# Techniques to Propagate Uncertainties

**Goal:** Consider the nonlinearly parameterized model

$$\Upsilon = f(Q) \; , \;\; Q = [Q_1, \ldots, Q_p]$$

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

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

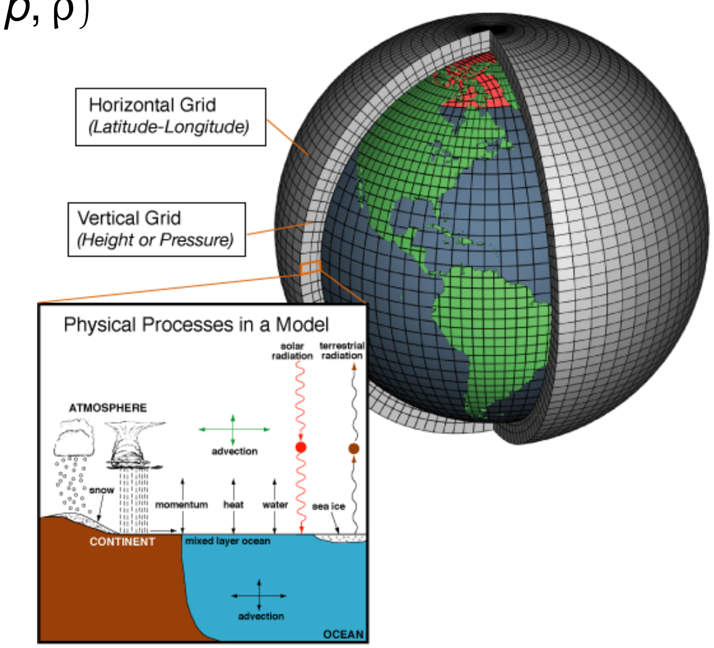
Momentum $$\frac{\partial v}{\partial t} = -v \cdot \nabla v - \frac{1}{\rho} \nabla p - g\hat{k} - 2\Omega \times v$$

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

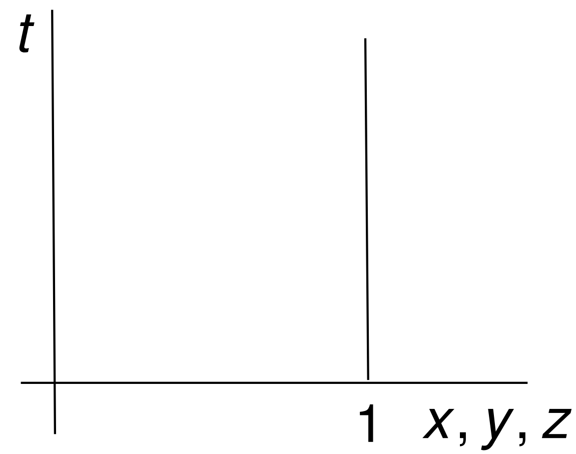
# Surrogate Models: Motivation

**Example:** Consider the heat equation

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

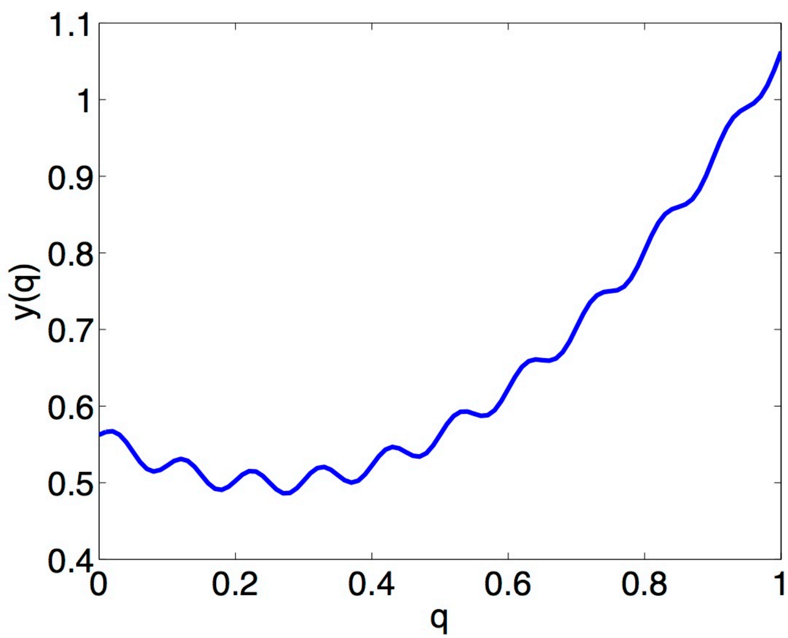
Boundary Conditions

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

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

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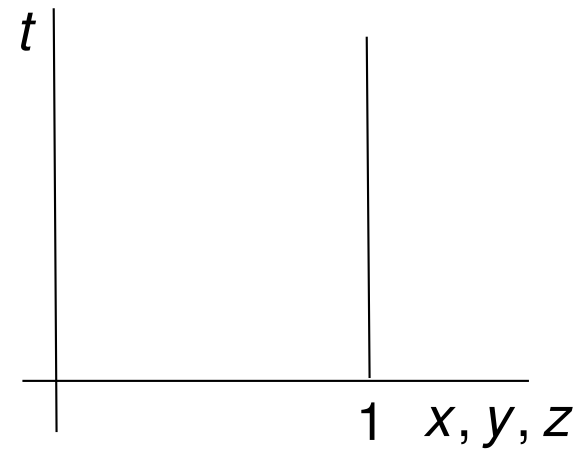
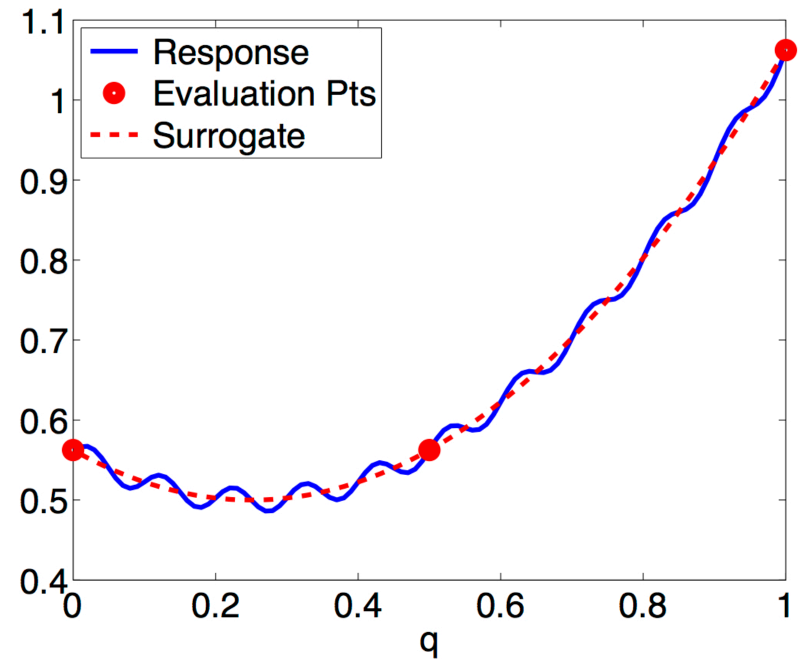



Surrogate: Quadratic

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




Question: How do you construct a polynomial surrogate?

- Regression
- Interpolation

# Surrogate Models

**Recall:** Consider the model

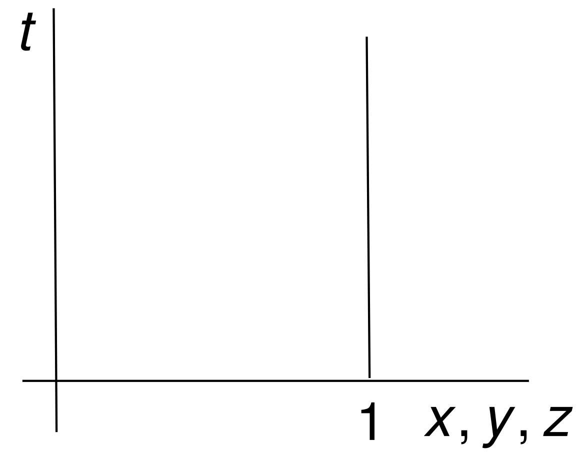
$$\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} + \frac{\partial^2 u}{\partial z^2} + f(q)$$

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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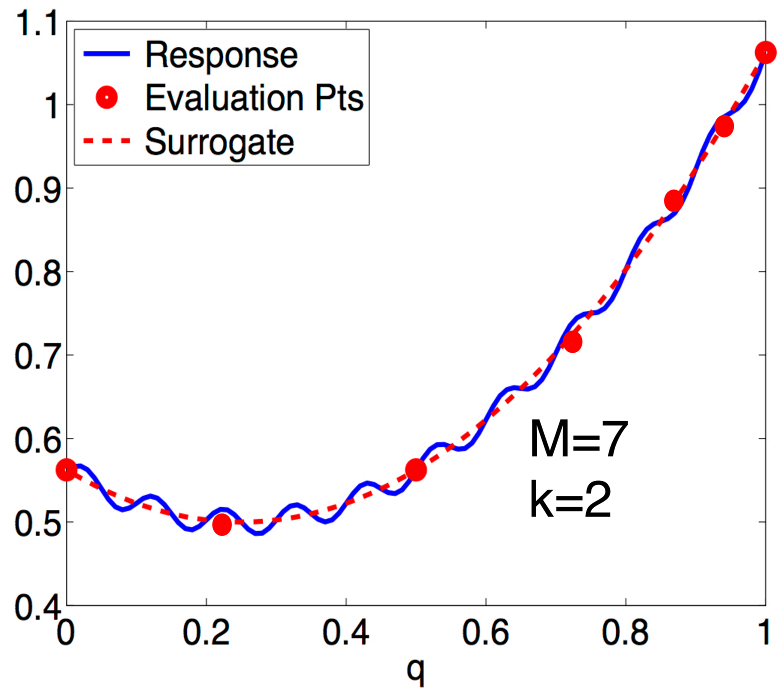



**Question:** How do you construct a polynomial surrogate?

- Interpolation
- Regression

# Surrogate Models

**Question:** How do we keep from fitting noise?

- Akaike Information Criterion (AIC)

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

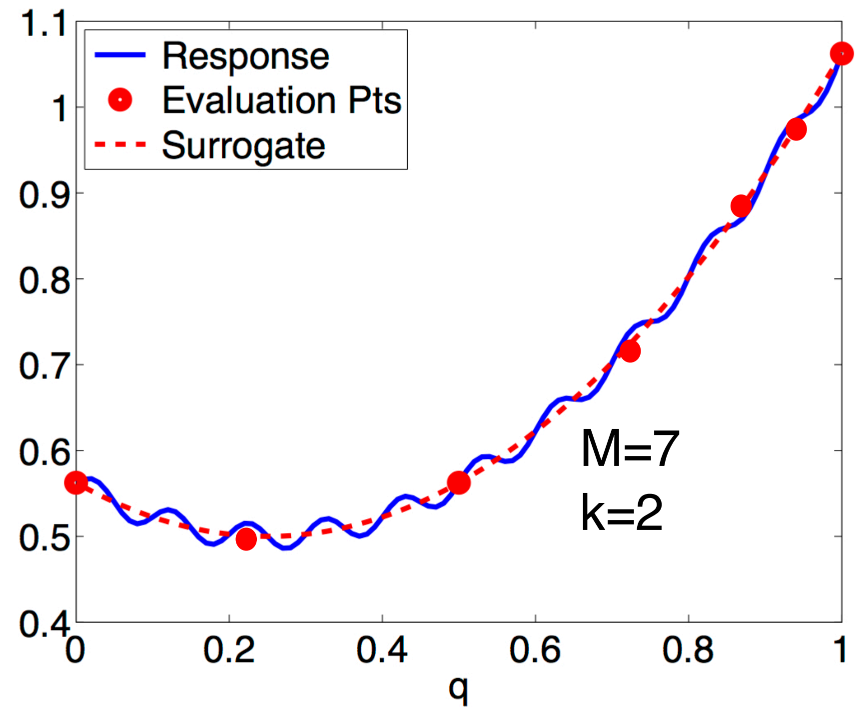
- Bayesian Information Criterion (BIC)

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

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

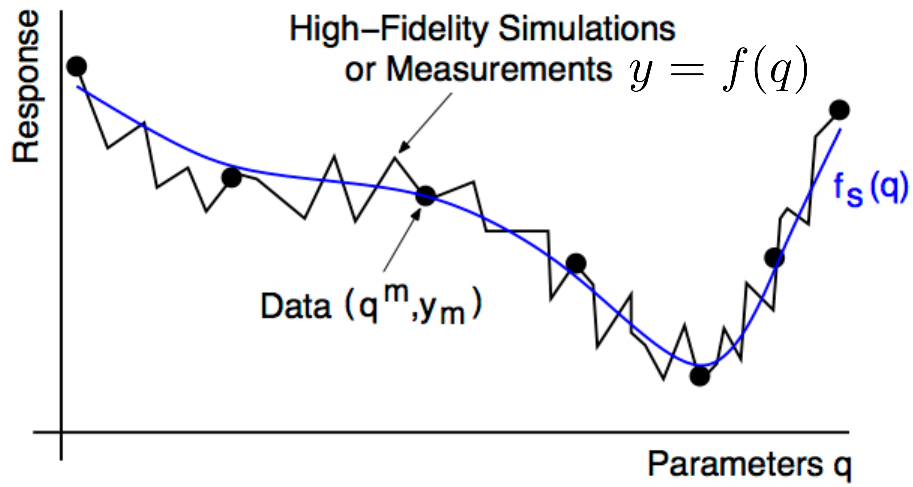
$$y = f(q)$$

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:**

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

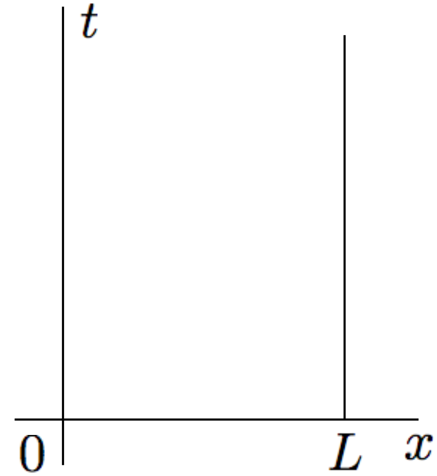
**Note:** $\Psi_k(Q)$ orthogonal with respect to inner product associated with pdf

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 on October 2




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

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

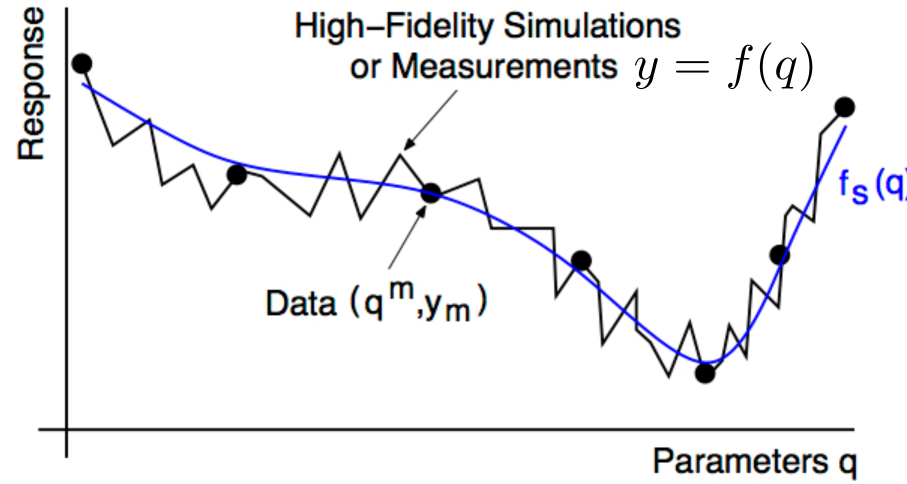
# Spectral Representation of Random Processes

**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:**

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

**Case 1:** Single random variable

**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

# Spectral Representation of Random Processes

**Hermite Polynomials:** $\boldsymbol{Q \sim N(0,1)}$

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

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

with the weight

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

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

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

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

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

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

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

Note: Can be used for:

- Uncertainty propagation
- Sobol-based global sensitivity analysis

**Issue:** How does one compute $y_k, k = 0, ..., K$?

- 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 produce 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: 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

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

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

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

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

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:**

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

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

# Spectral Representation of Random Processes

**Multiple Random Variables:**

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

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

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

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

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:**

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

**Goal:** For $i = 1, \ldots, N$, solve

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

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

**Stochastic Galerkin:** $y = f(Q)$

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

**Weak Formulation:** For i=0,…,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 $\alpha_1 \sim N(\overline{\alpha}_1, \sigma^2_{\alpha_1}) \Rightarrow \alpha_1 = \overline{\alpha}_1 + \sigma_{\alpha_1} Q_1$ 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,…,K

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

$$
\begin{aligned}
\Rightarrow \sum_{k=0}^{K} y_k \int_{\mathbb{R}} \psi_k(q_1)\psi_i(q_1)\rho(q_1)dq_1 \\
&= c_1 \int_{\mathbb{R}} (\overline{\alpha}_1 + \sigma_{\alpha_1} q_1)\, \psi_i(q_1)\rho(q_1)dq_1 \\
&= c_1\overline{\alpha}_1 \int_{\mathbb{R}} \psi_i(q_1)\rho(q_1)dq_1 + c_1\sigma_{\alpha_1} \int_{\mathbb{R}} q_1\psi_i(q_1)\rho(q_1)dq_1
\end{aligned}
$$

**Note:**

$$
\begin{aligned}
i = 0 &: \quad y_0 = \overline{\alpha}_1 c_1 \\
i = 1 &: \quad y_1 = \sigma_{\alpha_1} c_1 \\
i = 2 &: \quad 2! y_2 = 0 \\
i > 2 &: \quad i! y_i = 0
\end{aligned}
$$

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

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

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

# Stochastic Galerkin Example

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

$$\alpha_1 \sim N(\overline{\alpha}_1, \sigma^2_{\alpha_1})$$

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

$$\alpha_{11} \sim N(\overline{\alpha}_{11}, \sigma^2_{\alpha_{11}})$$

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

**Representation:**

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

**Weak Formulation:** For i=0,…,K

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

# Stochastic Galerkin Example

**Weak Formulation:** For i=0,…,K

$$\Rightarrow \sum_{k=0}^{K} y_k \int_{\mathbb{R}^2} \Psi_k(q)\Psi_i(q)\rho(q)dq$$

$$= c_1 \int_{\mathbb{R}^2} (\overline{\alpha}_1 + \sigma_{\alpha_1} q_1)\, \Psi_i(q)\rho(q)dq + c_2 \int_{\mathbb{R}^2} (\overline{\alpha}_{11} + \sigma_{\alpha_{11}} q_2)\, \Psi_i(q)\rho(q)dq$$

**Note:**

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

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

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

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

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

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

Thus

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

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

**Note:**

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

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

**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 -- $Q = [m, c, k] \sim N(\bar{q}, V)$

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

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

Parameters:

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

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

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

Response:

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

Representation:

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

Weak Formulation: i = 0,…,K

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

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

Construction of joint density often requires assumption of independent parameters

# Stochastic Galerkin Example

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

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

Coefficients:

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

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

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

Gauss-Hermite quadrature weights and points:

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

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

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

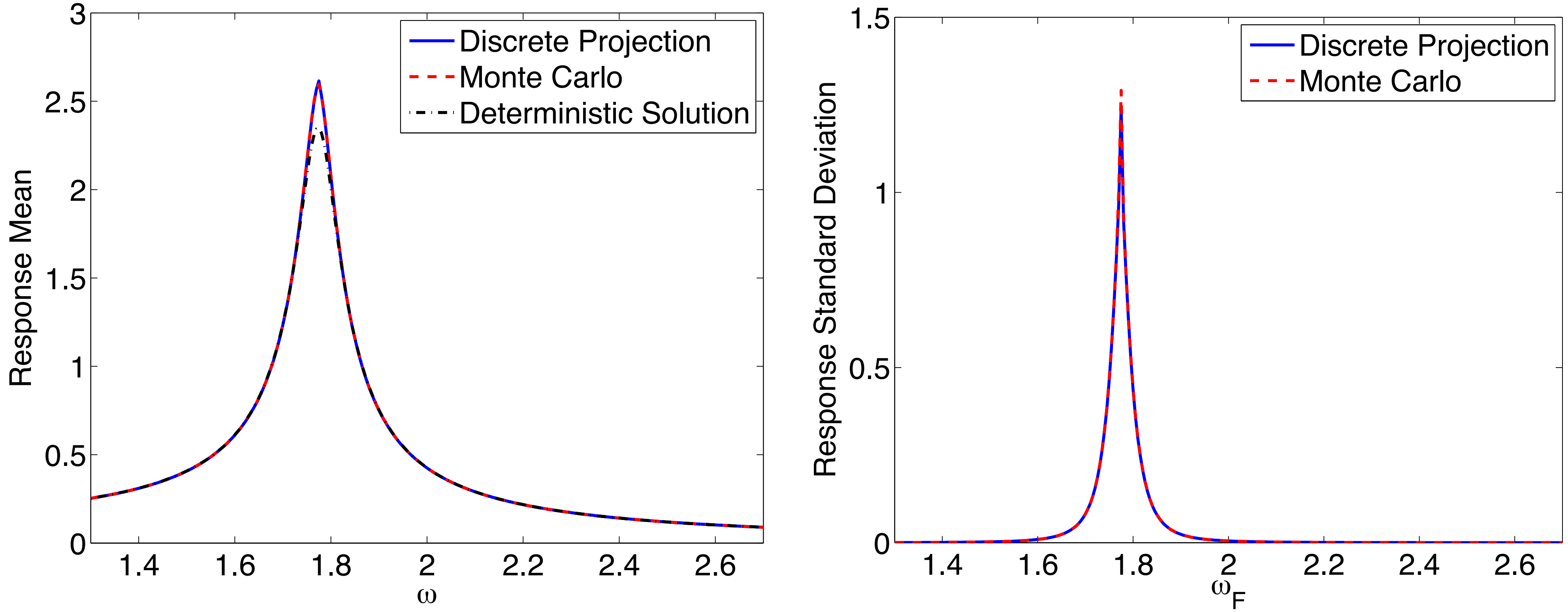
Note:

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

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

# Stochastic Galerkin Example

**Results:**




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

**Note:**

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

# Stochastic Galerkin Example

**Problem:**

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

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

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

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

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

**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, …, K

$$0 = \left\langle \frac{du^K}{dt} - f, \Psi_i \right\rangle_\rho$$

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

which is equivalent to

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

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

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

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

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

$$0 = \left\langle \frac{du^K}{dt} + \alpha^N u^K, \psi_i \right\rangle_\rho$$

$$= \int_{\mathbb{R}} \sum_{k=0}^{K} \frac{du_k}{dt}(t)\psi_k(q)\psi_i(q)\rho_Q(q)dq + \int_{\mathbb{R}} \alpha^N \sum_{k=0}^{K} u_k(t)\psi_k(q)\psi_i(q)\rho_Q(q)dq$$

which is equivalent to

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

where

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

$$e_{ink} = \mathbb{E}\left[\psi_i(q)\psi_n(q)\psi_k(q)\right] = \int_{\mathbb{R}} \psi_i(q)\psi_n(q)\psi_k(q)\rho_Q(q)dq$$

Initial Conditions:

$$u_k(0) = \beta_k\ ,\ k = 0, \cdots, K$$

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

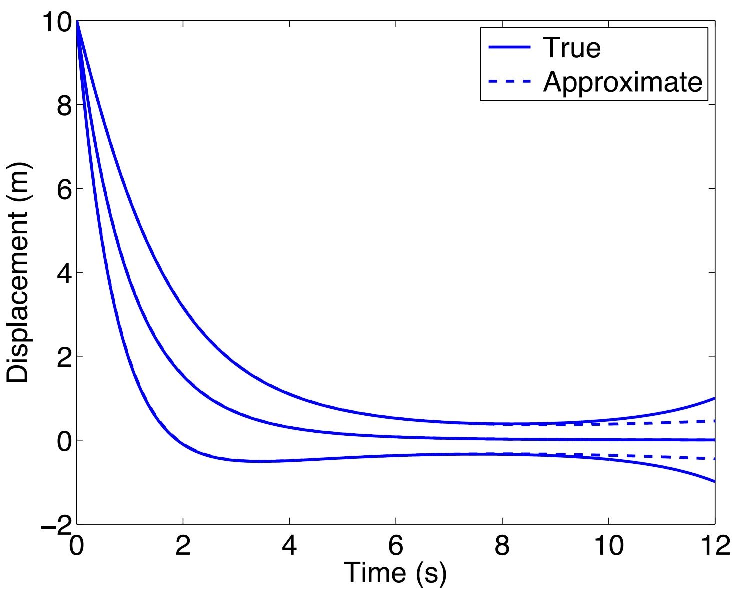
$$\mathbb{E}\left[u^K(t,Q)\right] = u_0(t)$$

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

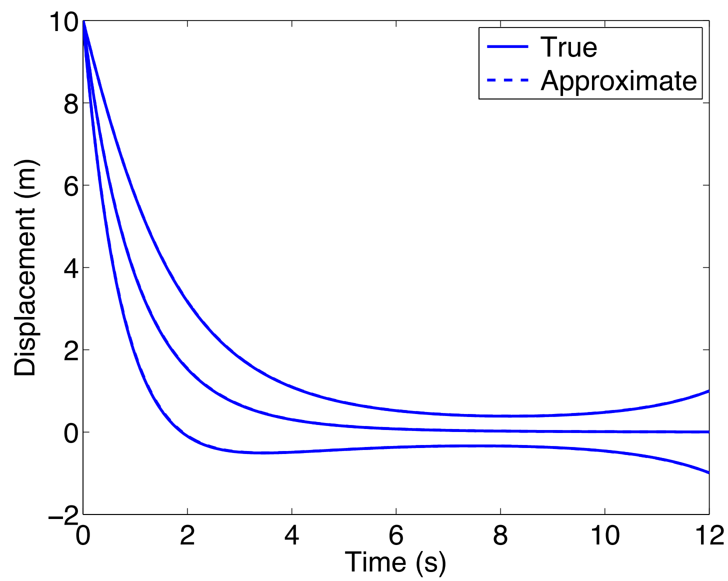
Exact Mean and Variance:

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

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




K = 8




K = 16

# 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:**

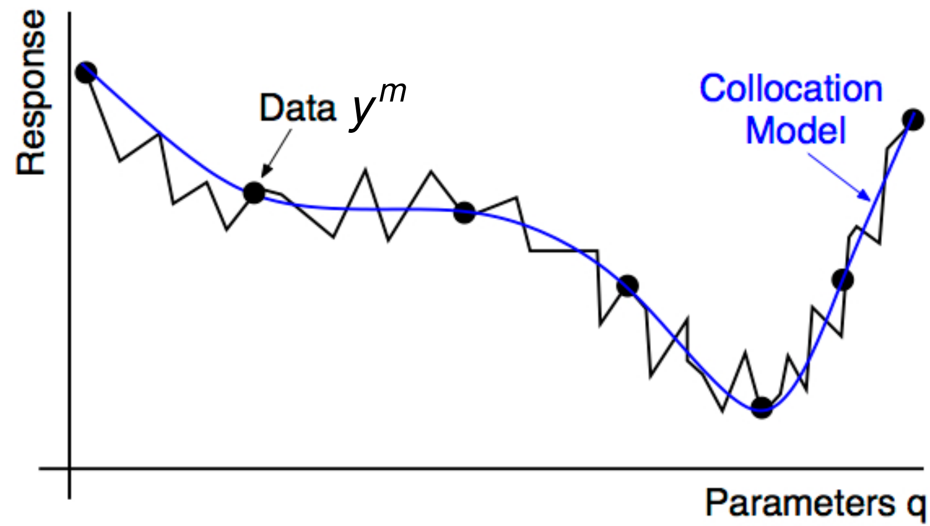
- Advantages
  - Like collocation, the method is nonintrusive and hence can be employed with post-processing to existing codes. The method is often referred to as nonintrusive PCE.
  - Projection method with associated error bounds.
  - Algorithms available in Sandia Dakota package.
- Disadvantages
  - 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 $y^m$ , $m = 1, ..., M$




Enforce

$$y^m = y^K(q^m) = \sum_{k=0}^{K} y_k \Psi_k(q^m) \; , \; m = 1, ..., M$$

**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

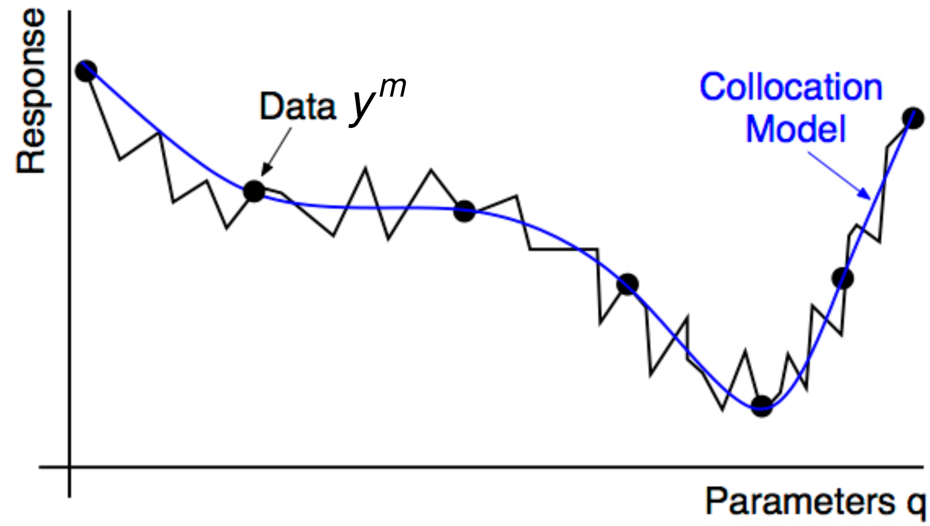
**Strategy:** Consider high fidelity model

$$y = f(q)$$

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

**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

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

**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:**

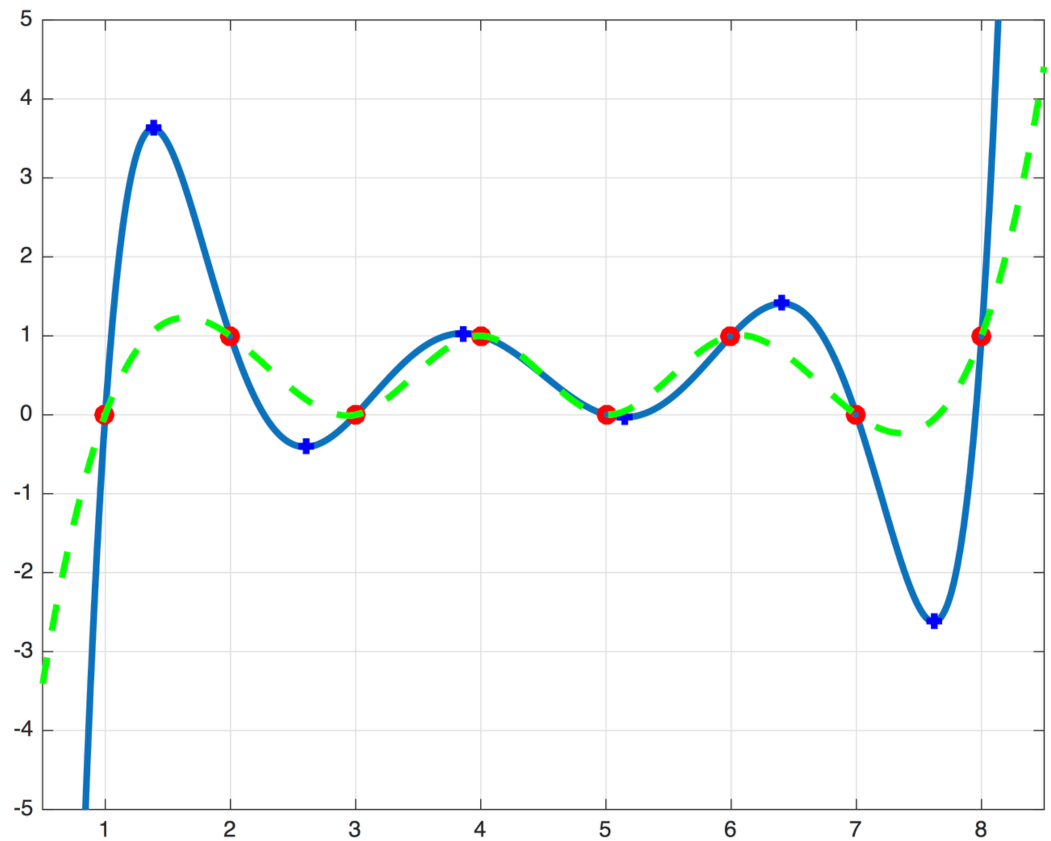
- Easy to add points
- Directly extendable to multiple-dim
- Can be highly oscillatory!

# 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:

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

**Note:** No quadrature rule associated with Lagrange polynomials

# Stochastic Collocation

Single Variable:

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

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

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

Variance: $\text{var}\left[y^M(\omega_F, Q)\right]$

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

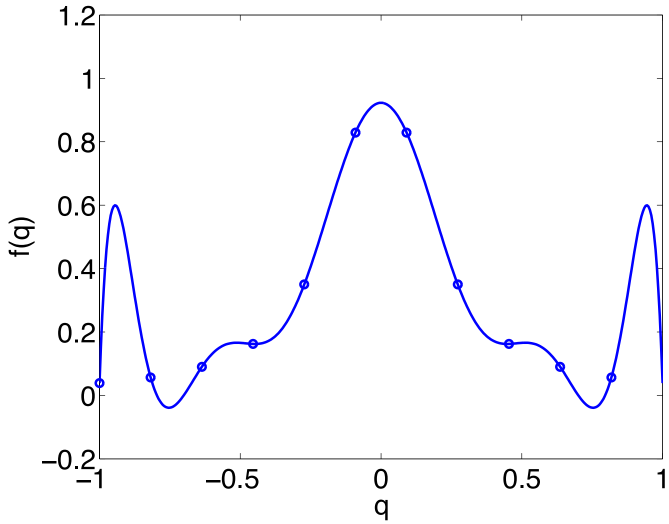
Take $q^r = q^m$

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

# Surrogate Models – Grid Choice

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

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



# Surrogate Models – Grid Choice

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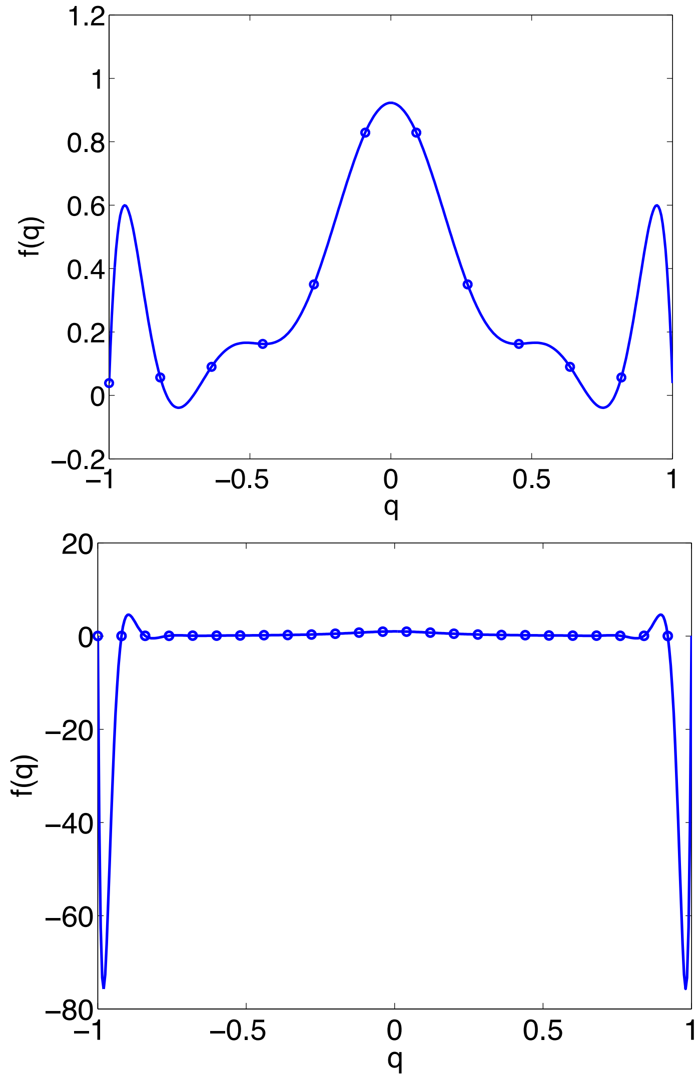
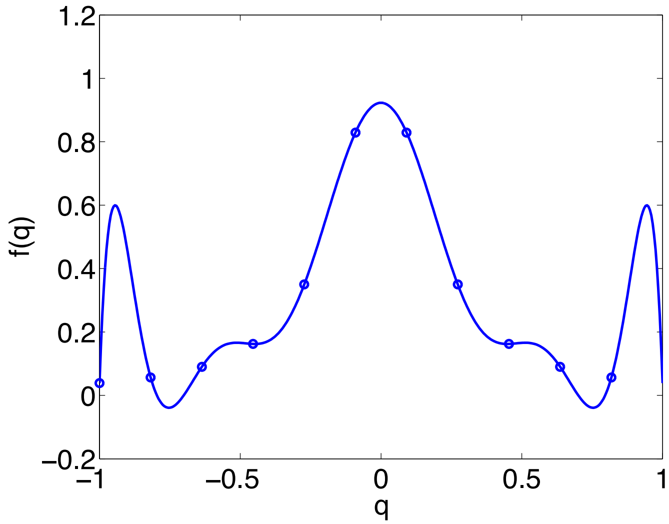
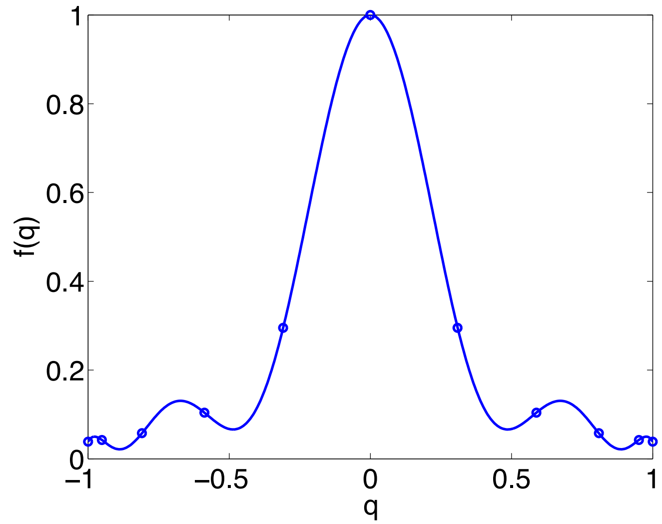


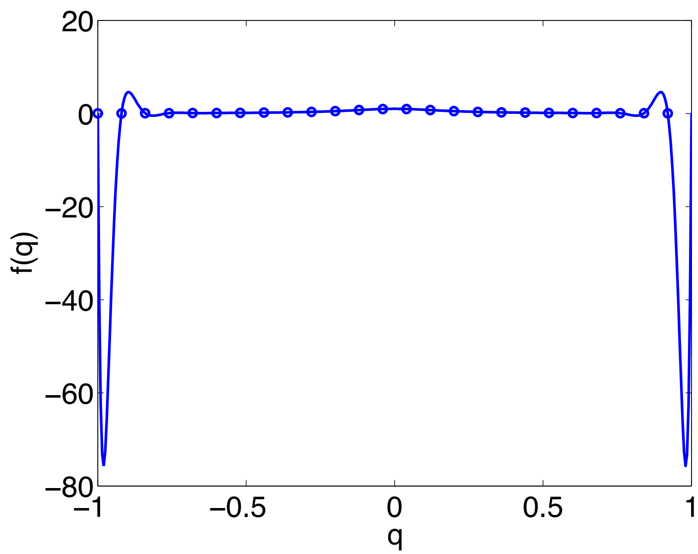
# Surrogate Models – Grid Choice

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

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



# Surrogate Models – Grid Choice

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

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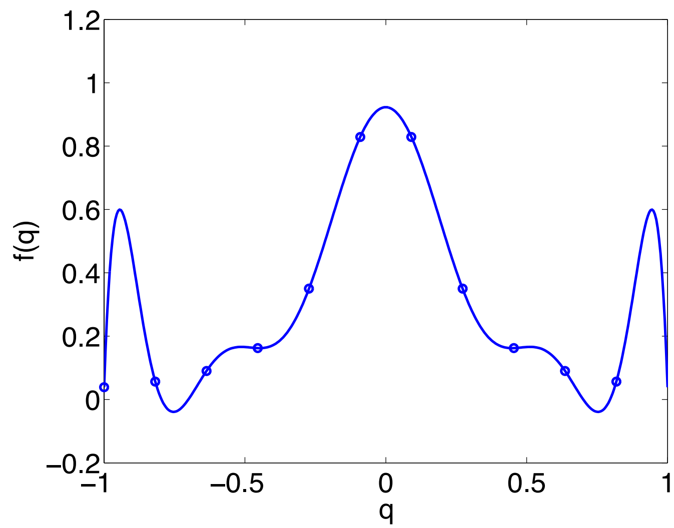
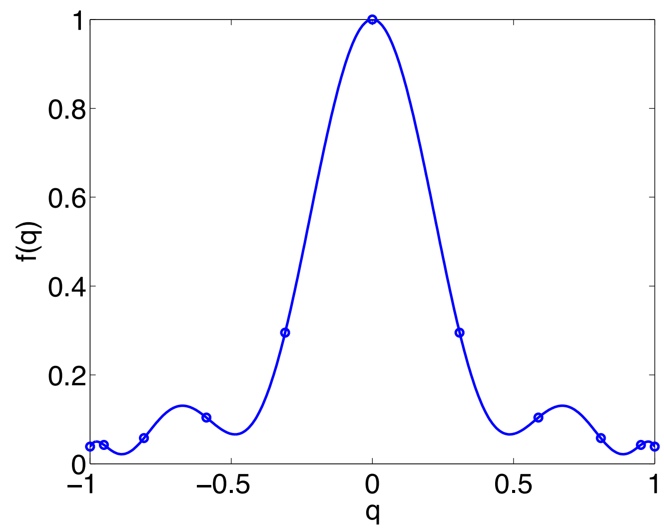
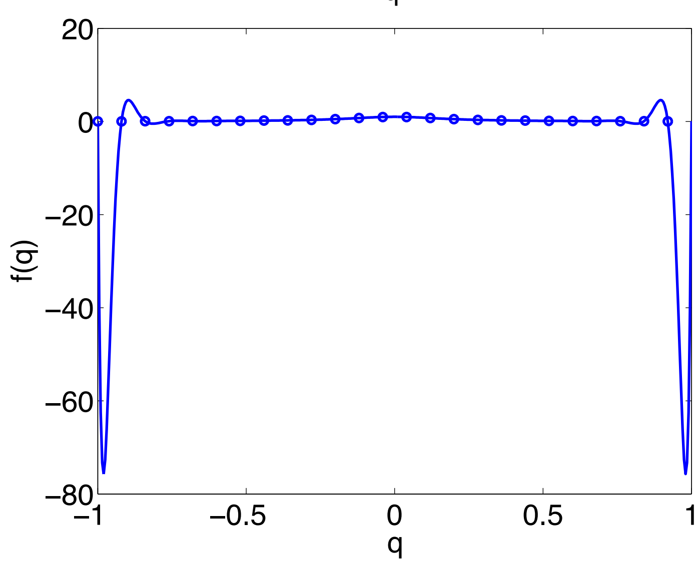
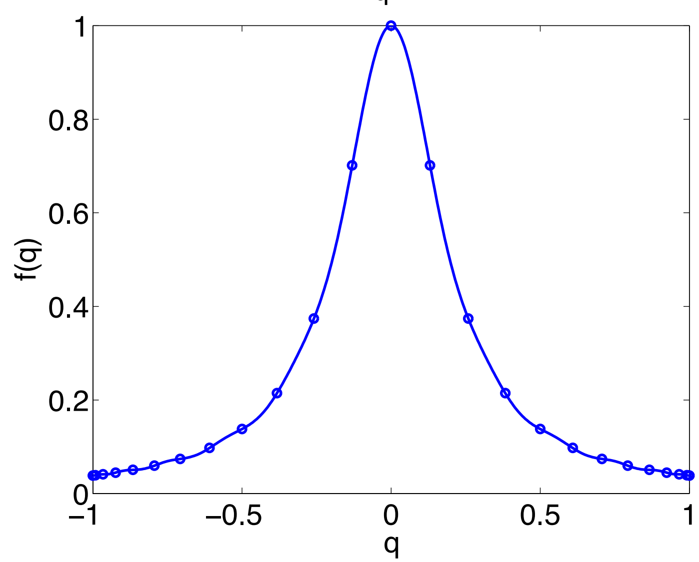


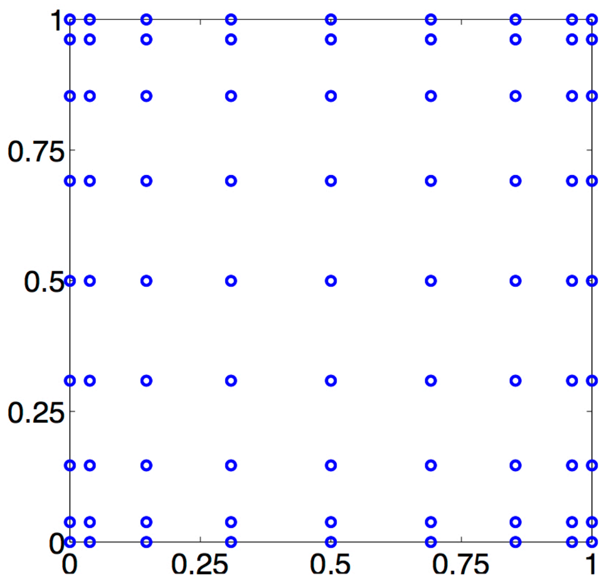



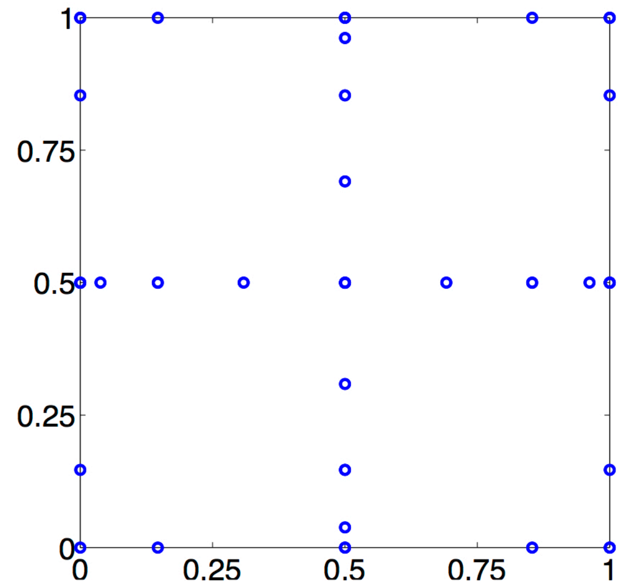



# Sparse Grid Techniques

Tensored Grids: Exponential growth




Sparse Grids: Same accuracy




| $p$ | $R_\ell$ | 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 | $> 2 \times 10^{95}$ |

**Sparse Grids:** More to follow in subsequent lectures