

Techniques to Propagate Uncertainties

Goal: Consider the nonlinearly parameterized model

$$\Upsilon = f(Q) , \quad Q = [Q_1, \dots, Q_p]$$

with a specified distribution for Q . What are appropriate techniques to determine a distribution or prediction intervals for Υ ?

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
 - Stochastic spectral methods
 - Gaussian process or Kriging representations

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

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

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

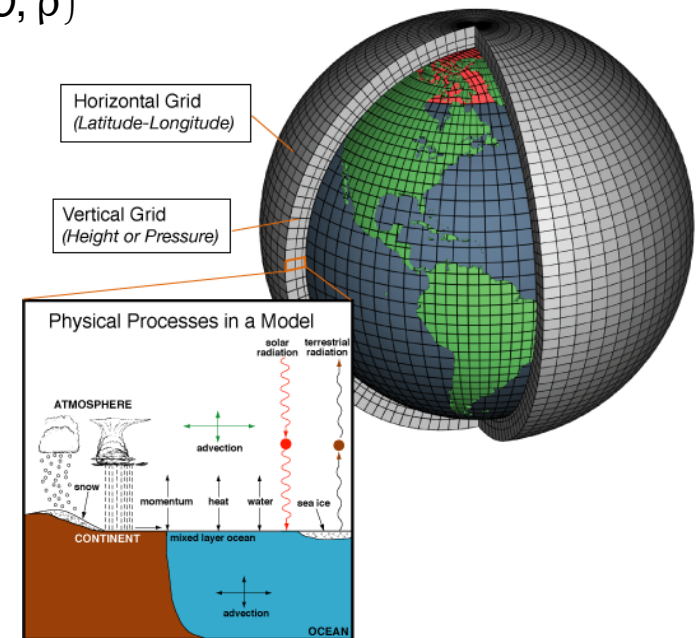
$$p = \rho R T$$

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

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

Solution: Construct surrogate models

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



Surrogate Models: Motivation

Example: Consider the heat equation

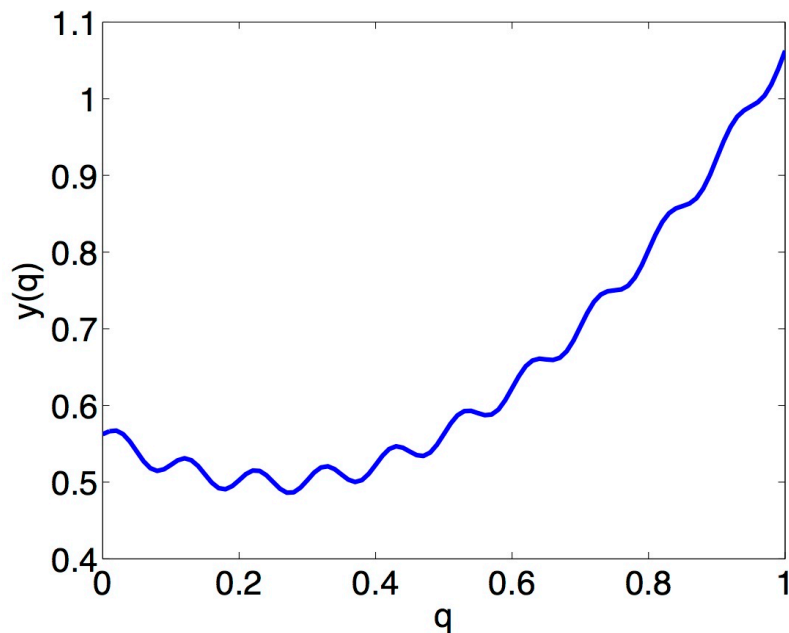
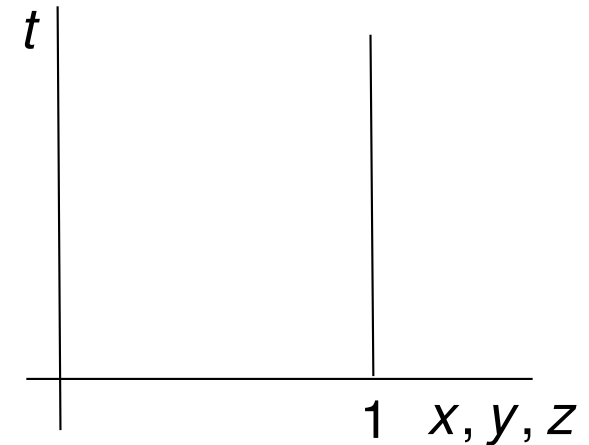
$$\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} + \frac{\partial^2 u}{\partial z^2} + f(q)$$

Boundary Conditions

Initial Conditions

with the response

$$y(q) = \int_0^1 \int_0^1 \int_0^1 \int_0^1 u(t, x, y, z) dx dy dz dt$$



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

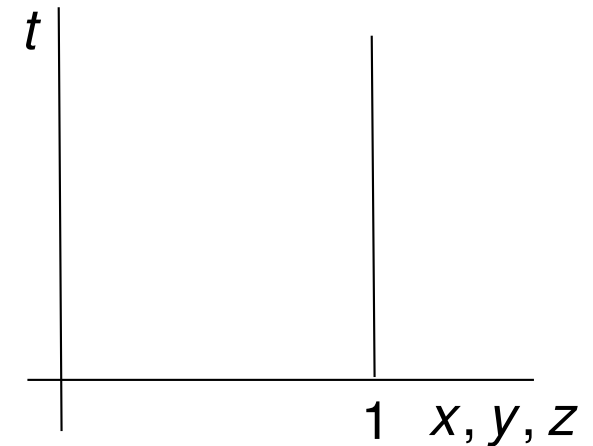
Initial Conditions

with the response

$$y(q) = \int_0^1 \int_0^1 \int_0^1 \int_0^1 u(t, x, y, z) dx dy dz dt$$

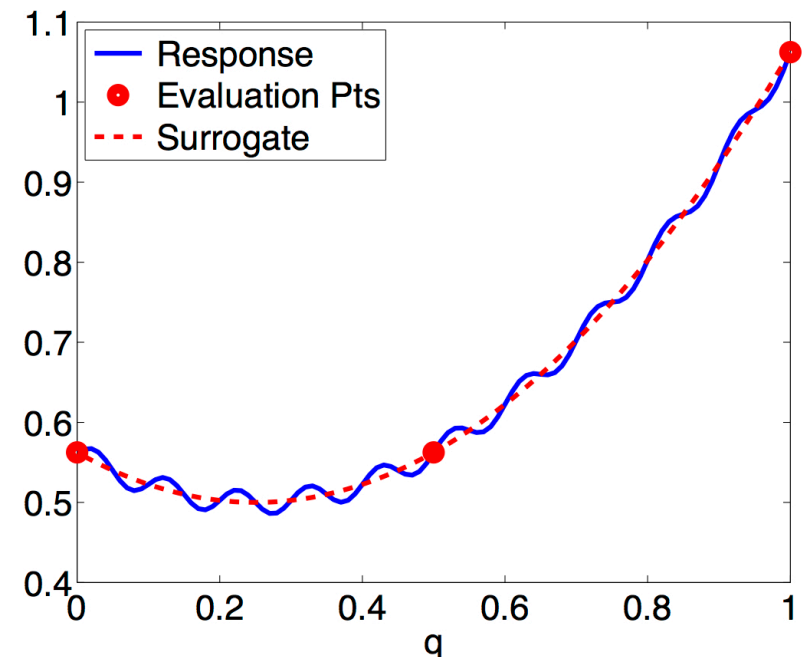
Question: How do you construct a polynomial surrogate?

- Regression
- **Interpolation**



Surrogate: Quadratic

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



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

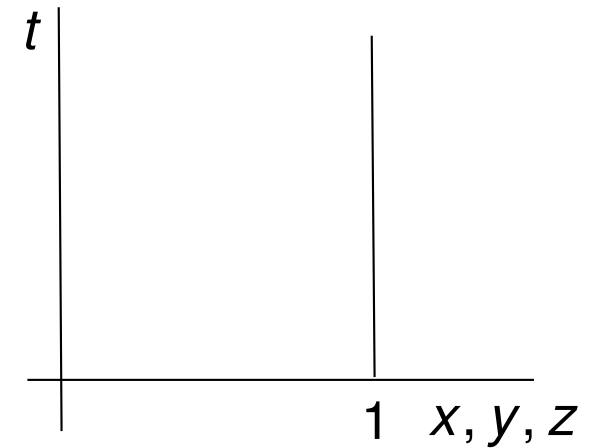
Initial Conditions

with the response

$$y(q) = \int_0^1 \int_0^1 \int_0^1 \int_0^1 u(t, x, y, z) dx dy dz dt$$

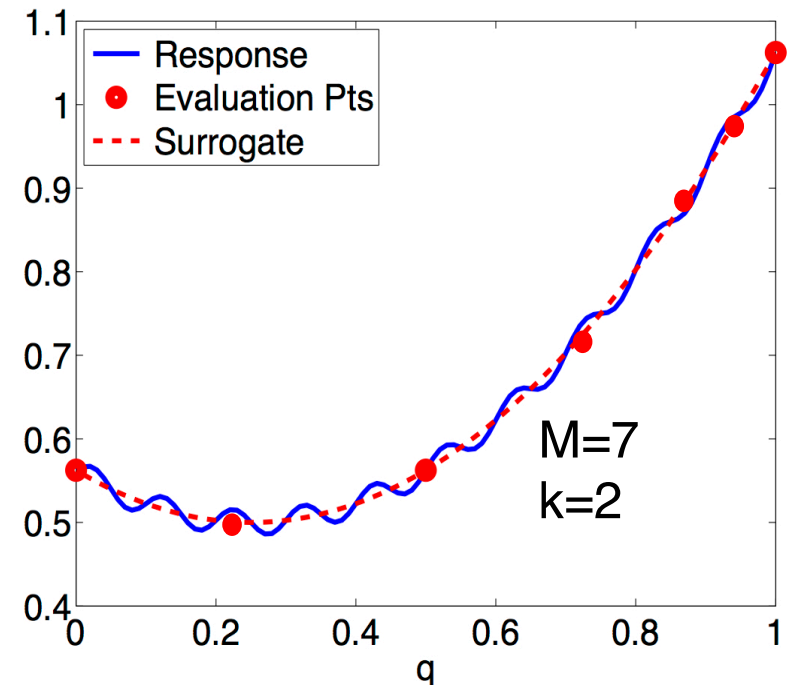
Question: How do you construct a polynomial surrogate?

- Interpolation
- Regression



Surrogate: Quadratic

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



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)

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

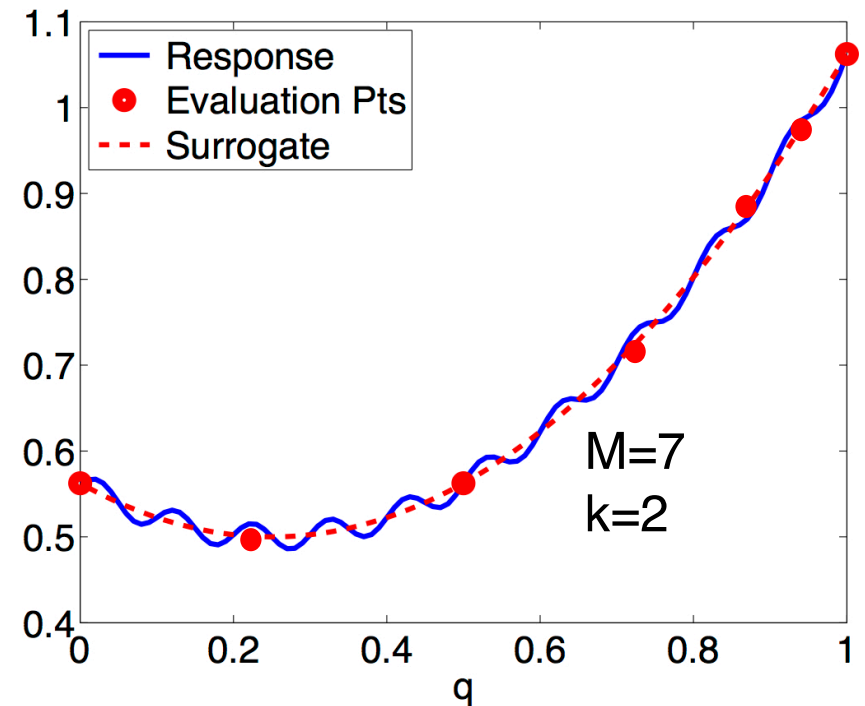
Likelihood:

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

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

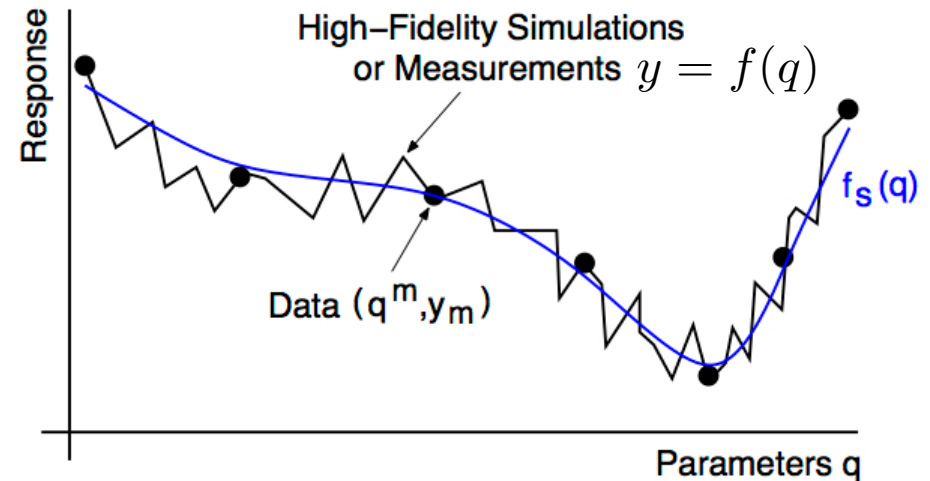
$$y = f(q)$$

with M model evaluations

$$y_m = f(q^m), \quad m = 1, \dots, M$$

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

$$y_m = f_s(q^m) + \varepsilon_m, \quad m = 1, \dots, M$$



Surrogate:

$$y^K(Q) = f_s(Q) = \sum_{k=0}^K y_k \Psi_k(Q)$$

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

e.g., $Q \sim N(0, 1)$: Hermite polynomials

$Q \sim U(-1, 1)$: Legendre polynomials

Motivation for Orthogonal Polynomial Methods

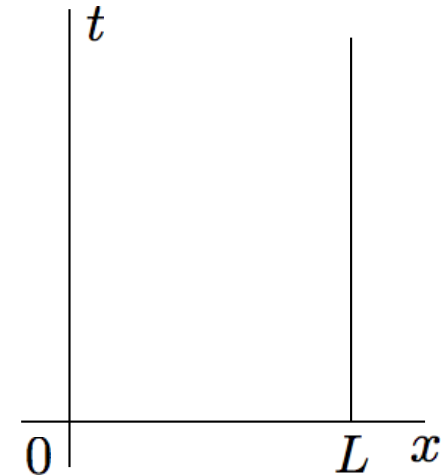
Heat Equation: See Lecture 6

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

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

$$y_m = f(q^m), \quad m = 1, \dots, M$$

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

$$y_m = f_s(q^m) + \varepsilon_m, \quad m = 1, \dots, M$$

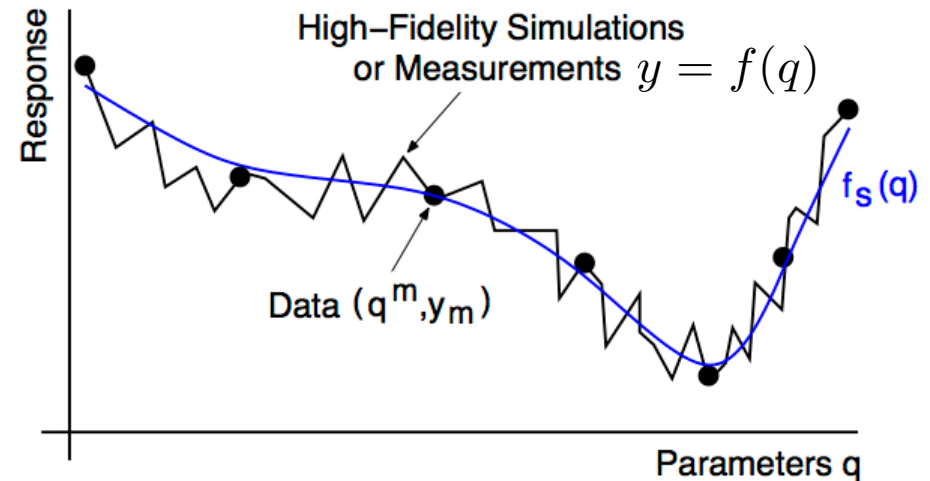
Surrogate:

$$y^k(Q) = f_s(Q) = \sum_{k=0}^K y_k \psi_k(Q)$$

Note: $\psi_k(Q)$ orthogonal with respect to inner product associated with pdf

e.g., $Q \sim N(0, 1)$: Hermite polynomials

$Q \sim U(-1, 1)$: Legendre polynomials



Case 1: Single random variable

Spectral Representation of Random Processes

Hermite Polynomials: $Q \sim N(0, 1)$

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

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

with the weight

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

$$\text{Normalization factor: } \gamma_i = \mathbb{E} [\psi_i^2(Q)] = \int_{\mathbb{R}} \psi_i^2(q) \rho_Q(q) dq = i!$$

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

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

$$P_3(Q) = \frac{5}{2}Q^3 - \frac{3}{2}Q \quad , \quad P_4(Q) = \frac{35}{8}Q^4 - \frac{15}{4}Q^2 + \frac{3}{8},$$

with the weight

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

Orthogonal Polynomial Representations

Representation:

$$y^K(Q) = \sum_{k=0}^K y_k \Psi_k(Q)$$

Note: $\Psi_0(Q) = 1$ implies that

$$\mathbb{E}[\Psi_0(Q)] = 1$$

$$\begin{aligned} \mathbb{E}[\Psi_i(Q)\Psi_j(Q)] &= \int_{\Gamma} \Psi_i(q)\Psi_j(q)\rho(q)dq \\ &= \delta_{ij}\gamma_i \end{aligned}$$

where $\gamma_i = \mathbb{E}[\Psi_i^2(Q)]$

Properties:

$$(i) \quad \mathbb{E}[y^K(Q)] = y_0$$

$$(ii) \quad \text{var}[y^K(Q)] = \sum_{k=1}^K y_k^2 \gamma_k$$

Note: Can be used for:

- Uncertainty propagation
- Sobol-based global sensitivity analysis

Issue: How does one compute $y_k, k = 0, \dots, K$?

- 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

Nonintrusive PCE: Take weighted inner product of $y(q) = \sum_{k=0}^{\infty} y_k \Psi_k(q)$ to obtain

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

Quadrature:

$$y_k \approx \frac{1}{\gamma_k} \sum_{r=1}^R y(q^r) \Psi_k(q^r) w^r$$

Note:

(i) Low-dimensional: Tensor 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

$$\min_{y \in \mathbb{R}^{K+1}} \|\Lambda y - d\|^2 \quad \text{subject to} \quad \sum_{k=0}^K |y_k| \leq \tau$$

Note: Sample points $\{q^m\}_{m=1}^M$

$$\Lambda \in \mathbb{R}^{M \times (K+1)} \quad \text{where} \quad \Lambda_{jk} = \Psi_k(q^j)$$

$$d = [y(q^1), \dots, y(q^m)]$$

e.g., SPGL1

• MATLAB Solver for large-scale sparse reconstruction

Spectral Representation of Random Processes

Example: Consider heat equation on Slide 8. Represent $u(t,x,Q)$ by

$$u^K(t, x, Q) = \sum_{k=0}^K u_k(t, x) \Psi_k(Q)$$

where $\Psi_k(Q)$ are orthogonal polynomials.

Single Random Variable:

Let $\psi_k(Q)$ be orthogonal with respect to $\rho_Q(q)$ with $\psi_0(Q) = 1$. Then

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

and

$$\begin{aligned} \mathbb{E}[\psi_i(Q)\psi_j(Q)] &= \int_{\Gamma} \psi_i(q)\psi_j(q)\rho_Q(q)dq \\ &= \langle \psi_i, \psi_j \rangle_{\rho} \\ &= \delta_{ij}\gamma_i \end{aligned}$$

Normalization factor:

$$\gamma_i = \mathbb{E}[\psi_i^2(Q)] = \langle \psi_i, \psi_i \rangle_{\rho}$$

Spectral Representation of Random Processes

Random Process:

$$\begin{aligned}\mathbb{E}[u^K(t, x, Q)] &= \mathbb{E}\left[\sum_{k=0}^K u_k(t, x)\psi_k(Q)\right] \\ &= u_0(t, x)\mathbb{E}[\psi_0(Q)] + \sum_{k=1}^K u_k(t, x)\mathbb{E}[\psi_k(Q)] \\ &= u_0(t, x)\end{aligned}$$

$$\begin{aligned}\text{var}[u^K(t, x, Q)] &= \mathbb{E}\left[\left(u^K(t, x, Q) - \mathbb{E}[u^K(t, x, Q)]\right)^2\right] \\ &= \mathbb{E}\left[\left(\sum_{k=0}^K u_k(t, x)\psi_k(Q) - u_0(t, x)\right)^2\right] \\ &= \mathbb{E}\left[\left(\sum_{k=1}^K u_k(t, x)\psi_k(Q)\right)^2\right] \\ &= \sum_{k=1}^K u_k^2(t, x)\gamma_k\end{aligned}$$

Spectral Representation of Random Processes

Multiple Random Variables:

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

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

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

Consider the p -variate basis functions

$$\Psi_{\mathbf{i}'}(Q) = \psi_{i_1}(Q_1), \dots, \psi_{i_p}(Q_p)$$

which satisfy

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

Spectral Representation of Random Processes

Multi-Index Representation:

$$u^K(t, x, Q) = \sum_{|\mathbf{k}'|=0}^K u_{\mathbf{k}'}(t, x) \Psi_{\mathbf{k}'}(Q)$$

Single Index Representation:

$$u^K(t, x, Q) = \sum_{k=0}^K u_k(t, x) \Psi_k(Q)$$

k	$ \mathbf{k}' $	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)	$\psi_0(Q_1)\psi_0(Q_2)\psi_2(Q_3)$

1. Stochastic Galerkin Method

Galerkin Method: Consider $Au = f$ defined on space X with inner product $\langle \cdot, \cdot \rangle$.

Approximate Solution: **Goal:** For $i = 1, \dots, N$, solve

$$u^N = \sum_{j=1}^N u_j \psi_j$$

$$\langle Au^N - f, \psi_i \rangle = 0$$

$$\Rightarrow \sum_{j=1}^N \langle A\psi_j, \psi_i \rangle u_j = \langle f, \psi_i \rangle$$

Stochastic Galerkin: $y = f(Q)$ **Representation:** $y^K(Q) = \sum_{k=0}^K y_k \Psi_k(Q)$

Weak Formulation: For $i=0, \dots, K$

$$\sum_{k=0}^K y_k \int_{\Gamma} \psi_k(q) \psi_i(q) \rho(q) dq = \int_{\Gamma} f(q) \psi_i(q) \rho(q) dq$$

$$\Rightarrow \begin{bmatrix} \gamma_0 & & & \\ & \gamma_1 & & \\ & & \ddots & \\ & & & \gamma_K \end{bmatrix} \begin{bmatrix} y_0 \\ y_1 \\ \vdots \\ y_K \end{bmatrix} = \begin{bmatrix} \int_{\Gamma} f(q) \psi_0(q) \rho(q) dq \\ \vdots \\ \int_{\Gamma} f(q) \psi_K(q) \rho(q) dq \end{bmatrix}$$

Stochastic Galerkin Example

Example: Consider the integrated Helmholtz energy

$$\begin{aligned}y &= f(Q) \\ &= \int_0^{0.8} [\alpha_1 P^2 + \alpha_{11} P^4 + \alpha_{111} P^6] dP \\ &= c_1 \alpha_1 + c_2 \alpha_{11} + c_3 \alpha_{111}\end{aligned}$$

Case 1: $q = \alpha_1$ so $f(Q) = c_1 \alpha_1$

Take $\alpha_1 \sim N(\bar{\alpha}_1, \sigma_{\alpha_1}^2) \Rightarrow \alpha_1 = \bar{\alpha}_1 + \sigma_{\alpha_1} Q_1$ where $Q_1 \sim N(0, 1)$

Hence $\rho(q_1) = \frac{1}{\sqrt{2\pi}} e^{-q_1^2/2}$

Representation:

$$y^K(Q_1) = \sum_{k=0}^K y_k \psi_k(Q_1)$$

Stochastic Galerkin Example

Weak Formulation: For $i=0, \dots, K$

$$\begin{aligned} 0 &= \langle y^K(q_1) - f(q_1), \psi_i(q_1) \rangle_\rho \\ &= \int_{\mathbb{R}} [y^K(q_1) - f(q_1)] \psi_i(q_1) \rho(q_1) dq_1 \\ &= \int_{\mathbb{R}} \left[\sum_{k=0}^K y_k \psi_k(q_1) - c_1 (\bar{\alpha}_1 + \sigma_{\alpha_1} q_1) \right] \psi_i(q_1) \rho(q_1) dq_1 \\ &\Rightarrow \sum_{k=0}^K y_k \int_{\mathbb{R}} \psi_k(q_1) \psi_i(q_1) \rho(q_1) dq_1 \\ &= c_1 \int_{\mathbb{R}} (\bar{\alpha}_1 + \sigma_{\alpha_1} q_1) \psi_i(q_1) \rho(q_1) dq_1 \\ &= c_1 \bar{\alpha}_1 \int_{\mathbb{R}} \psi_i(q_1) \rho(q_1) dq_1 + c_1 \sigma_{\alpha_1} \int_{\mathbb{R}} q_1 \psi_i(q_1) \rho(q_1) dq_1 \end{aligned}$$

Note: $i = 0$: $y_0 = \bar{\alpha}_1 c_1$
 $i = 1$: $y_1 = \sigma_{\alpha_1} c_1$
 $i = 2$: $2! y_2 = 0$
 $i > 2$: $i! y_i = 0$

Result: $y^K(Q_1) = c_1 [\bar{\alpha}_1 + \sigma_{\alpha_1} Q_1]$

Recall: $\mathbb{E} [y^K(Q)] = c_1 \bar{\alpha}_1$

$$\text{var} [y^K(Q)] = \sum_{k=1}^K y_k^2 \gamma_k = c_1^2 \sigma_{\alpha_1}^2$$

Stochastic Galerkin Example

Case 2: $Q = [\alpha_1, \alpha_{11}]$ so $f(Q) = c_1 \alpha_1 + c_2 \alpha_{11}$

$$\alpha_1 \sim N(\bar{\alpha}_1, \sigma_{\alpha_1}^2)$$

$$\Rightarrow \alpha_1 = \bar{\alpha}_1 + \sigma_{\alpha_1} Q_1 \text{ where } Q_1 \sim N(0, 1)$$

$$\alpha_{11} \sim N(\bar{\alpha}_{11}, \sigma_{\alpha_{11}}^2)$$

$$\Rightarrow \alpha_{11} = \bar{\alpha}_{11} + \sigma_{\alpha_{11}} Q_2 \text{ where } Q_2 \sim N(0, 1)$$

Representation:

$$y^K(Q) = \sum_{k=0}^K y_k \psi_k(Q)$$

Weak Formulation: For $i=0, \dots, K$

$$\begin{aligned} 0 &= \int_{\mathbb{R}^2} [y^K(q) - f(q)] \psi_i(q) \rho(q) dq \\ &= \int_{\mathbb{R}^2} \left[\sum_{k=0}^K y_k \psi_k(q) - c_1(\bar{\alpha}_1 + \sigma_{\alpha_1} q_1) - c_2(\bar{\alpha}_{11} + \sigma_{\alpha_{11}} q_2) \right] \psi_i(q) \rho(q) dq \end{aligned}$$

Stochastic Galerkin Example

Weak Formulation: For $i=0,\dots,K$

$$\begin{aligned} \Rightarrow \sum_{k=0}^K y_k \int_{\mathbb{R}^2} \Psi_k(q) \Psi_i(q) \rho(q) dq \\ = c_1 \int_{\mathbb{R}^2} (\bar{\alpha}_1 + \sigma_{\alpha_1} q_1) \Psi_i(q) \rho(q) dq + c_2 \int_{\mathbb{R}^2} (\bar{\alpha}_{11} + \sigma_{\alpha_{11}} q_2) \Psi_i(q) \rho(q) dq \end{aligned}$$

Note:

$$i = 0 : (0, 0) \Rightarrow \Psi_0(q) = \psi_0(q_1) \psi_0(q_2)$$

$$y_0 = c_1 \bar{\alpha}_1 + c_2 \bar{\alpha}_{11}$$

$$i = 1 : (1, 0) \Rightarrow \Psi_1(q) = \psi_1(q_1) \psi_0(q_2)$$

$$y_1 = c_1 \sigma_{\alpha_1}$$

$$i = 2 : (0, 1) \Rightarrow \Psi_2(q) = \psi_0(q_1) \psi_1(q_2)$$

$$y_2 = c_2 \sigma_{\alpha_{11}}$$

Thus

$$y^K(Q) = y_0 + y_1 Q_1 + y_2 Q_2$$

$$= (c_1 \bar{\alpha}_1 + c_2 \bar{\alpha}_{11}) + c_1 \sigma_{\alpha_1} Q_1 + c_2 \sigma_{\alpha_{11}} Q_2$$

Note:

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

$$\text{var} [y^K(Q)] = c_1^2 \sigma_{\alpha_1}^2 + c_2^2 \sigma_{\alpha_{11}}^2$$

Recall:

$$\mathbb{E} \left(\sum_{i=1}^n a_i X_i \right) = \sum_{i=1}^n a_i \mathbb{E}(X_i)$$

$$\text{var} \left(\sum_{i=1}^n a_i X_i \right) = \sum_{i=1}^n a_i^2 \text{var}(X_i) + 2 \sum_{i < j} a_i a_j \text{cov}(X_i, X_j)$$

Stochastic Galerkin Example

Spring Model: See perturbation notes -- $Q = [m, c, k] \sim N(\bar{q}, V)$

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

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

Response:

$$y(\omega_F, Q) = \frac{1}{\sqrt{(k - m\omega_F^2)^2 + (c\omega_F)^2}}$$

Parameters:

$$m = \bar{m} + \sigma_m Q_1$$

$$c = \bar{c} + \sigma_c Q_2$$

$$k = \bar{k} + \sigma_k Q_3$$

Representation:

$$y^K(\omega_F, Q) = \sum_{k=0}^K y_k(\omega_F) \Psi_k(Q)$$

Weak Formulation: $i = 0, \dots, K$

$$0 = \int_{\mathbb{R}^3} \left[\sum_{k=0}^K y_k(\omega_F) \Psi_k(q) - \frac{1}{\sqrt{[(\bar{k} + \sigma_k q_3) - (\bar{m} + \sigma_m q_1)\omega_F^2]^2 + (\bar{c} + \sigma_c q_2)^2 \omega_F^2}} \right] \Psi_i(q) \rho(q) dq$$

$$\Rightarrow \sum_{k=0}^K y_k(\omega_F) \int_{\mathbb{R}^3} \Psi_k(q) \Psi_i(q) \rho(q) dq = \int_{\mathbb{R}^3} \frac{\Psi_i(q) \rho(q) dq}{\sqrt{[(\bar{k} + \sigma_k q_3) - (\bar{m} + \sigma_m q_1)\omega_F^2]^2 + (\bar{c} + \sigma_c q_2)^2 \omega_F^2}}$$

Construction of joint density often requires assumption of independent parameters

Stochastic Galerkin Example

Easy Case: $c = 0, k = 1$

$$\sum_{k=0}^K \frac{y_k(\omega_F)}{\sqrt{2\pi}} \int_{\mathbb{R}} \psi_k(q_1) \psi_i(q_1) e^{-q_1^2/2} dq_1 = \frac{1}{\sqrt{2\pi}} \int_{\mathbb{R}} \frac{\psi_i(q_1) e^{-q_1^2/2} dq_1}{\sqrt{[1 - (\bar{m} + \sigma_m q_1) \omega_F^2]^2}}$$

Coefficients:

$$i = 0: \quad y_0(\omega_F) \approx \sum_{r=1}^R \frac{\hat{w}^r}{\sqrt{[1 - (\bar{m} + \sigma_m q_1^r) \omega_F^2]^2}}$$

$$i = 1: \quad y_1(\omega_F) \approx \sum_{r=1}^R \frac{q_1^r \hat{w}^r}{\sqrt{[1 - (\bar{m} + \sigma_m q_1^r) \omega_F^2]^2}}$$

$$i = 2: \quad y_2(\omega_F) \approx \frac{1}{2} \sum_{r=1}^R \frac{[(q_1^r)^2 - 1] \hat{w}^r}{\sqrt{[1 - (\bar{m} + \sigma_m q_1^r) \omega_F^2]^2}}$$

Gauss-Hermite quadrature weights and points:

$$\hat{w}^r = \frac{w^r}{\sqrt{\pi}}, \quad q^r = \sqrt{2} \cdot x^r$$

where w^r, x^r from tables

Notes:

- For this problem, same as discrete projection (nonintrusive PCE)

Stochastic Galerkin Example

Harder Case: $Q = [m,c,k]$ random

Representation:

$$y^K(\omega_F, Q) = \sum_{k=0}^K y_k(\omega_F) \Psi_k(Q)$$

where

$$\begin{aligned} y_k(\omega_F) &= \frac{1}{\gamma_k} \int_{\mathbb{R}^3} y(\omega_F Q) \Psi_k(q) \rho(q) dq \\ &= \frac{1}{\gamma_k} \int_{\mathbb{R}^3} \frac{\Psi_k(q) \rho(q) dq}{\sqrt{[(\bar{k} + \sigma_k q_3) - (\bar{m} + \sigma_m q_1) \omega_F^2]^2 + (\bar{c} + \sigma_c q_2)^2 \omega_F^2}} \\ &\approx \frac{1}{\gamma_k} \sum_{r_1=1}^{R_{\ell_1}} \sum_{r_2=1}^{R_{\ell_2}} \sum_{r_3=1}^{R_{\ell_3}} \frac{\Psi_k(q^r) \hat{w}^r}{\sqrt{[(\bar{k} + \sigma_k q_3^{r_3}) - (\bar{m} + \sigma_m q_1^{r_1}) \omega_F^2]^2 + (\bar{c} + \sigma_c q_2^{r_2})^2 \omega_F^2}} \end{aligned}$$

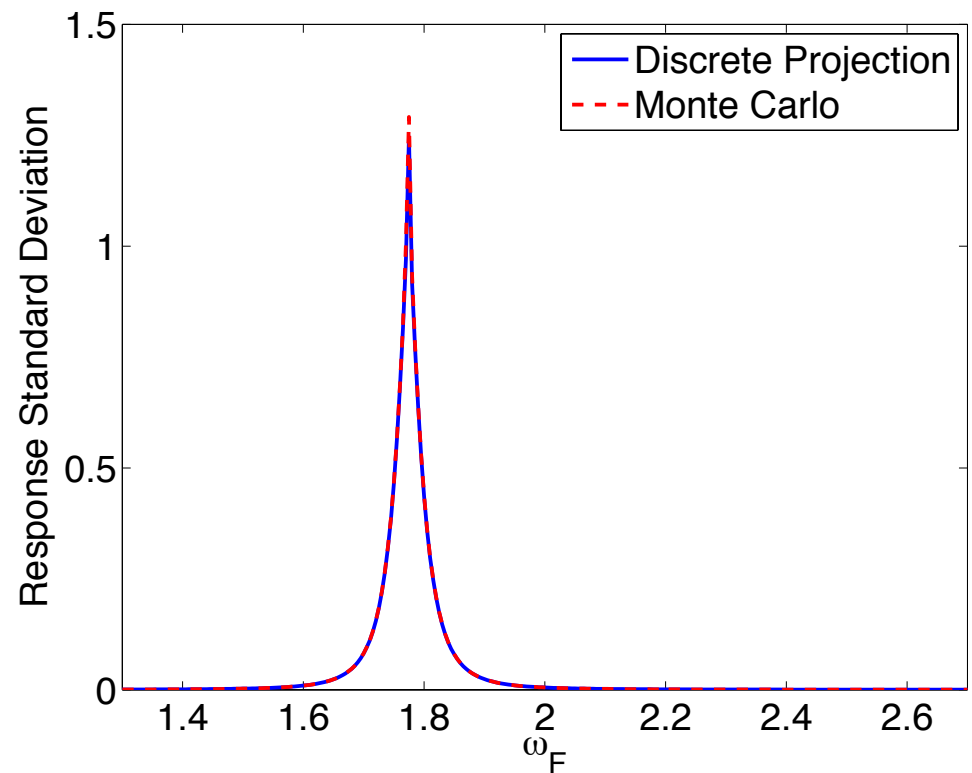
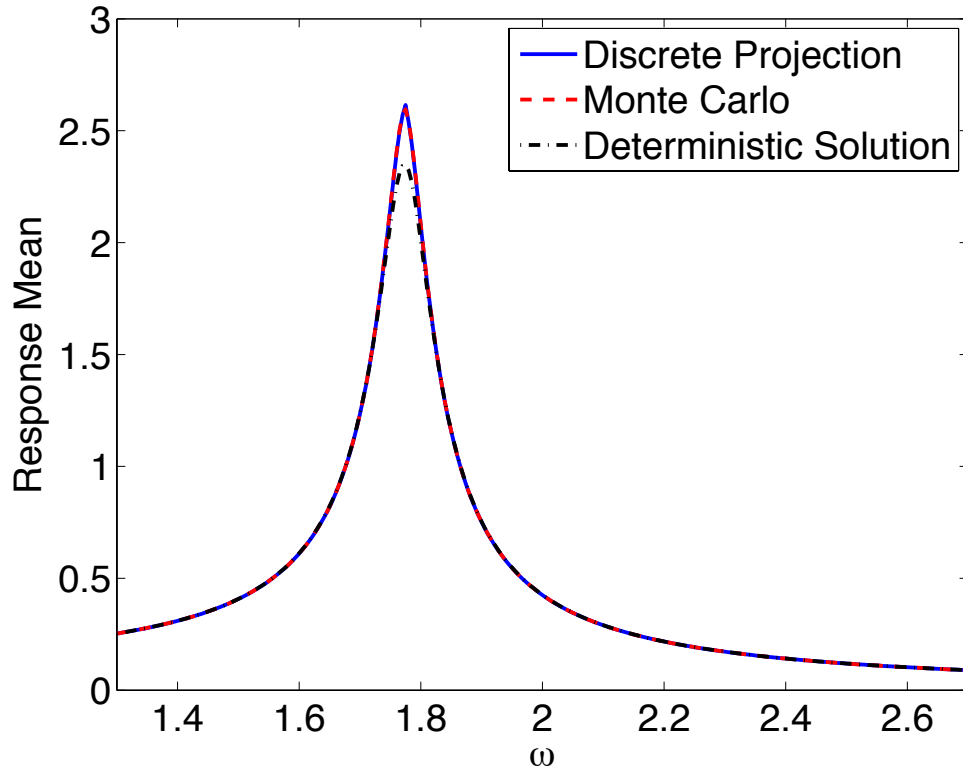
Note:

$$\mathbb{E} [y^k(\omega_F, Q)] = y_0(\omega_F)$$

$$\text{var} [y^k(\omega_F, Q)] = \sum_{k=1}^K y_k^2(\omega_F) \gamma_k$$

Stochastic Galerkin Example

Results:



Code: http://www4.ncsu.edu/~rsmith/UQ_TIA/CHAPTER10/index_chapter10.html

Note:

- Deterministic solution $y(\omega_F, \bar{q})$
- Due to nonlinearity, $y(\omega_F, \bar{q}) \neq \mathbb{E}[y(\omega_F, Q)]$ near the natural frequency

Stochastic Galerkin Example

Problem:

$$\frac{du}{dt} = f(t, Q, u), \quad t > 0$$

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

Quantity of Interest:

$$y(t) = \int_{\Gamma} u(t, q) \rho_Q(q) dq$$

Finite-Dimensional Representation:

$$u^K(t, Q) = \sum_{k=0}^K u_k(t) \Psi_k(Q)$$

where

$$u_k(t) = \frac{1}{\gamma_k} \int_{\Gamma} u(t, q) \Psi_k(q) \rho_Q(q) dq$$

$$\approx \frac{1}{\gamma_k} \sum_{r=1}^R u(t, q^r) \Psi(q^r) \hat{w}^r$$

Note:

- Discrete projection
- Nonintrusive and treat code as black box
- Parameters often assumed independent to construct joint density

Stochastic Galerkin Method

Weak Stochastic Formulation: For $i=0, \dots, K$

$$\begin{aligned} 0 &= \left\langle \frac{du^K}{dt} - f, \Psi_i \right\rangle_\rho \\ &= \int_\Gamma \left[\sum_{k=0}^K \frac{du_k}{dt}(t) \Psi_k(q) - f \left(t, q, \sum_{k=0}^K u_k(t) \Psi_k(q) \right) \right] \Psi_i(q) \rho_Q(q) dq \end{aligned}$$

which is equivalent to

$$\mathbb{E} \left[\frac{du^K(t, Q)}{dt} \Psi_i(Q) \right] = \mathbb{E} [f(t, Q, u^K) \Psi_i(Q)]$$

Quadrature yields

$$\sum_{r=1}^R \Psi_i(q^r) \rho_Q(q^r) w^r \left[\sum_{k=0}^K \frac{du_k}{dt}(t) \Psi_k(q^r) - f \left(t, q^r, \sum_{k=0}^K u_k(t) \Psi_k(q^r) \right) \right] = 0$$

 Must modify code and hence intrusive.
This is often prohibitive.

Stochastic Galerkin Method

Example: Consider

$$\frac{du}{dt} = -\alpha(\omega)u$$

$$u(0, \omega) = \bar{\beta}$$

where $\bar{\beta}$ is fixed and $\alpha \sim N(\bar{\alpha}, \sigma_\alpha^2)$ with $\bar{\alpha} > 0$. Here

$$\alpha = \alpha^N = \sum_{n=0}^N \alpha_n \psi_n(Q) \quad , \quad \alpha_0 = \bar{\alpha}, \alpha_1 = \sigma_\alpha, \alpha_n = 0, n > 1$$

$$\beta = \beta^N = \sum_{n=0}^N \beta_n \psi_n(Q) \quad , \quad \beta_0 = \bar{\beta}, \beta_n = 0, n > 0$$

Analytic solution:

$$u(t, Q) = \bar{\beta} e^{-(\bar{\alpha} + \sigma_\alpha Q)t}$$

Stochastic Galerkin Method

Approximate solution: Find

$$u^K(t, Q) = \sum_{k=0}^K u_k(t) \psi_k(Q)$$

subject to

$$\begin{aligned} 0 &= \left\langle \frac{du^K}{dt} + \alpha^N u^K, \psi_i \right\rangle_{\rho} \\ &= \int_{\mathbb{R}} \sum_{k=0}^K \frac{du_k}{dt}(t) \psi_k(q) \psi_i(q) \rho_Q(q) dq + \int_{\mathbb{R}} \alpha^N \sum_{k=0}^K u_k(t) \psi_k(q) \psi_i(q) \rho_Q(q) dq \end{aligned}$$

which is equivalent to

$$\frac{du_i}{dt} = \frac{1}{\gamma_i} \sum_{n=0}^N \sum_{k=0}^K \alpha_n u_k(t) \mathbf{e}_{ink}$$

where

$$\gamma_i = \mathbb{E} [\psi_i^2(Q)] = \int_{\mathbb{R}} \psi_i^2(q) \rho_Q(q) dq = i!$$

$$\mathbf{e}_{ink} = \mathbb{E} [\psi_i(q) \psi_n(q) \psi_k(q)] = \int_{\mathbb{R}} \psi_i(q) \psi_n(q) \psi_k(q) \rho_Q(q) dq$$

Initial Conditions:

$$u_k(0) = \beta_k, \quad k = 0, \dots, K$$

since

$$u^K(0, Q) = \sum_{k=0}^K u_k(0) \psi_k(Q) = \beta = \sum_{n=1}^N \beta_n \psi_n(Q)$$

Stochastic Galerkin Method

Note: To evaluate QoI, we observe that

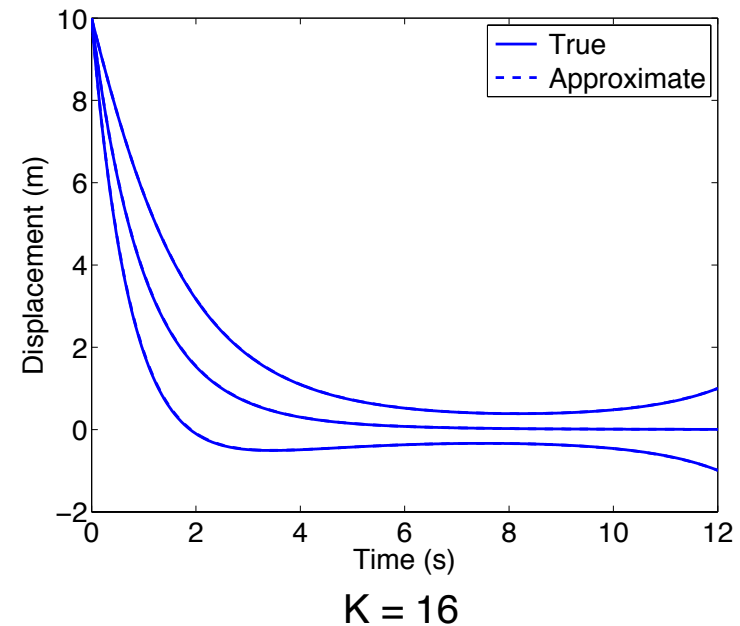
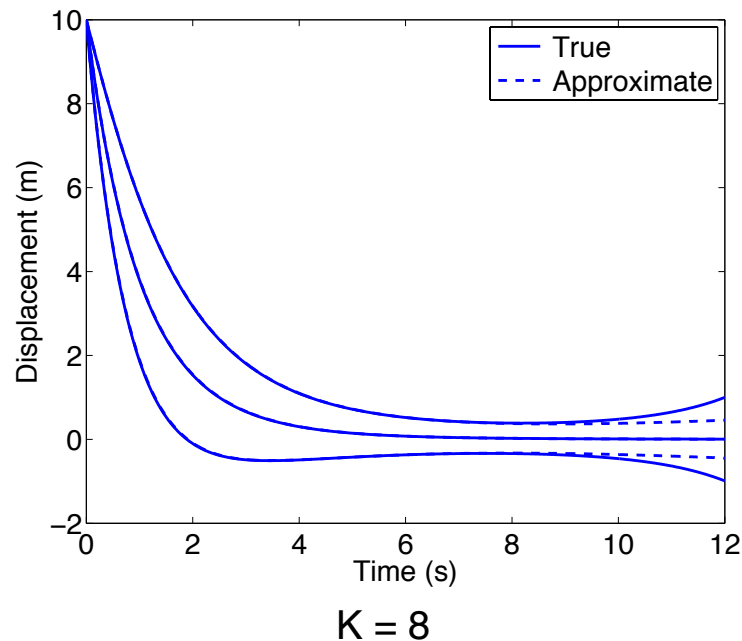
$$\mathbb{E} [u^K(t, Q)] = u_0(t)$$

$$\text{var}[u^K(t, Q)] = \sum_{k=1}^K u_k^2(t) \gamma_k.$$

Exact Mean and Variance:

$$\begin{aligned} \bar{u}(t) &= \int_{\mathbb{R}} \bar{\beta} e^{-(\bar{\alpha} + \sigma_{\alpha} q)t} \cdot \frac{1}{\sqrt{2\pi}} e^{-q^2/2} dq \\ &= \bar{\beta} e^{-\bar{\alpha}t} e^{\sigma_{\alpha}^2 t^2 / 2} \end{aligned}$$

$$\begin{aligned} \text{var}[u] &= \mathbb{E} [u^2(t)] - \bar{u}^2(t) \\ &= e^{-2\bar{\alpha}t} \bar{\beta}^2 \left(e^{2\sigma_{\alpha}^2 t^2} - e^{-\sigma_{\alpha}^2 t^2} \right) \end{aligned}$$



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.

Stochastic Collocation

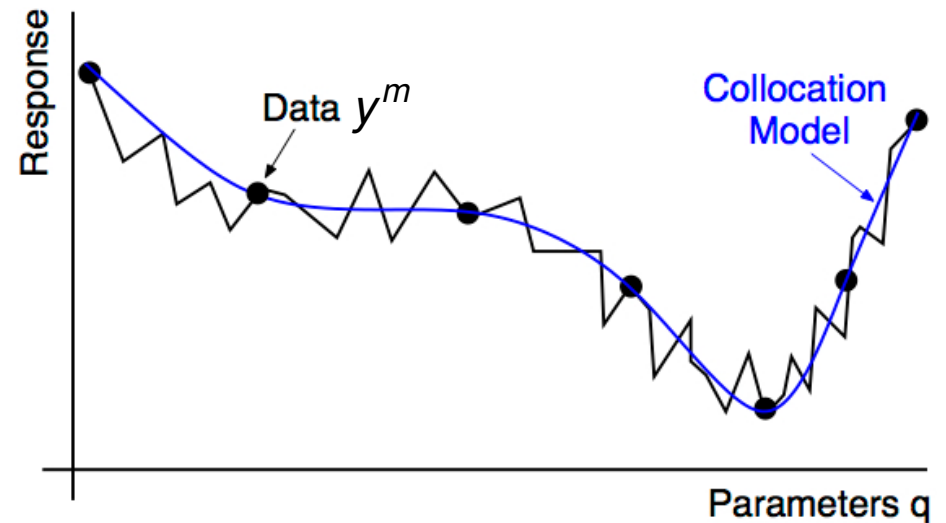
Strategy: Consider high fidelity model

$$y = f(q)$$

with M samples y^m , $m = 1, \dots, M$

Enforce

$$y^m = y^K(q^m) = \sum_{k=0}^K y_k \psi_k(q^m), \quad m = 1, \dots, M$$



Vandemonde System:

$$\begin{bmatrix} \psi_0(q^1) & \cdots & \psi_K(q^1) \\ \vdots & & \vdots \\ \psi_0(q^M) & \cdots & \psi_K(q^M) \end{bmatrix} \begin{bmatrix} y_0 \\ \vdots \\ y_K \end{bmatrix} = \begin{bmatrix} y^1 \\ \vdots \\ y^M \end{bmatrix}$$

Problem:

- Ill-posed and dense so difficult to extent to multiple dimensions

Stochastic Collocation

Strategy: Consider high fidelity model

$$y = f(q)$$

with M samples y^m , $m = 1, \dots, M$

Alternative: Collocation surrogate

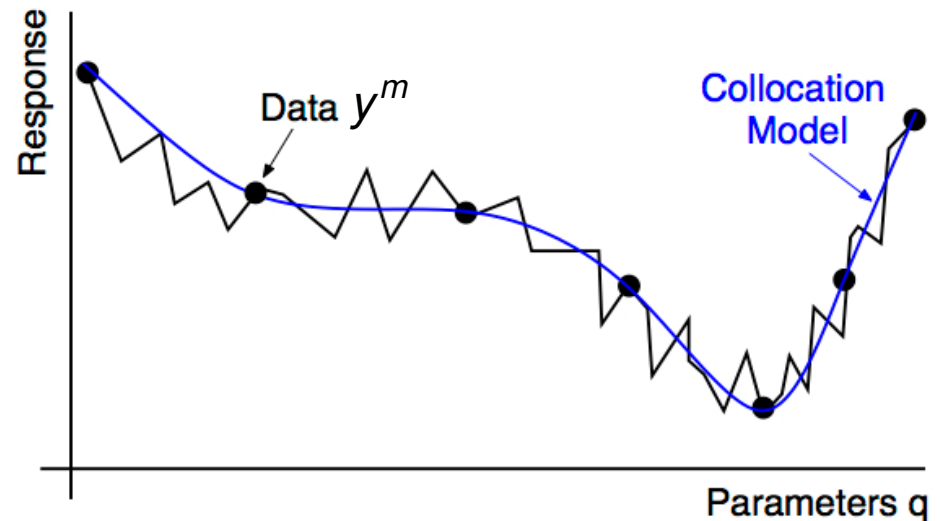
$$y^M(q) = \sum_{m=1}^M y_m L_m(q)$$

where $L_m(q)$ is a Lagrange polynomial, which in 1-D, is represented by

$$L_m(q) = \prod_{\substack{j=0 \\ j \neq m}}^M \frac{q - q^j}{q^m - q^j} = \frac{(q - q^1) \dots (q - q^{m-1})(q - q^{m+1}) \dots (q - q^M)}{(q^m - q^1) \dots (q^m - q^{m-1})(q^m - q^{m+1}) \dots (q^m - q^M)}$$

Note:

$$L_m(q^j) = \delta_{jm} = \begin{cases} 0 & , \quad j \neq m \\ 1 & , \quad j = m \end{cases}$$



Result: $y^M(q^m) = y_m$

Properties:

- Easy to add points
- Directly extendable to multiple-dim
- Can be highly oscillatory!

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);
```

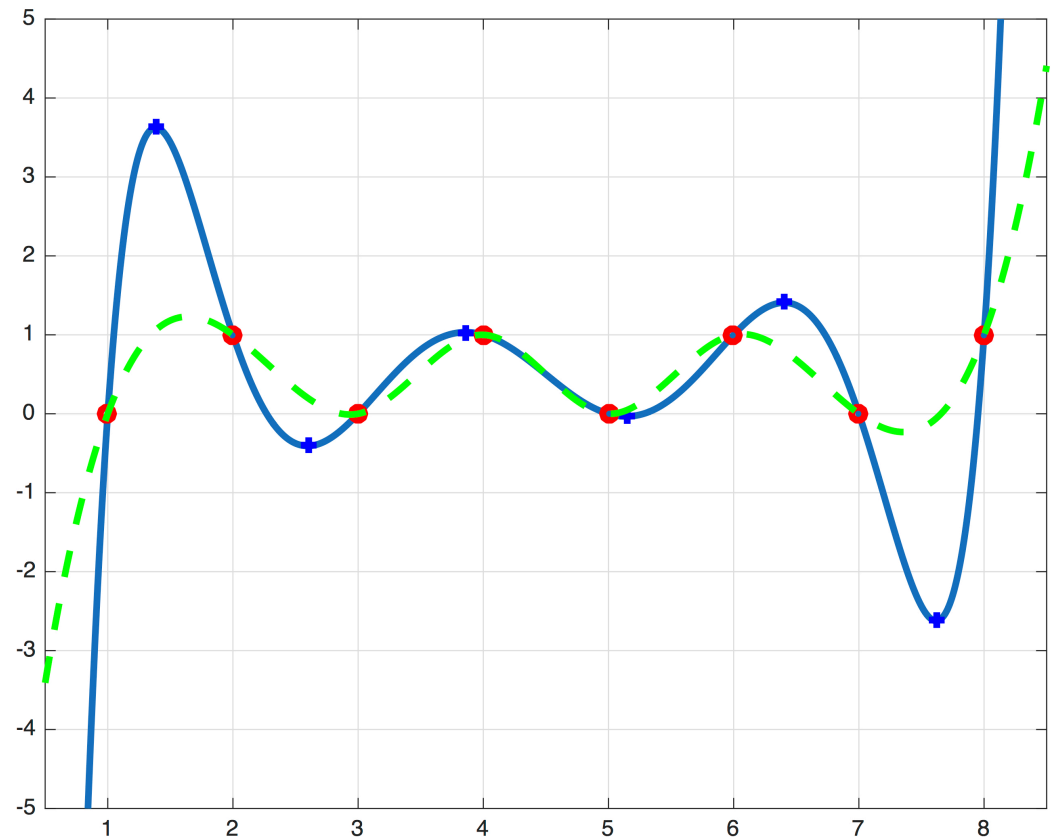
```
xx = 0.5 : 0.01 : 8.5;
```

```
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: More discussion to follow on point choices



Stochastic Collocation

Note: Analytic expressions for expected value and variance no longer hold for Lagrange basis!

Example: Consider spring response

$$y(\omega_F, Q) = \frac{1}{\sqrt{(k - m\omega_F^2)^2 + (c\omega_F)^2}}$$

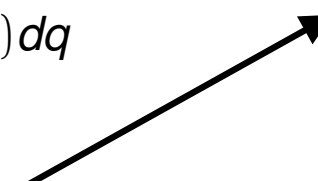
and

$$y^M(\omega_F, Q) = \sum_{m=1}^M y(\omega_F, q_m) L_m(Q)$$

Single Variable:

$$\begin{aligned} \mathbb{E} [y^M(\omega_F, Q)] &= \int_{\mathbb{R}} y^M(\omega_f, q) \rho(q) dq \\ &= \sum_{m=1}^M y(\omega_F, q^m) \int_{\mathbb{R}} L_m(q) \rho(q) dq \\ &\approx \sum_{m=1}^M y(\omega_F, q^m) \sum_{r=1}^R L_m(q^r) \rho(q^r) w^r \end{aligned}$$

Note: No quadrature rule associated with Lagrange polynomials



Stochastic Collocation

Single Variable:

$$\mathbb{E} [y^M(\omega_F, \mathbf{Q})] \approx \sum_{m=1}^M y(\omega_F, q^m) \sum_{r=1}^R L_m(q^r) \rho(q^r) w^r$$

Note: 2nd exercise
on Project 5

Strategy: Take $q^r = q^m$

$$\bar{y}^M(\omega_F) = \mathbb{E} [y^M(\omega_F, \mathbf{Q})] \approx \sum_{m=1}^M y(\omega_F, q^m) \rho(q^m) w^m$$

$$\begin{aligned} \text{Variance: } \text{var} [y^M(\omega_F, \mathbf{Q})] &= \int_{\mathbb{R}} [y^M(\omega_F, q) - \bar{y}^M(\omega_F)]^2 \rho(q) dq \\ &= \int_{\mathbb{R}} [y^M(\omega_F, q)]^2 \rho(q) dq - [\bar{y}^M(\omega_F)]^2 \\ &= \int_{\mathbb{R}} \left[\sum_{m=1}^M y^M(\omega_F, q^m) L_m(q) \right]^2 \rho(q) - [\bar{y}^M(\omega_F)]^2 \\ &\approx \sum_{r=1}^R \left[\sum_{m=1}^M y^M(\omega_F, q^m) L_m(q^r) \right]^2 \rho(q^r) w^r - [\bar{y}^M(\omega_F)]^2 \end{aligned}$$

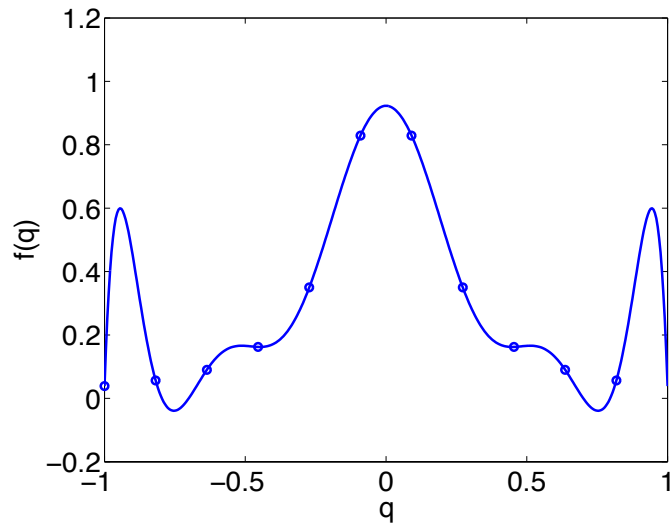
Take $q^r = q^m$

$$\text{var} [y^M(\omega_F, \mathbf{Q})] \approx \sum_{m=1}^M [y^M(\omega_F, q^m)]^2 \rho(q^m) w^m - [\bar{y}^M(\omega_F)]^2$$

Surrogate Models – Grid Choice

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

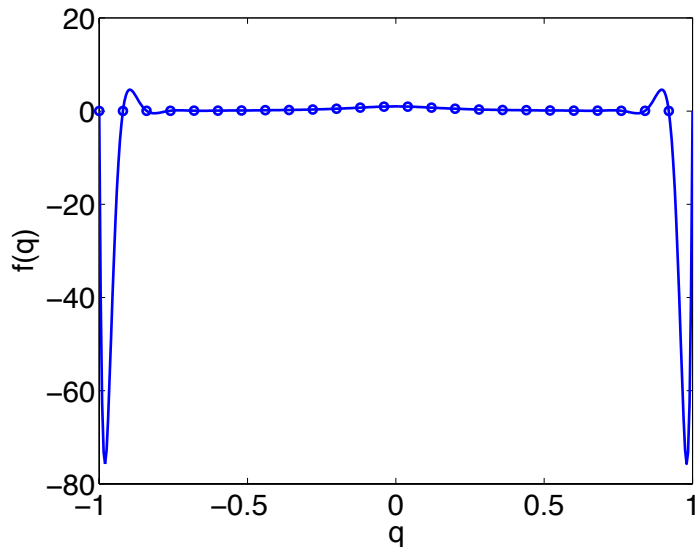
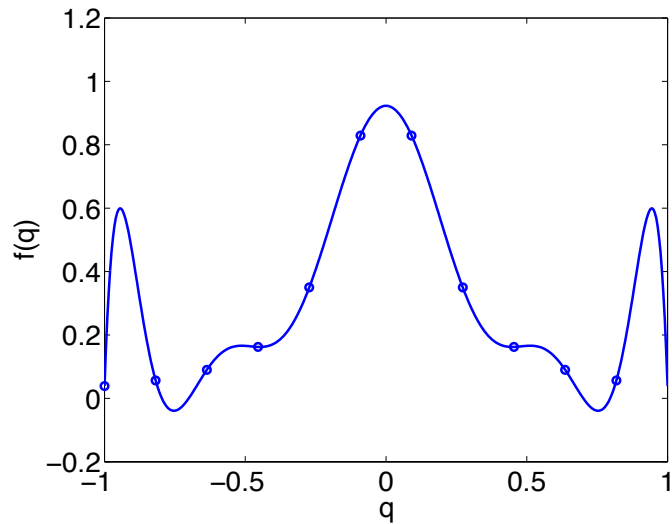
$$q^j = -1 + (j-1) \frac{2}{M}, \quad j = 1, \dots, M$$



Surrogate Models – Grid Choice

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

$$q^j = -1 + (j-1) \frac{2}{M}, \quad j = 1, \dots, M$$

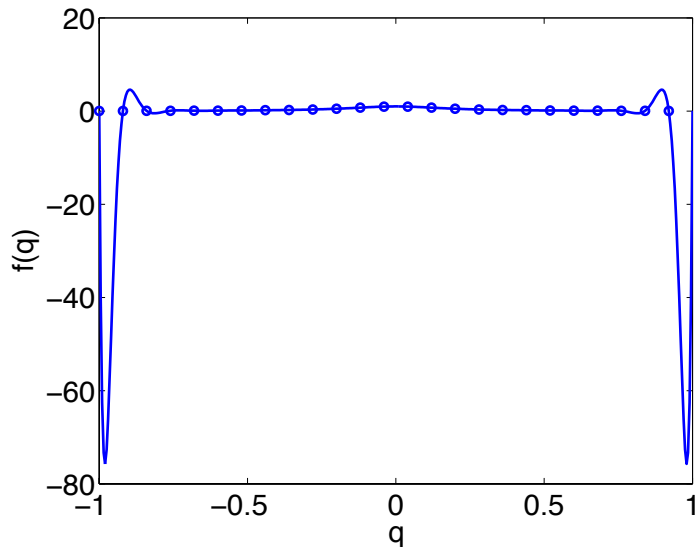
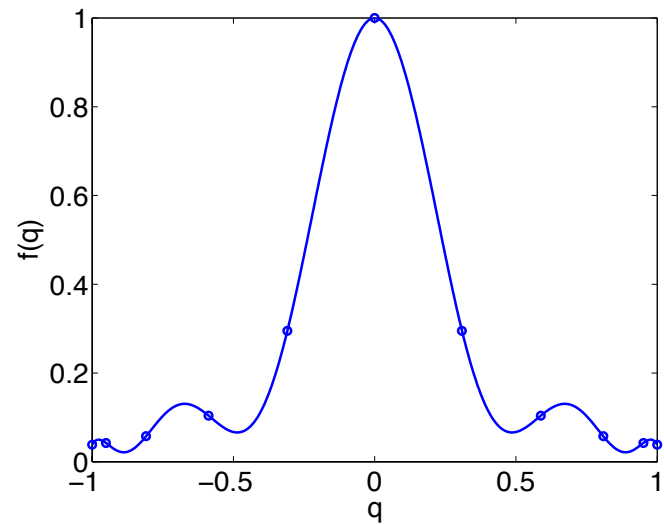
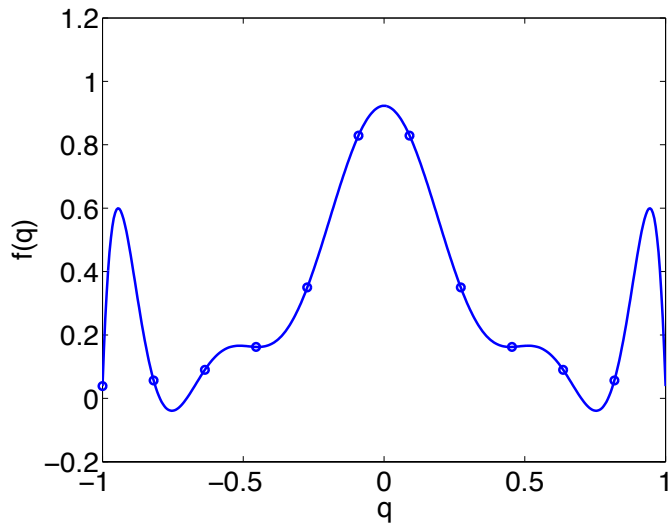


Surrogate Models – Grid Choice

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

$$q^j = -1 + (j-1) \frac{2}{M}, \quad j = 1, \dots, M$$

$$q^j = -\cos \frac{\pi(j-1)}{M-1}, \quad j = 1, \dots, M$$

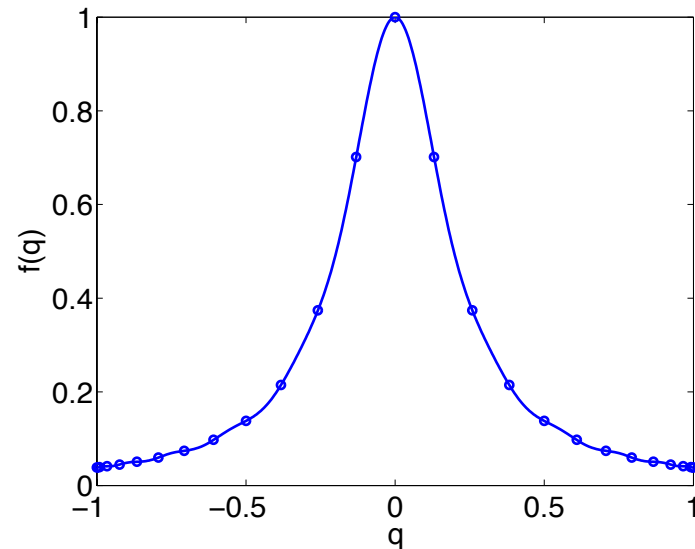
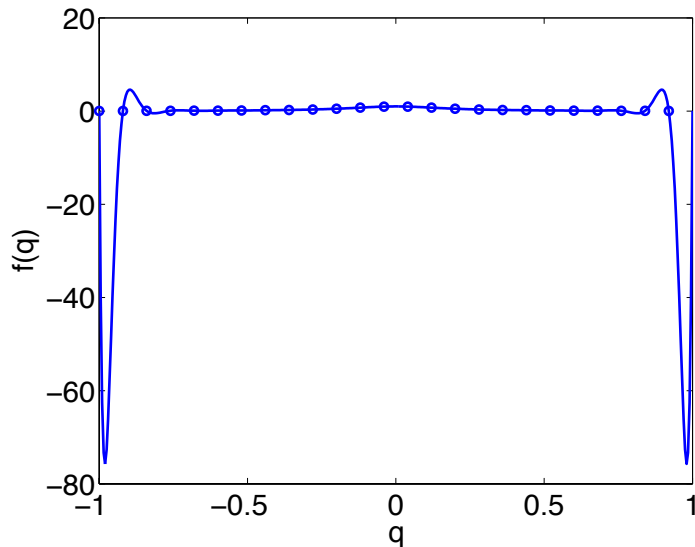
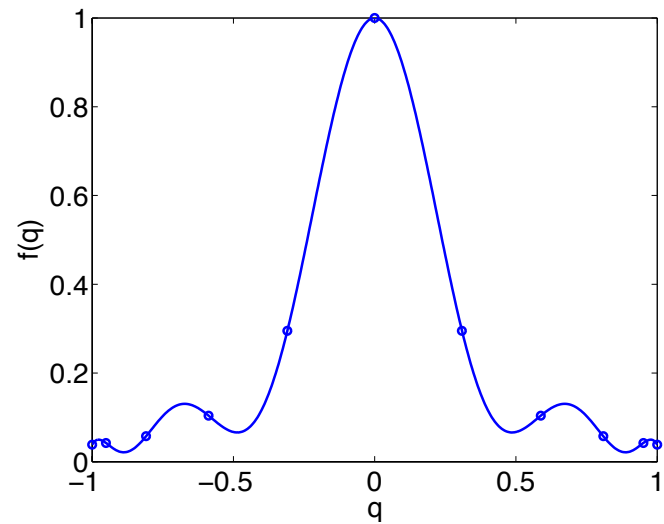
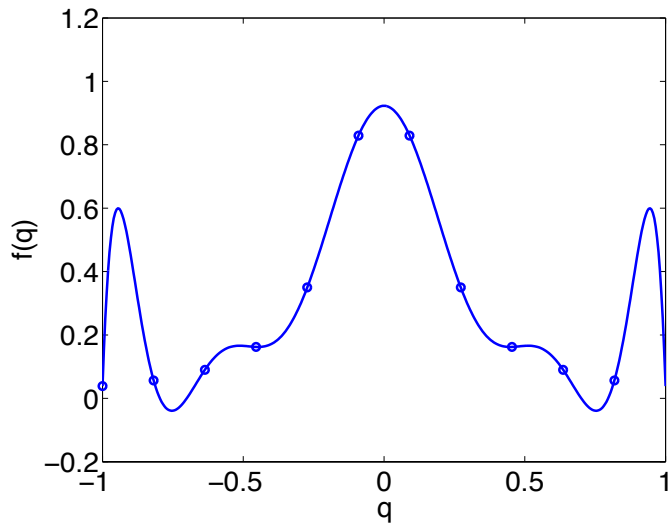


Surrogate Models – Grid Choice

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

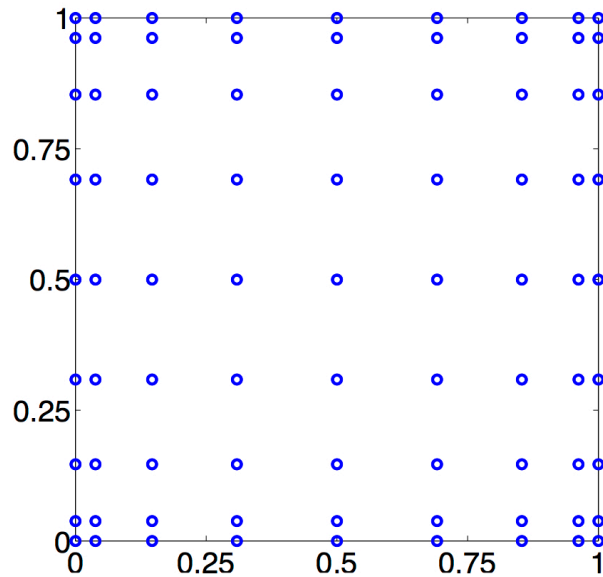
$$q^j = -1 + (j-1) \frac{2}{M}, \quad j = 1, \dots, M$$

$$q^j = -\cos \frac{\pi(j-1)}{M-1}, \quad j = 1, \dots, M$$

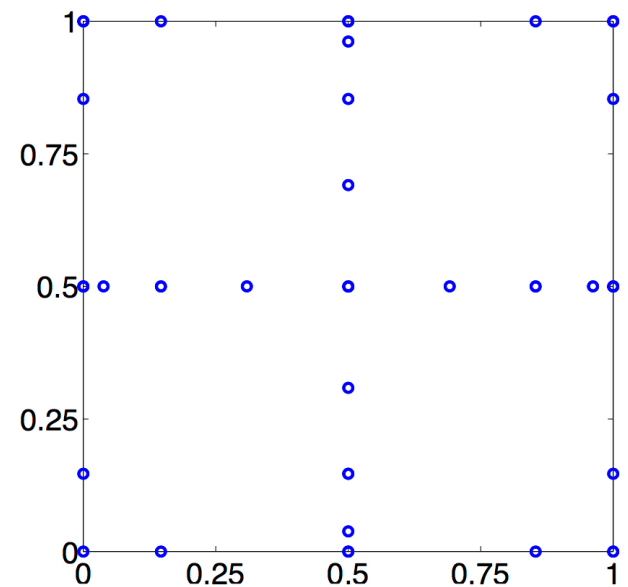


Sparse Grid Techniques

Tensor Grids: Exponential growth



Sparse Grids: Same accuracy



p	R_ℓ	Sparse Grid \mathcal{R}	Tensor 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	$> 2 \times 10^{95}$

Sparse Grids: More to follow in subsequent lectures