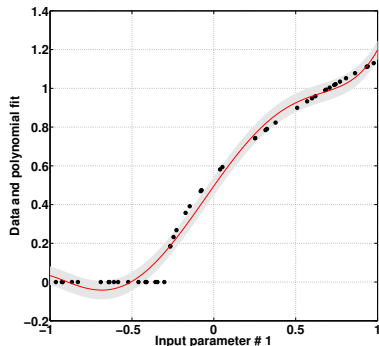


Illustration of piecewise PC construction

Piecewise 5-th order surrogate

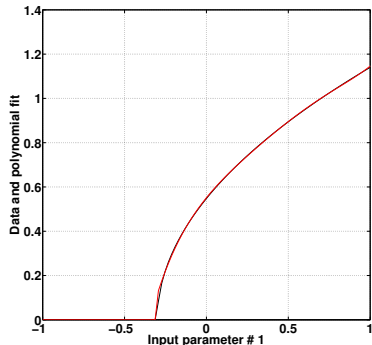
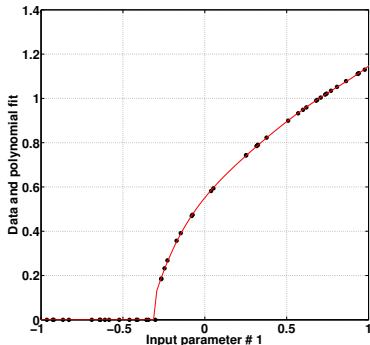
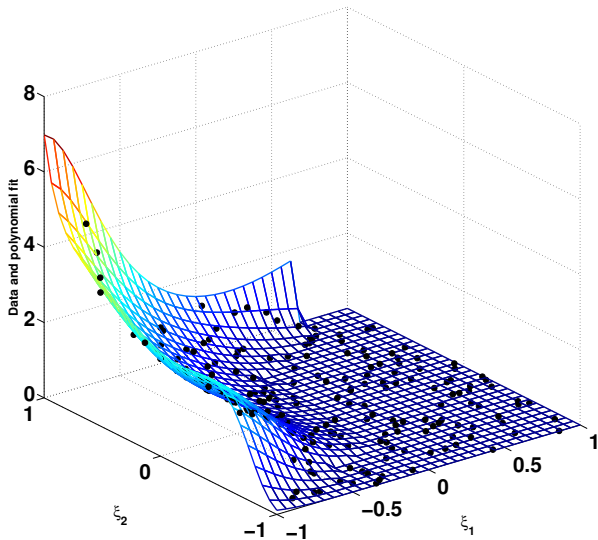
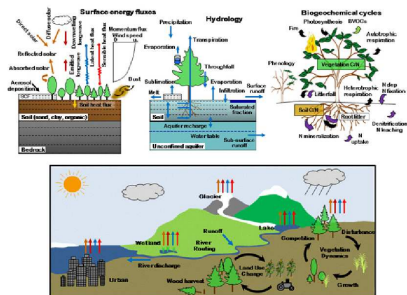


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$$g(x_1, \dots, x_d) = \sum_{k=0}^{K-1} c_k \Psi_k(\mathbf{x})$$

- Main effect sensitivity indices

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

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

- Joint sensitivity indices

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

\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

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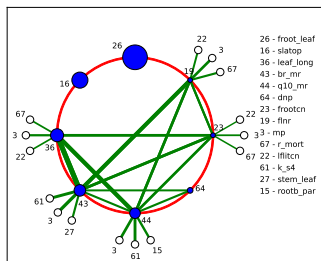
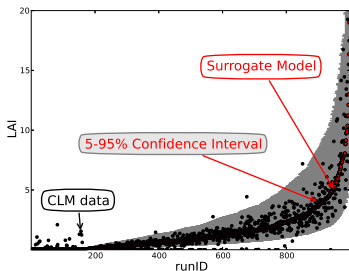
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- For piecewise PC, need to resort to Monte-Carlo estimation
[Saltelli, 2002].

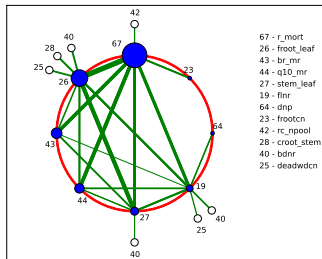
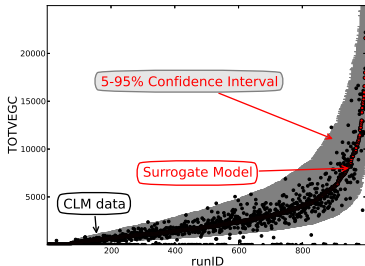
Sparse PC surrogate for the Community Land Model - 10K ensemble

- iBCS leads to about 200 polynomial basis terms in the 70-dimensional space
- Main effect sensitivities : rank input parameters
- Joint sensitivities : most influential input couplings
- Sparse PC will further be used for
 - sampling in a reduced space
 - parameter calibration against experimental data



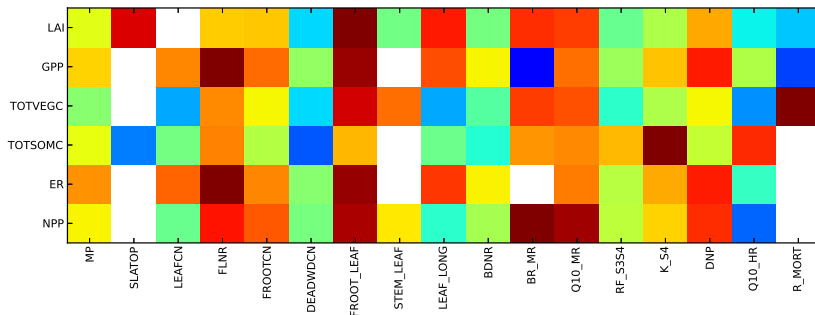
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Summary

- 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 *iterative* Bayesian CS algorithm that reduces dimensionality and increases order on-the-fly.
- Dependent inputs
 - Rosenblatt transformation
- Nonlinear behavior
 - Data clustering and classification-driven piecewise PC
- Applied to CLM
 - Dimensionality reduction, Sensitivity analysis
 - Coming up: lower-dim surrogate and calibration

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Thank You