Techniques to Propagate Uncertainties

Goal: Consider the nonlinearly parameterized model

$$y = f(q)\ ,\ q = [q_1, \ldots, q_p]$$

with a specified distribution for q. What are appropriate techniques to determine a distribution or prediction interval for Y?

Techniques for Uncertainty Propagation:

- Monte Carlo sampling: General but slow convergence
- Analytic techniques for linearly parameterized models
- Perturbation techniques for nonlinear models
- Techniques utilizing surrogate models
  - General polynomial models (Chapter 16)
  - Stochastic spectral methods (Chapters 16 and 17)
  - Gaussian process or Kriging representations (Chapter 18)

Surrogate and Reduced-Order Models

Problem: Difficult to obtain sufficient number of realizations of discretized PDE models for Bayesian model calibration, design and control.

Mass
$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho v) = 0$$

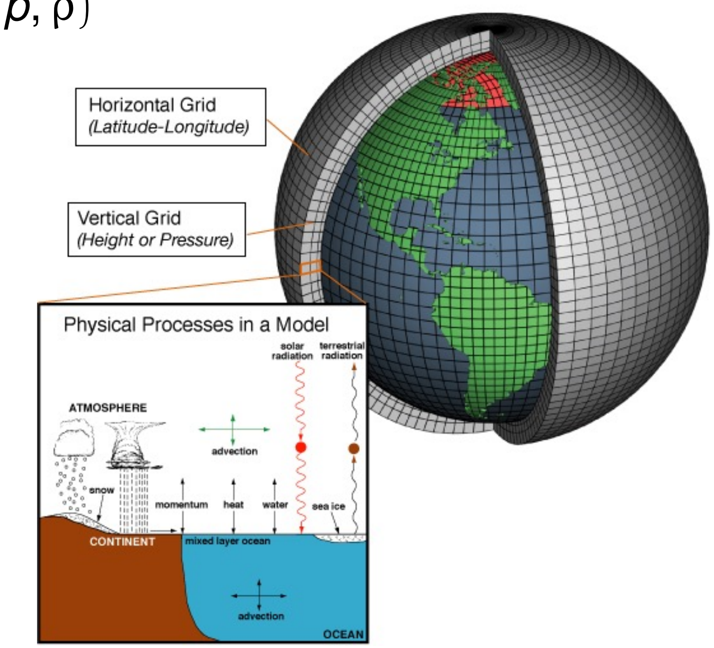
Momentum
$$\frac{\partial v}{\partial t} = -v \cdot \nabla v - \frac{1}{\rho}\nabla p - g\hat{k} - 2\Omega \times v$$

Energy
$$\rho c_V \frac{\partial T}{\partial t} + p\nabla \cdot v = -\nabla \cdot F + \nabla \cdot (k \nabla T) + \rho \dot{q}(T, p, \rho)$$

$$p = \rho R T$$

Water
$$\frac{\partial m_j}{\partial t} = -v \cdot \nabla m_j + S_{m_j}(T, m_j, \chi_j, \rho) \ , \ j = 1, 2, 3,$$

Aerosol
$$\frac{\partial \chi_j}{\partial t} = -v \cdot \nabla \chi_j + S_{\chi_j}(T, \chi_j, \rho) \ , \ j = 1, \cdots, J,$$



Solution: Construct surrogate models

- Also termed data-fit models, response surface models, emulators, meta-models
- Projection-based models often called reduced-order models (Chapter 19)

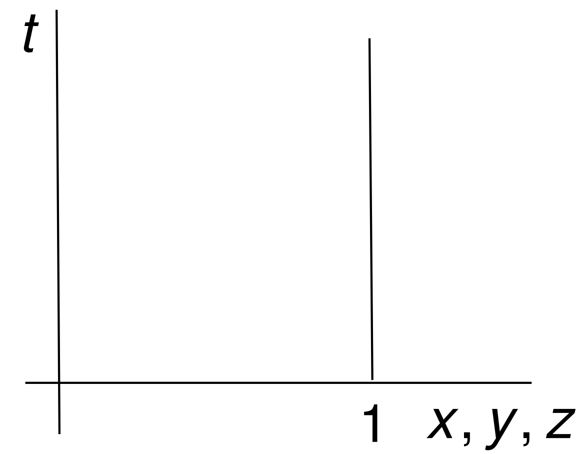
Surrogate Models: Motivation

Example: Consider the heat equation

$$\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} + \frac{\partial^2 u}{\partial z^2} + f(q)$$

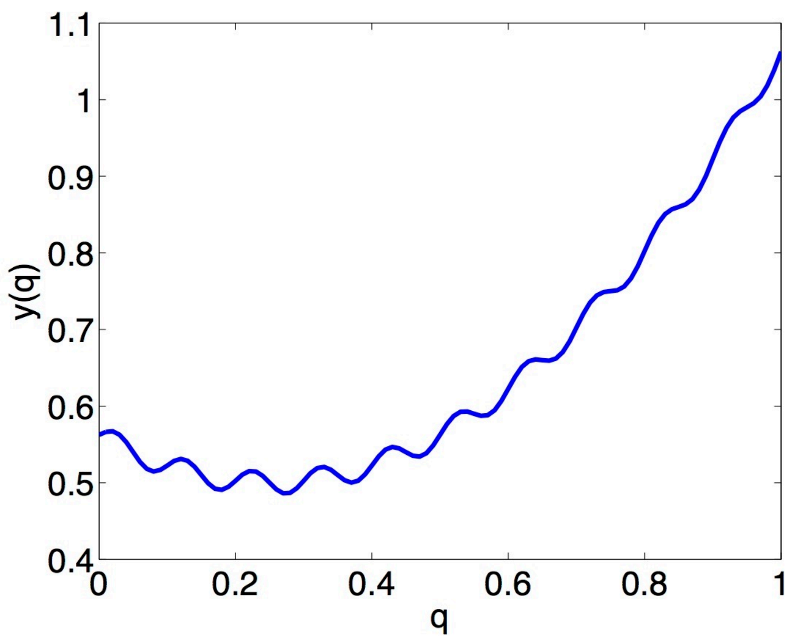
Boundary Conditions

Initial Conditions



with the response

$$y(q) = \int_0^1 \int_0^1 \int_0^1 \int_0^1 u(t,x,y,z)\,dxdydzdt$$



Notes:

- Requires approximation of PDE in 3-D
- What would be a simple surrogate?

Surrogate Models: Motivation

Example: Consider the heat equation

$$\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} + \frac{\partial^2 u}{\partial z^2} + f(q)$$

Boundary Conditions

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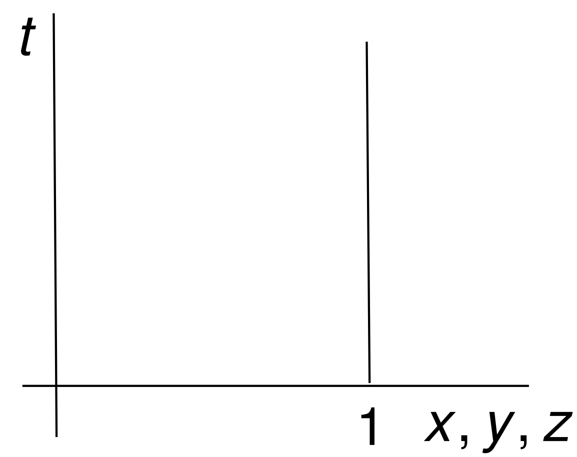
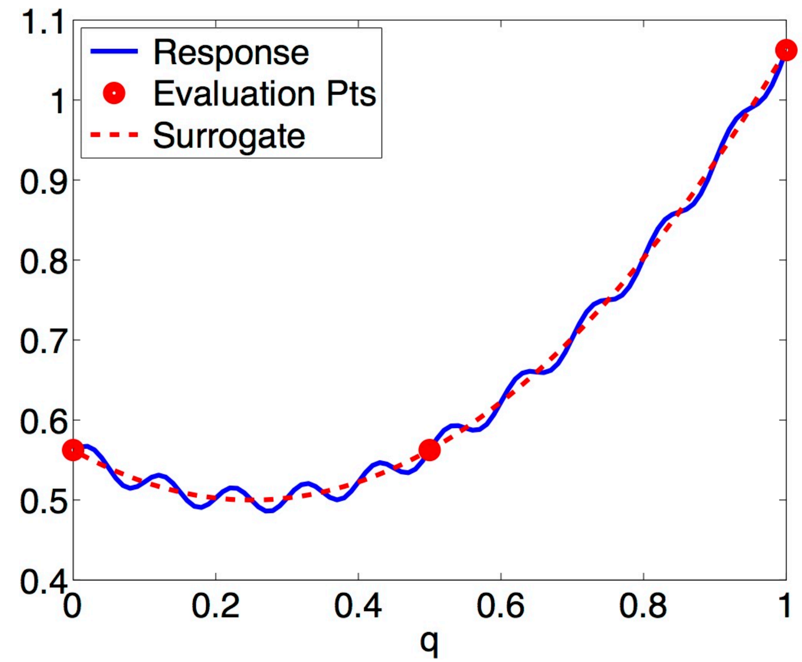


Surrogate: Quadratic

$$y_s(q) = (q - 0.25)^2 + 0.5$$



Question: How do you construct a polynomial surrogate?

- Regression
- Interpolation

Surrogate Models

Recall: Consider the model

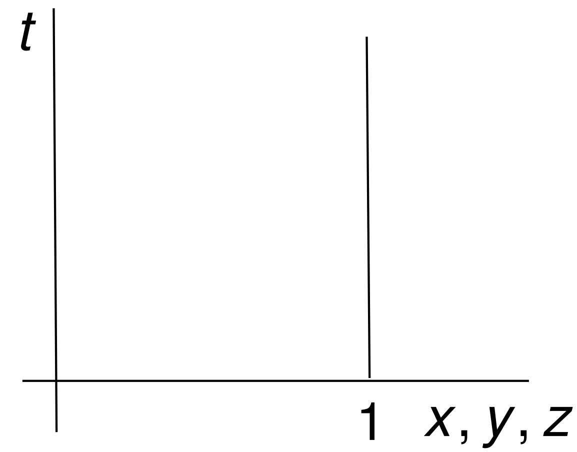
$$\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} + \frac{\partial^2 u}{\partial z^2} + f(q)$$

Boundary Conditions

Initial Conditions

with the response

$$y(q) = \int_0^1 \int_0^1 \int_0^1 \int_0^1 u(t,x,y,z)\, dxdydzdt$$



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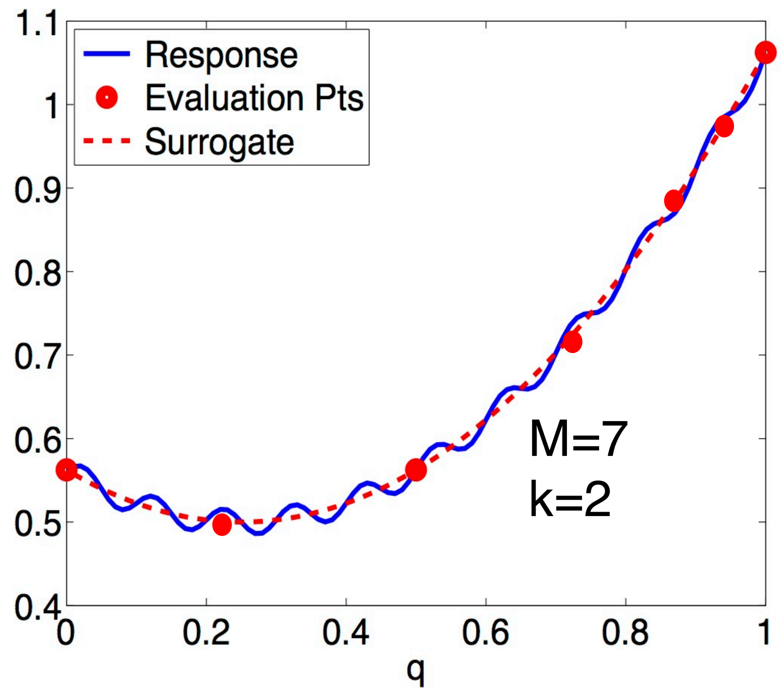


Question: How do you construct a polynomial surrogate?

- Interpolation
- Regression

Surrogate Models

Question: How do we keep from fitting noise?

- Akaike Information Criterion (AIC)

$$AIC = 2k - 2\log[\pi(y|q)]$$

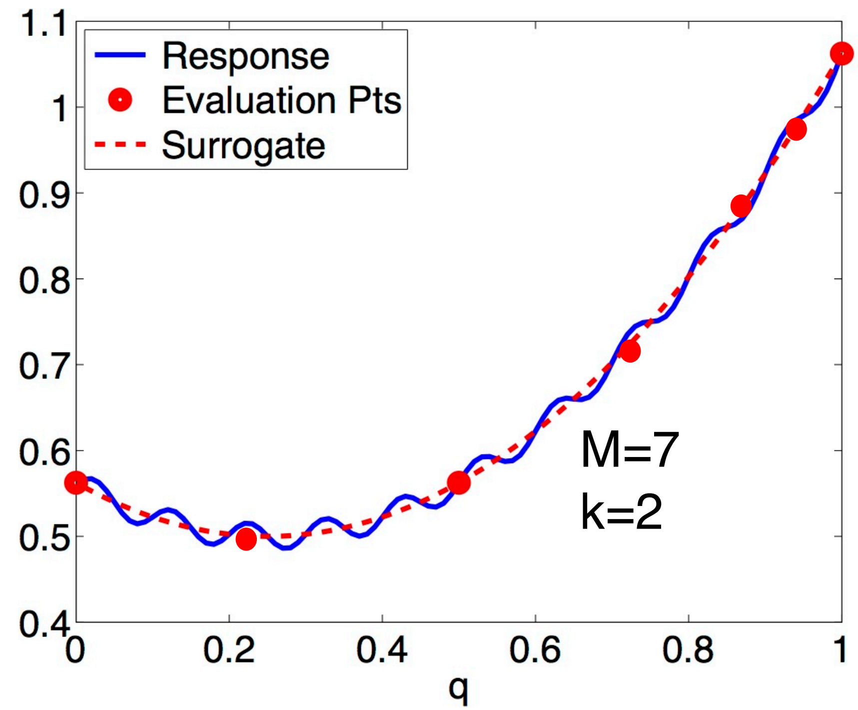
- Bayesian Information Criterion (BIC)

$$BIC = k\log(M) - 2\log[\pi(y|q)]$$

Likelihood:

$$\pi(y|q) = \frac{1}{(2\pi\sigma^2)^{M/2}} e^{-SS_q/2\sigma^2}$$ Maximize

$$SS_q = \sum_{m=1}^{M} [y_m - y_s(q^m)]^2$$ Minimize



Data-Fit Models

Notes:

• Often termed response surface models, surrogates, emulators, meta-models.

• Rely on interpolation or regression.

• Data can consist of high-fidelity simulations or experiments.

• Common techniques: polynomial models, kriging (Gaussian process regression), orthogonal polynomials.

Strategy: Consider high fidelity model

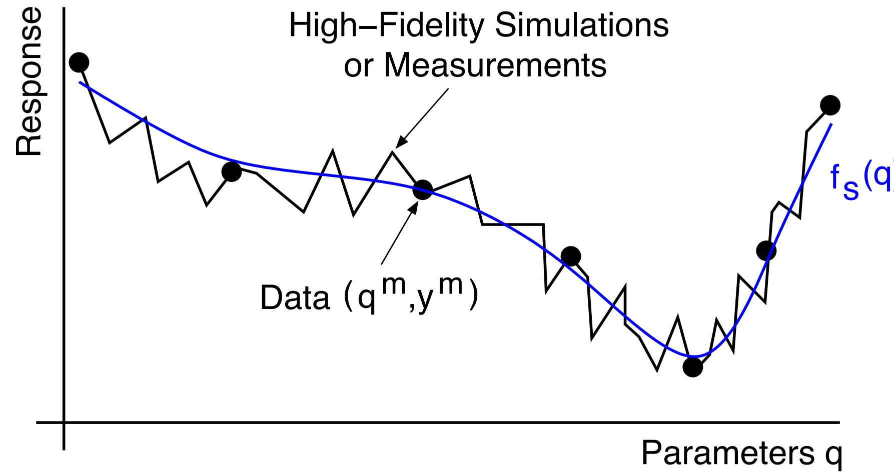
$$y = f(q)$$

with M model evaluations

$$y^m = f(q^m) \; , \;\; m = 1, \ldots , M$$

Statistical Model: $f_s(q)$: Surrogate for $f(q)$

$$y^m = f_s(q^m) + \varepsilon^m \; , \;\; m = 1, \ldots , M$$



Surrogate:

$$f_s^K(q,u) = \sum_{k=0}^{K} u_k \Psi_k(q) + P(q)$$

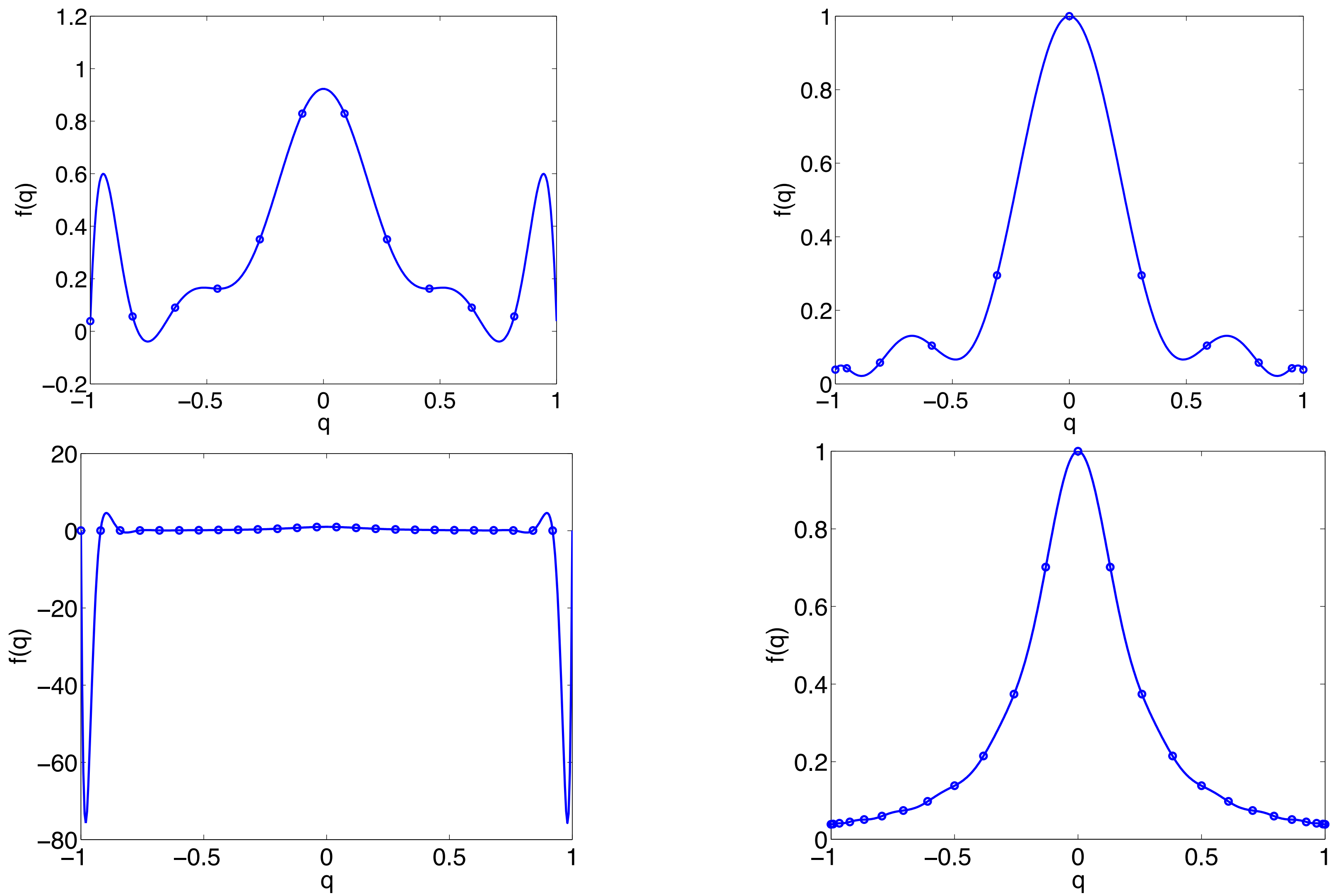
Options:

- Numerical: Often based on smoothness
- Statistical: Determined by covariance structure

Surrogate Models – Grid Choice

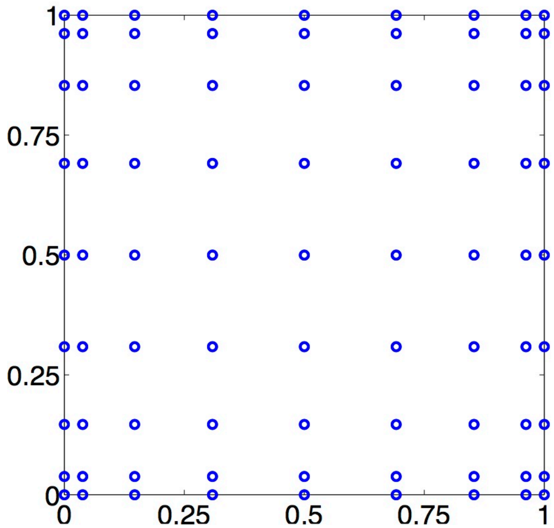
Example: Consider the Runge function $f(q) = \frac{1}{1+25q^2}$ with points

$$q^j = -1 + (j-1)\frac{2}{M}\ ,\ j = 1, \ldots, M \qquad q^j = -\cos\frac{\pi(j-1)}{M-1}\ ,\ j = 1, \ldots, M$$

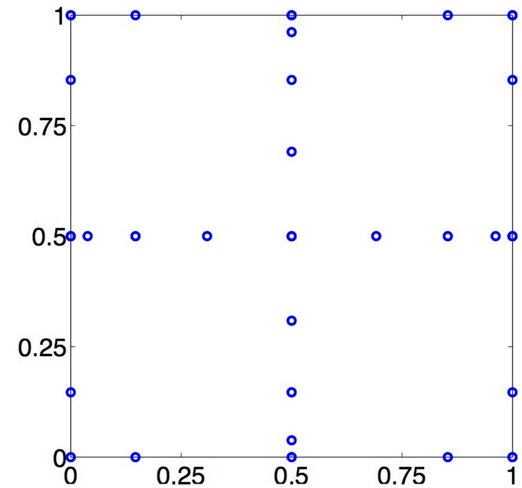


Sparse Grid Techniques

Tensored Grids: Exponential growth as a function of dimension



Sparse Grids: Same accuracy with significantly reduce number of points

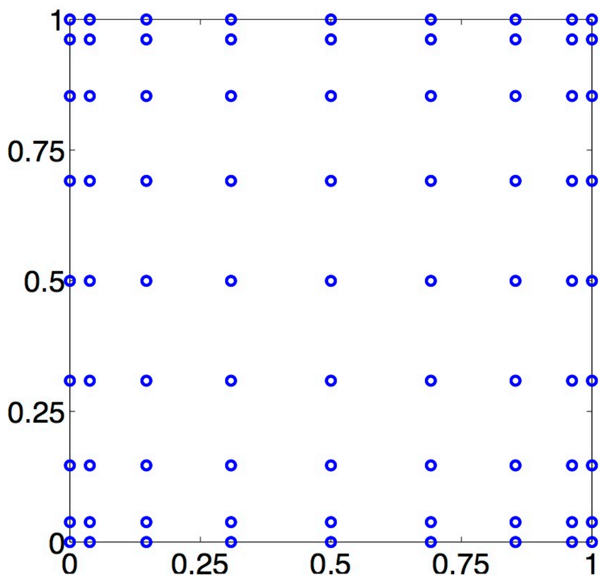


Motivation: Do not need full set of points to achieve same degree of accuracy

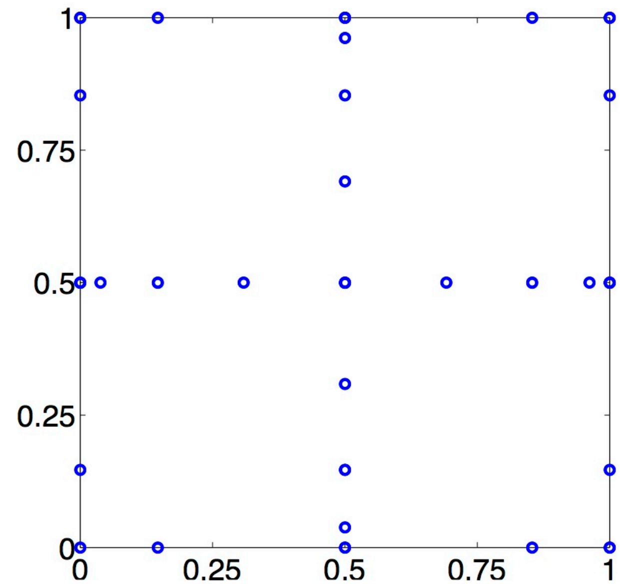
R									
0					1				
1				x		y			
2			x^2		xy		y^2		
3		x^3		x^2y		xy^2		y^3	
4	x^4		x^3y		x^2y^2		xy^3		y^4

Sparse Grid Techniques

Tensored Grids: Exponential growth



Sparse Grids: Same accuracy



p	R_ℓ	Sparse Grid $\mathcal{R}$	Tensored Grid $R = (R_\ell)^p$
2	9	29	81
5	9	241	59,049
10	9	1581	$> 3 \times 10^9$
50	9	171,901	$> 5 \times 10^{47}$
100	9	1,353,801	$> 2 \times 10^{95}$

Numerical Surrogate Models

Polynomial Surrogates:

$$f_s^K(q) = \sum_{k=0}^{K} u_k \Psi_k(q),$$

Notes:

- $\Psi_k(q)$ are univariate or multivariate polynomials
- Use interpolation or regression to determine weights $u = [u_0, \ldots, u_K]^T$

Univariate Interpolation: Consider

$$f_s^K(q) = \sum_{k=0}^{K} u_k \cdot (q)^k$$

Vandemonde System: y = Xu where

$$X = \begin{bmatrix} 1 & q^1 & (q^1)^2 & \cdots & (q^1)^K \\ \vdots & & & & \vdots \\ 1 & q^M & (q^M)^2 & \cdots & (q^M)^K \end{bmatrix} \quad , \quad y = \begin{bmatrix} y^0 \\ \vdots \\ y^M \end{bmatrix}$$

Warning: Typically ill-conditions so best avoided!

Polynomial Interpolation

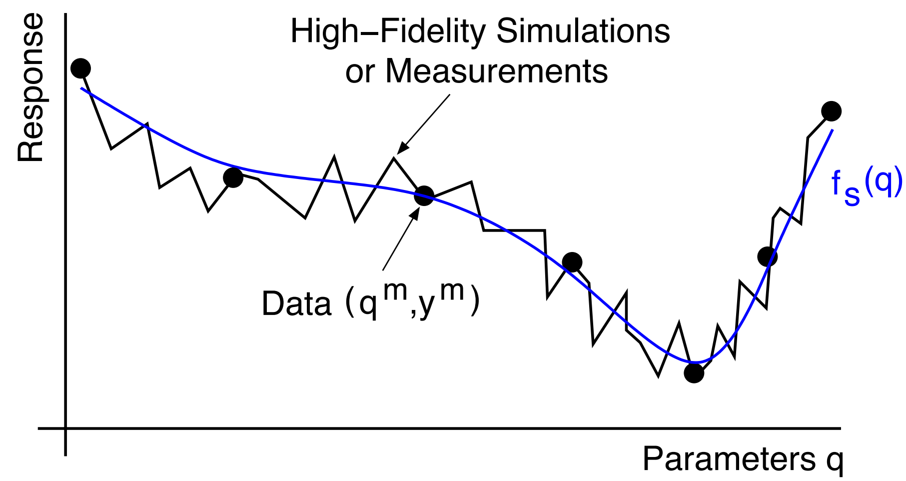
Lagrange representation: Take

$$f_s^M(q) = \sum_{m=0}^{M} y^m L_m(q)$$

where

$$L_m(q) = \prod_{\substack{j=0 \\ j \neq m}}^{M} \frac{q - q^j}{q^m - Q^j}$$

$$= \frac{(q-q^0)\cdots(q-q^{m-1})(q-q^{m+1})\cdots(q-q^M)}{(q^m-q^0)\cdots(q^m-q^{m-1})(q^m-q^{m+1})\cdots(q^m-q^M)}$$



Note: Because

$$L_m(q^j) = \delta_{mj}\ ,\ 0 \leqslant m, j \leqslant M$$

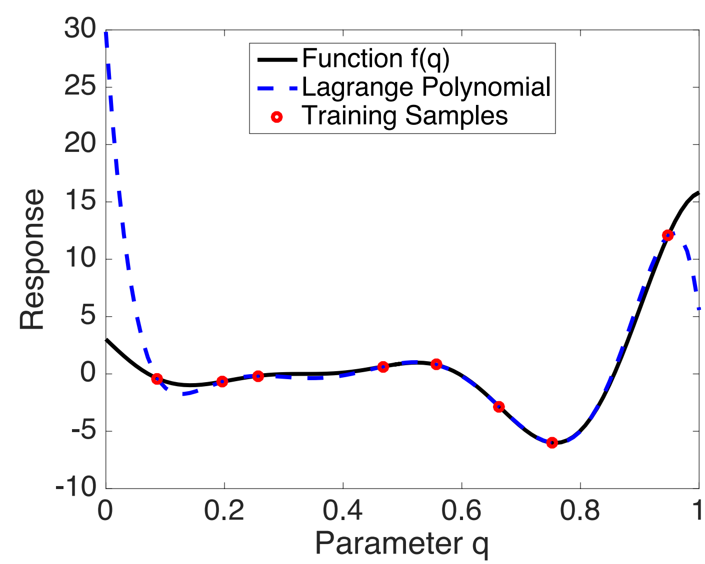
it follows that

$$f_s^M(q^m) = y^m$$

Warning: Be careful of extrapolation!

Multivariate: Tensor of 1-D relations

Example: $f(q) = (6q-2)^2 \sin(12q-4)$



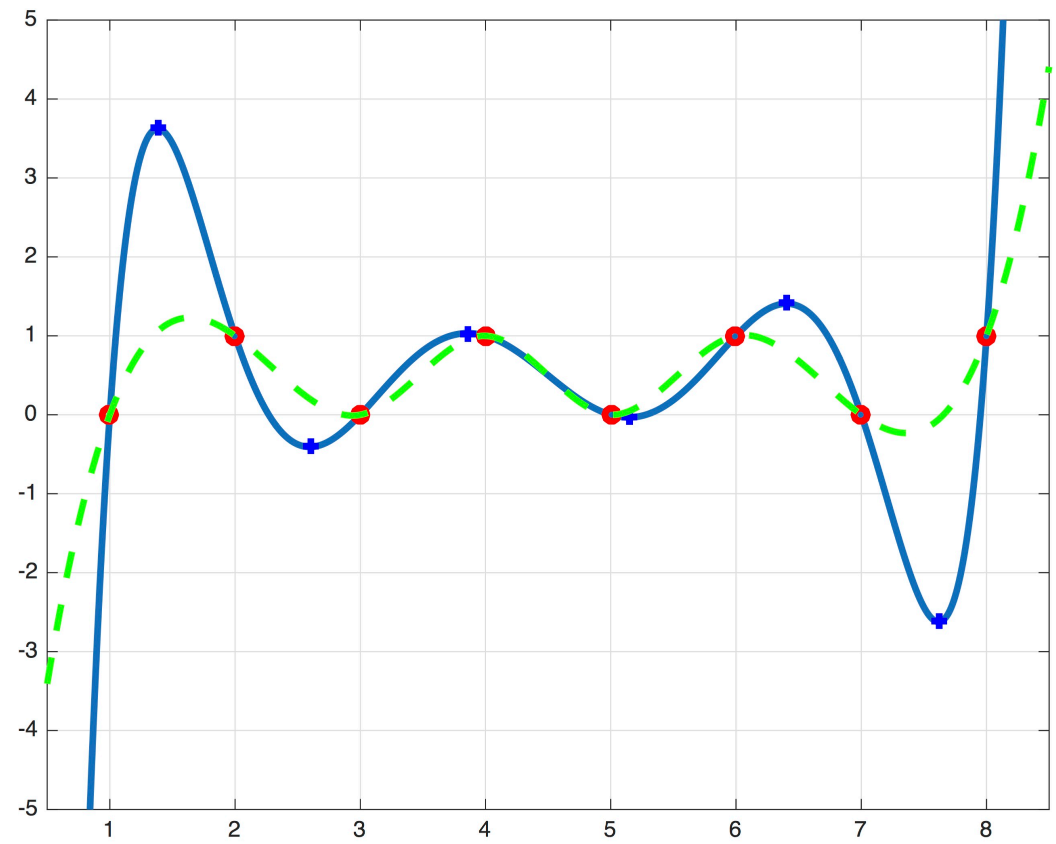
Stochastic Collocation

MATLAB Code: lagrangepoly.m

```
X = [1 2 3 4 5 6 7 8];
Y = [0 1 0 1 0 1 0 1];
[P,R,S] = lagrangepoly(X,Y);

xx = 0.5 : 0.01 : 8.5;
plot(xx,polyval(P,xx),X,Y,'or',R,S,'+b',xx,spline(X,Y,xx),'--g','linewidth',3)
grid
axis([0.5 8.5 -5 5])
```

Note: Recall use of unequally spaced points.



Polynomial Interpolation

Response Mean and Variance: Note that

$$
\begin{aligned}
\mathbb{E}[f_s^M(q)] &= \int_\Gamma f_s^M(q)\rho(q)dq \\
&= \sum_{m=0}^M f(q^m) \int_\Gamma L_m(q)\rho(q)dq \\
&\approx \sum_{m=0}^M f(q^m) \sum_{r=0}^R L_m(q^r)\rho(q^r)w^r,
\end{aligned}
$$

Strategy: Quadrature with $q^r = q^m$ and $R = M$

Mean:

$$\mathbb{E}[f_s^M(q)] \approx \bar{f}_s^M = \sum_{m=0}^M f(q^m)\rho(q^m)w^m$$

Monte Carlo:

$$\bar{f}_s^M = \frac{1}{M+1}\sum_{m=0}^M f(q^m)$$

Note: Same computational complexity but Newton-Cotes, Clenshaw-Curtis or Gaussian quadrature are MUCH more accurate than Monte Carlo!!

Polynomial Interpolation

Response Variance:

$$
\begin{aligned}
\text{var}[f_s^M(q)] &= \int_\Gamma \left[f_s^M(q) - \mathbb{E}[f_s^M(q)]\right]^2 \rho(q)dq \\
&\approx \sum_{r=0}^{R} \left[\sum_{m=0}^{M} f(q^m)L_m(q^r) - \bar{f}_s^M\right]^2 \rho(q^r)w^r \\
&= \sum_{m=0}^{M} \left[f(q^m) - \bar{f}_s^M\right]^2 \rho(q^m)w^m
\end{aligned}
$$

Sample Variance:

$$
\text{var}[f_s^M(q)] = \frac{1}{M}\sum_{m=0}^{M}[f(q^m) - \bar{f}_s^M]^2
$$

Note:

- Same computational complexity but Newton-Cotes, Clenshaw-Curtis or Gaussian quadrature are MUCH more accurate than Monte Carlo!!
- Often cannot use Monte Carlo for PDE examples.

Polynomial Regression

Strategy: Take M+1 > K+1 training points and minimize

$$\mathcal{J}(u) = \sum_{m=0}^{M} \left[y^m - \sum_{k=0}^{K} u_k \cdot (q^m)^k \right]^2$$
$$= (y - Xu)^T (y - Xu)$$

for

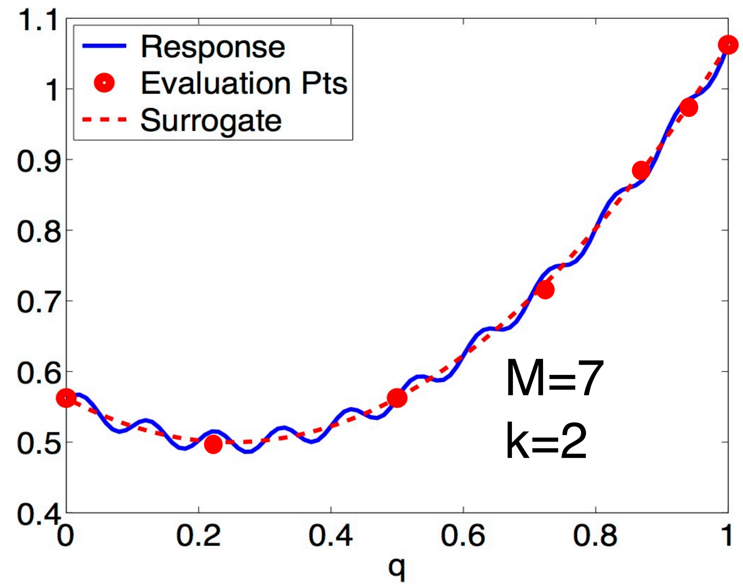
$$X = \begin{bmatrix} 1 & q^1 & (q^1)^2 & \cdots & (q^1)^K \\ \vdots & & & & \vdots \\ 1 & q^M & (q^M)^2 & \cdots & (q^M)^K \end{bmatrix} \quad , \quad y = \begin{bmatrix} y^0 \\ \vdots \\ y^M \end{bmatrix}$$

Least Squares Solution:

$$u = (X^T X)^{-1} X^T y = X^{\dagger} y$$

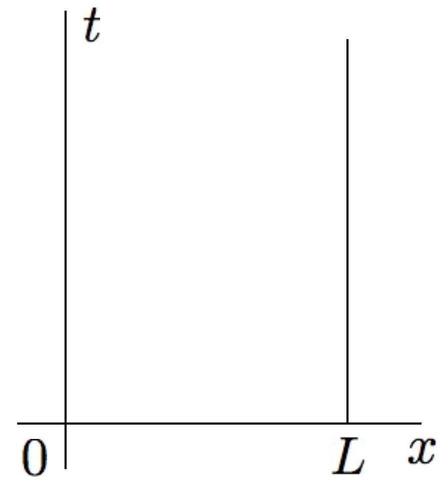
MATLAB: u = X\y

PDE Example:



Motivation for Orthogonal Polynomial Methods

Heat Equation:



$$\frac{\partial u}{\partial t} = \alpha \frac{\partial^2 u}{\partial x^2}$$

Note: $q = \alpha$

$$u(t,0) = u(t,L) = 0$$

$$u(0,x) = u_0(x)$$

Separation of Variables: Take

$$u(t,x) = T(t)X(x)$$

General Solution: Surrogate – truncate to upper limit of N

$$u(t,x) = \sum_{n=1}^{\infty} \beta_n e^{-\alpha \lambda_n^2 t} \sin(\lambda_n x) \quad , \quad \lambda_n = \frac{n\pi}{L}$$

Coefficients:

$$\beta_n = \frac{2}{L} \int_0^L u_0(x) \sin(\lambda_n x) dx$$

Recall: Trig functions orthogonal

$$\int_{-L}^{L} \sin\left(\frac{m\pi x}{L}\right) \sin\left(\frac{n\pi x}{L}\right) dx = \delta_{mn} L$$

Response: $y(t,x) = \int_\Gamma u(t,x,q)\rho(q)dq$

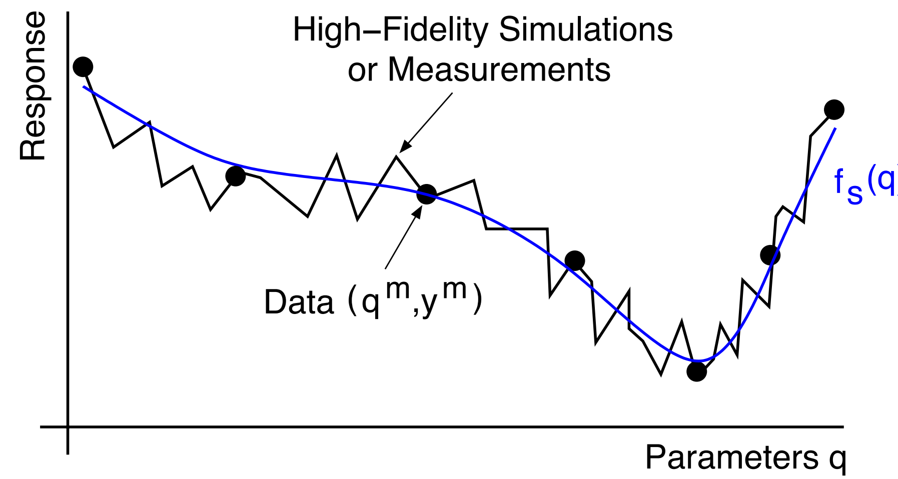
Spectral Representation of Random Processes

Strategy: Consider high fidelity model

$$y = f(q)$$

with M model evaluations

$$y^m = f(q^m)\ ,\ m = 1, \ldots, M$$



Statistical Model: $f_s(q)$: Surrogate for $f(q)$

$$y^m = f_s(q^m) + \varepsilon^m\ ,\ m = 1, \ldots, M$$

Surrogate:

$$f_s^K(q,u) = \sum_{k=0}^{K} u_k \Psi_k(q) + P(q)$$

Case 1: Single random variable

Note: $\Psi_k(q)$ orthogonal with respect to inner product associated with pdf

e.g., $q \sim \mathcal{N}(0,1)$: Hermite polynomials

$q \sim \mathcal{U}(-1,1)$: Legendre polynomials

Spectral Representation of Random Processes

Hermite Polynomials: $q \sim \mathcal{N}(0,1)$

$$H_0(q) = 1 \quad , \quad H_1(q) = q \quad , \quad H_2(q) = q^2 - 1,$$

$$H_3(q) = q^3 - 3q \quad , \quad H_4(q) = q^4 - 6q^2 + 3$$

with the weight

$$\rho(q) = \frac{1}{\sqrt{2\pi}} e^{-q^2/2},$$

Normalization factor: $\gamma_k = \int_{\mathbb{R}} \psi_k^2(q)\rho(q)dq = k!$

Legendre Polynomials: $q \sim \mathcal{U}(-1,1)$

$$P_0(q) = 1 \quad , \quad P_1(q) = q \quad , \quad P_2(q) = \frac{1}{2}(3q^2 - 1),$$

$$P_3(q) = \frac{1}{2}(5q^3 - 3q) \quad , \quad P_4(q) = \frac{1}{8}(35q^4 - 30q^2 + 3),$$

with the weight

$$\rho(q) = \frac{1}{2}$$

Normalization factor: $\gamma_k = \frac{1}{2k+1}$

Orthogonal Polynomial Representations

Representation:

$$f_s^K(q) = \sum_{k=0}^{K} u_k \psi_k(q)$$

Note: $\psi_0(q) = 1$ implies that

$$\mathbb{E}[\psi_0(q)] = 1$$

$$\mathbb{E}[\psi_j(q)\psi_k(q)] = \int_\Gamma \psi_j(q)\psi_k(q)\rho(q)dq$$

$$= \delta_{jk}\gamma_k$$

where $\gamma_k = \mathbb{E}[\psi_k^2(q)]$

Properties:

(i) $\mathbb{E}[f_s^K(q)] = u_0$

(ii) $\text{var}[f_s^K(q)] = \sum_{k=1}^{K} u_k^2 \gamma_k$

Note: Can be used for:

- Uncertainty propagation
- Sobol-based global sensitivity analysis

Issue: How does one compute u_k , $k = 0, \ldots K$?

- Stochastic Galerkin techniques (Polynomial Chaos Expansion – PCE)
- Nonintrusive PCE (Discrete projection)
- Stochastic collocation
- Regression-based methods with sparsity control (Lasso)

Note: Methods nonintrusive and treat code as blackbox.

Orthogonal Polynomial Representations

Properties:

$$\begin{aligned}
\mathbb{E}\left[f_s^K(q)\right] &= \mathbb{E}\left[\sum_{k=0}^{K} u_k \Psi_k(q)\right] \\
&= u_0 \mathbb{E}[\Psi_0(q)] + \sum_{k=1}^{K} u_k \mathbb{E}[\Psi_k(q)] \\
&= u_0
\end{aligned}$$

and

$$\begin{aligned}
\mathrm{var}[f_s^K(q)] &= \mathbb{E}\left[\left(f_s^K(q) - \mathbb{E}[f_s^K(q)]\right)^2\right] \\
&= \mathbb{E}\left[\left(\sum_{k=0}^{K} u_k \Psi_k(q) - u_0\right)^2\right] \\
&= \mathbb{E}\left[\left(\sum_{k=1}^{K} u_k \Psi_k(q)\right)^2\right] \\
&= \sum_{k=1}^{K} u_k^2 \gamma_k,
\end{aligned}$$

Orthogonal Polynomial Representations

Multiple Random Variables:

Definition: (p-Dimensional Multi-Index): a p-tuple

$$\mathbf{k}' = (k_1, \cdots, k_p) \in \mathbb{N}_0^p$$

of non-negative integers is termed a p-dimensional multi-index with magnitude $|\mathbf{k}'| = k_1 + k_2 + \cdots + k_p$ and satisfying the ordering $\mathbf{j}' \leq \mathbf{k}' \Leftrightarrow j_i \leq k_i$ for $i = 1, \cdots, p$.

Consider the p-variate basis functions

$$\Psi_{\mathbf{k}'}(q) = \psi_{k_1}(q_1), \ldots, \psi_{k_p}(q_p)$$

which satisfy

$$\begin{aligned}
\mathbb{E}[\Psi_{\mathbf{j}'}(q)\Psi_{\mathbf{k}'}(q)] &= \int_\Gamma \Psi_{\mathbf{j}'}(q)\Psi_{\mathbf{k}'}(q)\rho(q)dq \\
&= \langle \Psi_{\mathbf{j}'}, \Psi_{\mathbf{k}'} \rangle_\rho \\
&= \delta_{\mathbf{j}'\mathbf{k}'}\gamma_{\mathbf{k}'},
\end{aligned}$$

Orthogonal Polynomial Representations

Multi-Index Representation:

$$f_s^K(q) = \sum_{|\mathbf{k}'|=0}^{K} u_{\mathbf{k}'} \Psi_{\mathbf{k}'}(q)$$

Single Index Representation:

$$f_s^K(q) = \sum_{k=0}^{K} u_k \Psi_k(q)$$

k	$\lvert\mathbf{k}'\rvert$	Multi-Index	Polynomial
0	0	$(0,0,0)$	$\psi_0(q_1)\psi_0(q_2)\psi_0(q_3)$
1	1	$(1,0,0)$	$\psi_1(q_1)\psi_0(q_2)\psi_0(q_3)$
2		$(0,1,0)$	$\psi_0(q_1)\psi_1(q_2)\psi_0(q_3)$
3		$(0,0,1)$	$\psi_0(q_1)\psi_0(q_2)\psi_1(q_3)$
4	2	$(2,0,0)$	$\psi_2(q_1)\psi_0(q_2)\psi_0(q_3)$
5		$(1,1,0)$	$\psi_1(q_1)\psi_1(q_2)\psi_0(q_3)$
6		$(1,0,1)$	$\psi_1(q_1)\psi_0(q_2)\psi_1(q_3)$
7		$(0,2,0)$	$\psi_0(q_1)\psi_2(q_2)\psi_0(q_3)$
8		$(0,1,1)$	$\psi_0(q_1)\psi_1(q_2)\psi_1(q_3)$
9		$(0,0,2)$	$\psi_0(q_1)\psi_0(q_2)\psi_2(q_3)$

Orthogonal Polynomial Representations

Discrete Projection: Take weighted inner product of $f(q) = \sum_{k=0}^{\infty} u_k \Psi_k(q)$ to obtain

$$u_k = \frac{1}{\gamma_k} \int_\Gamma f(q) \Psi_k(q) \rho(q) dq$$

Quadrature:

$$u_k \approx \frac{1}{\gamma_k} \sum_{r=1}^{R} f(q^r) \Psi(q^r) w^r$$

Note:

(i) Low-dimensional: Tensored 1-D quadrature rules – e.g., Gaussian

(ii) Moderate-dimensional: Sparse grid (Smolyak) techniques

(iii) High-dimensional: Monte Carlo or quasi-Monte Carlo (QMC) techniques

Regression-Based Methods with Sparsity Control (Lasso): Solve

$$\min_{u \in \mathbb{R}^{K+1}} \|Xu - y\|^2 \text{ subject to } \sum_{k=0}^{K} |u_k| \leqslant \tau,$$

Note: Sample points $\{q^m\}_{m=0}^{M}$

$$[X]_{ij} = \Psi_j(q^i)$$

$$y = [f(q^0), \ldots, f(q^M)]^T$$

e.g., SPGL1

- MATLAB Solver for large-scale sparse reconstruction

Orthogonal Polynomial Representations

Galerkin: Seek solutions $f_s^K(q)$ that satisfy

$$\left\langle f_s^K(q) - f(q), \Psi_i \right\rangle_\rho = 0$$

which yields

$$\sum_{k=0}^{K} u_k \int_\Gamma \Psi_k(q)\Psi_i(q)\rho(q)dq = \int_\Gamma f(q)\Psi_i(q)\rho(q)dq$$

Equivalent Formulation:

$$\mathbb{E}\left[f_s^K(q)\Psi_i(q)\right] = \mathbb{E}\left[f(q)\Psi_i(q)\right]$$

Result:

$$u_k = \frac{1}{\gamma_k}\int_\Gamma f(q)\Psi_k(q)\rho(q)dq$$

Note: This technique is often invasive in the sense that it requires the modification of existing codes.

General Uniform Distributions

Note: Consider $q \sim \mathcal{U}(a, b)$ with mean and variance

$$\mu = \frac{a+b}{2} \quad , \quad \sigma^2 = \frac{(b-a)^2}{12}$$

Then

$$q = g(\xi) = \mu + \sqrt{3}\sigma\xi = \frac{a+b}{2} + \frac{b-a}{2}\xi$$

where $\xi \sim \mathcal{U}(-1, 1)$.

Random Vector:

$$q = g(\xi) = [\mu_1 + \sqrt{3}\sigma_1\xi_1, \ldots, \mu_p + \sqrt{3}\sigma_p\xi_p]$$

Spectral Surrogate:

$$f_s^K(q) = f_s^K(g(\xi)) = \sum_{k=0}^{K} u_k \Psi_k(\xi)$$

General Uniform Distributions

Spectral Surrogate:

$$f_s^K(q) = f_s^K(g(\xi)) = \sum_{k=0}^{K} u_k \Psi_k(\xi)$$

Discrete Projection:

$$\begin{aligned} u_k &= \frac{1}{\gamma_k} \int_\Gamma f(g(\xi)) \Psi_k(\xi) \rho(\xi) d\xi \\ &\approx \frac{1}{\gamma_k} \sum_{r=1}^{R} f(g(\xi^r)) \Psi_k(\xi^r) w^r \end{aligned}$$

Galerkin:

$$\sum_{k=0}^{K} u_k \int_\Gamma \Psi_k(\xi) \Psi_i(\xi) \rho(\xi) d\xi = \int_\Gamma f(g(\xi)) \Psi_i(\xi) \rho(\xi) d\xi \,, \;\; i = 0, 1, \ldots, K$$

General Uniform Distributions

Example: Consider

$$f(\alpha_1, \alpha_{11}) = \int_0^{0.8} [\alpha_1 P^2 + \alpha_{11} P^4] dP = c_1 \alpha_1 + c_2 \alpha_{11},$$

where $c_1 = \frac{0.8^3}{3}$ and $c_2 = \frac{0.8^5}{5}$ and $q = [\alpha_1, \alpha_{11}]$

Approach: Take $\alpha_1 \sim \mathcal{U}(a_1, b_1)$ and $\alpha_{11} \sim \mathcal{U}(a_2, b_2)$ so

$$\alpha_1 = \bar{\alpha}_1 + \sqrt{3}\sigma_1 \xi_1 \quad , \quad \bar{\alpha}_1 = \frac{a_1 + b_1}{2}, \; \sqrt{3}\sigma_1 = \frac{b_1 - a_1}{2}$$

$$\alpha_{11} = \bar{\alpha}_{11} + \sqrt{3}\sigma_{11} \xi_2 \quad , \quad \bar{\alpha}_{11} = \frac{a_2 + b_2}{2}, \; \sqrt{3}\sigma_{11} = \frac{b_2 - a_2}{2},$$

where $\xi, \xi_2 \sim \mathcal{U}(-1, 1)$ and $\rho(\xi_1) = \rho(\xi_2) = \frac{1}{2}$

Response:

$$f(q) = f(g(\xi)) = c_1 \left(\bar{\alpha}_1 + \sqrt{3}\sigma_1 \xi_1 \right) + c_2 \left(\bar{\alpha}_{11} + \sqrt{3}\sigma_{11} \xi_2 \right)$$

General Uniform Distributions

Response:

$$f(q) = f(g(\xi)) = c_1 \left(\bar{\alpha}_1 + \sqrt{3}\sigma_1 \xi_1\right) + c_2 \left(\bar{\alpha}_{11} + \sqrt{3}\sigma_{11}\xi_2\right)$$

Surrogate:

$$f_s^K(q) = f_s^K(g(\xi)) = \sum_{k=0}^{K} u_k \Psi_k(\xi),$$

where $\Psi_k(\xi)$ are tensored Legendre polynomials on $\Gamma = [-1, 1]^2$

Galerkin: From

$$\int_\Gamma [f_s^K(\xi) - f(\xi)]\Psi_i(\xi)\rho(\xi)d\xi = 0$$

it follows that

$$\begin{aligned}\sum_{k=0}^{K} u_k \int_\Gamma \Psi_k(\xi)\Psi_i(\xi)\rho(\xi)d\xi &= c_1 \int_\Gamma (\bar{\alpha}_1 + \sqrt{3}\sigma_1\xi_1)\Psi_i(\xi)\rho(\xi)d\xi \\ &+ c_2 \int_\Gamma (\bar{\alpha}_{11} + \sqrt{3}\sigma_{11}\xi_2)\Psi_i(\xi)\rho(\xi)d\xi\end{aligned}$$

General Uniform Distributions

Note:

$$\sum_{k=0}^{K} u_k \int_\Gamma \Psi_k(\xi)\Psi_i(\xi)\rho(\xi)d\xi = c_1 \int_\Gamma (\bar{\alpha}_1 + \sqrt{3}\sigma_1 \xi_1)\Psi_i(\xi)\rho(\xi)d\xi$$

$$+c_2 \int_\Gamma (\bar{\alpha}_{11} + \sqrt{3}\sigma_{11}\xi_2)\Psi_i(\xi)\rho(\xi)d\xi$$

For $i = 0, 1$ and 2, the Legendre basis functions and weights are

$$\Psi_0(\xi) = \psi_0(\xi_1)\psi_0(\xi_2) \quad \Rightarrow \quad u_0 = c_1\bar{\alpha}_1 + c_2\bar{\alpha}_{11}$$

$$\Psi_1(\xi) = \psi_1(\xi_1)\psi_0(\xi_2) \quad \Rightarrow \quad u_1 = c_1\sqrt{3}\sigma_1$$

$$\Psi_2(\xi) = \psi_0(\xi_1)\psi_1(\xi_2) \quad \Rightarrow \quad u_2 = c_2\sqrt{3}\sigma_{11}$$

Surrogate:

$$f_s^K(q) = f_s^K(g(\xi)) = (c_1\bar{\alpha}_1 + c_2\bar{\alpha}_{11}) + c_1\sqrt{3}\sigma_1\xi_1 + c_2\sqrt{3}$$

Moments:

$$\mathbb{E}[f_s^K(q)] = c_1\bar{\alpha}_1 + c_2\bar{\alpha}_{11}$$

$$\text{var}[f_s^K(q)] = 3c_1^2\sigma_1^2 + 3c_2^2\sigma_{11}^2$$

Note: Employ physical parameters in the model and transformed parameters in weak formulation and computation of weights.

Discrete Projection Example

Spring Model: See perturbation notes

$$m\frac{d^2z}{\partial t^2} + c\frac{dz}{dt} + kz = f_0 \cos(\omega_F t)$$

$$z(0) = z_0 \quad , \quad \frac{dz}{dt}(0) = z_1$$

Parameters:

$$m \sim \mathcal{U}(\bar{m} - \sigma_m, \bar{m} + \sigma_m)$$

$$c \sim \mathcal{U}(\bar{c} - \sigma_c, \bar{c} + \sigma_c)$$

$$k \sim \mathcal{U}(\bar{k} - \sigma_k, \bar{k} + \sigma_k)$$

Response:

$$z(\omega_F, q) = \frac{1}{\sqrt{(k - m\omega_F^2)^2 + (c\omega_f)^2}}$$

Representation:

$$f_s^K(\omega_F, q) = f_s^K(\omega_F, g(\xi)) = \sum_{k=0}^{K} u_k(\omega_F)\Psi_k(\xi)$$

Discrete Projection Example

Discrete Projection:

$$u_k(\omega_F) = \frac{1}{\gamma_k} \int_\Gamma f(g(\omega_F, \xi))\Psi_k(\xi)\rho(\xi)d\xi$$

$$= \frac{1}{\gamma_k} \int_\Gamma \frac{\Psi_k(\xi)\rho(\xi)d\xi}{\sqrt{\left[(\bar{k} + \sqrt{3}\sigma_k\xi_3) - (\bar{m} + \sqrt{3}\sigma_m\xi_1)\omega_F^2\right]^2 + (\bar{c} + \sqrt{3}\sigma_c\xi_2)^2\omega_F^2}}$$

$$\approx \frac{1}{\gamma_k} \sum_{r_1=1}^{R_1} \sum_{r_2=1}^{R_2} \sum_{r_3=1}^{R_3} \frac{\Psi_k(\xi^r)w^r}{\sqrt{\left[(\bar{k} + \sqrt{3}\sigma_k\xi_3^{r_3}) - (\bar{m} + \sqrt{3}\sigma_m\xi_1^{r_1})\omega_F^2\right]^2 + (\bar{c} + \sqrt{3}\sigma_c\xi_2^{r_2})^2\omega_F^2}},$$

Surrogate: Mean and variance

$$\mathbb{E}[f_s^K(\omega_F, q)] = u_0(\omega_F)$$

$$\text{var}[f_s^K(\omega_F, q)] = \sum_{k=1}^{K} u_k^2(\omega_F)\gamma_k$$

Monte Carlo: With M = 1e+5

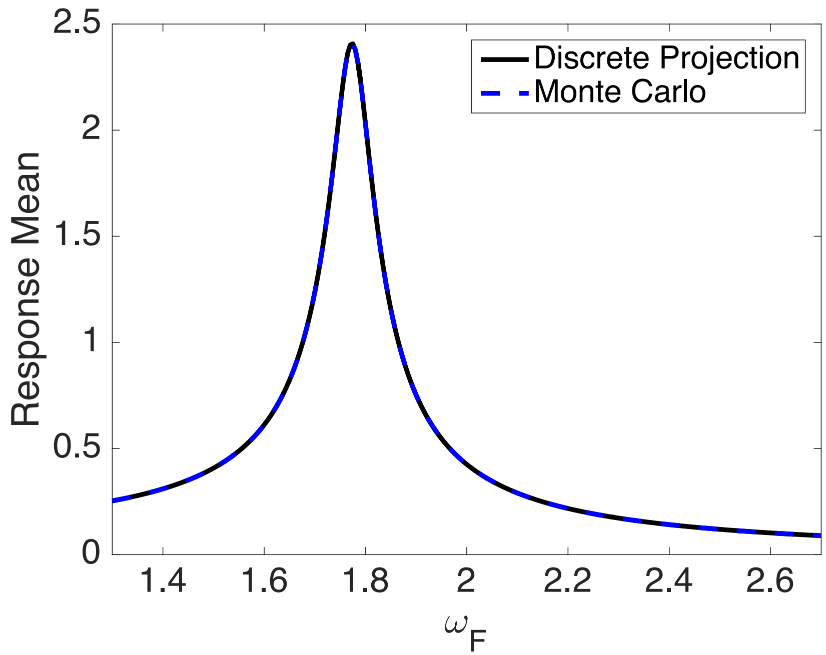
$$\bar{f}_s^K(\omega_F) = \frac{1}{M} \sum_{i=1}^{M} f(\omega_F, q^m),$$

$$\sigma_s^K(\omega_F) = \left[\frac{1}{M-1} \sum_{i=1}^{M} \left[f(\omega_F, q^m) - \bar{f}_s^K(\omega_F)\right]^2\right]^{1/2}$$

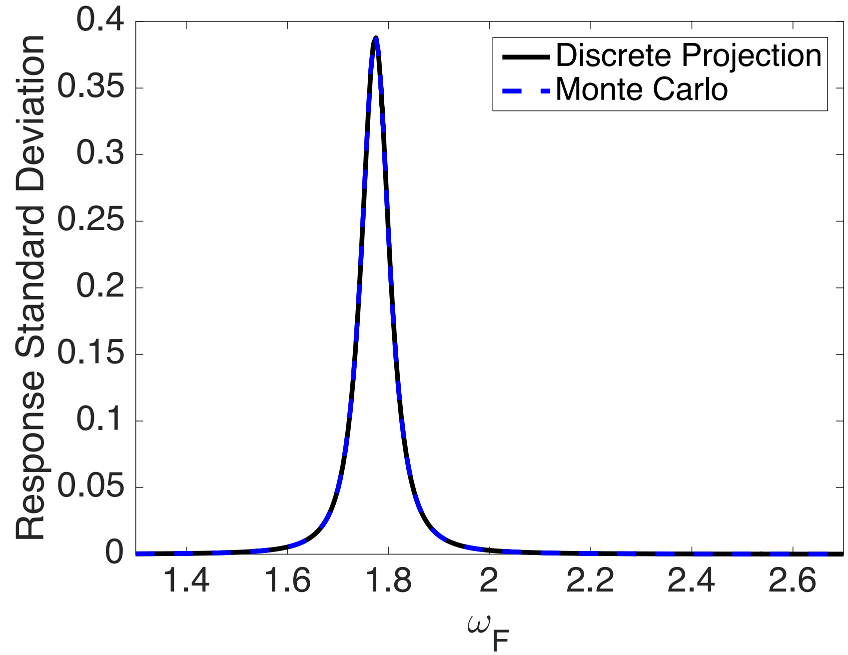
Note: We plot the standard deviations

Discrete Projection Example

Result: Mean and standard deviation



Mean



Standard Deviation

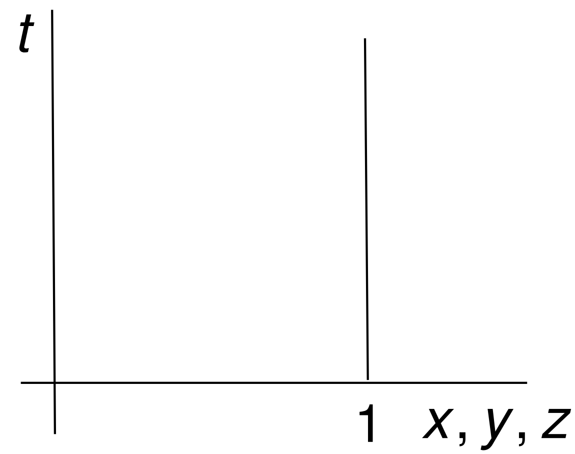
Surrogate Models

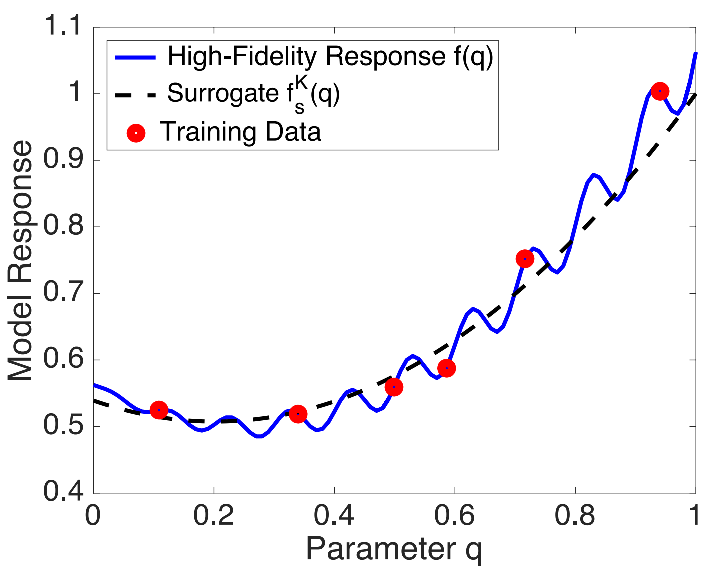
Example: Consider the heat equation

$$\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} + \frac{\partial^2 u}{\partial z^2} + f(q)$$

with the response

$$y(q) = \int_0^1 \int_0^1 \int_0^1 \int_0^1 u(t,x,y,z)\, dxdydzdt$$





Note: Regression with sparsity control

$$u = [0.6406, 0.2305, 0.1289, 0, 0]^T$$

Surrogate:

$$f_s^K(q) = \sum_{k=0}^{K} u_k \psi_k(q)$$

Note:

$$\phi_0(q) = 1$$

$$\phi_1(q) = 2q - 1$$

$$\phi_2(q) = \frac{3}{2}(2q-1)^2 - \frac{1}{2}$$

Stochastic Galerkin Method

Properties:

• Accuracy is optimal in L2 sense.

• Projection method with associated error bounds.

• Disadvantages

- Method is intrusive and hence difficult to implement with legacy codes or codes for which only executable is available.
- Method requires densities with associated orthogonal polynomials. These can sometimes be constructed from empirical histograms.
- Method requires mutually independent parameters.

Note:

• Very commonly termed polynomial chaos expansion [Weiner, 1938]. However, no chaos in the present use.

Discrete Projection

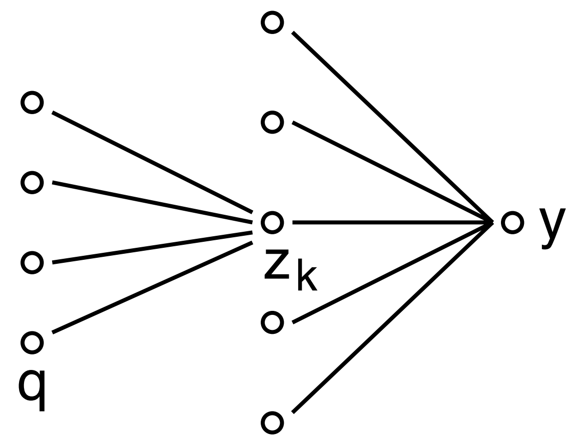
Properties:

- Advantages
  - Like collocation, the method is nonintrusive and hence can be employed with post-processing to existing codes. The method is often referred to as nonintrusive PCE.
  - Projection method with associated error bounds.
  - Algorithms available in Sandia Dakota package.
- Disadvantages
  - Requires the construction of the joint density which often relies on mutually independent parameters.

Neural Networks

Single Perceptron:

$$z_k = h\left(\sum_{j=1}^{p} v_{jk} q_j + b_k^0\right) = h(\mathbf{v}_k^T \tilde{q})$$



Activation Functions:

$$h(\mathbf{v}_k^T \tilde{q}) = \tanh(\mathbf{v}_k^T \tilde{q})$$

$$h(\mathbf{v}_k^T \tilde{q}) = \frac{2}{1 + \exp(-2\mathbf{v}_k^T \tilde{q})} - 1$$

Regression:

$$y = \sum_{k=1}^{N_H} u_k h(\mathbf{v}_k^T \tilde{q}) + b^1 = \mathbf{u}^T z$$