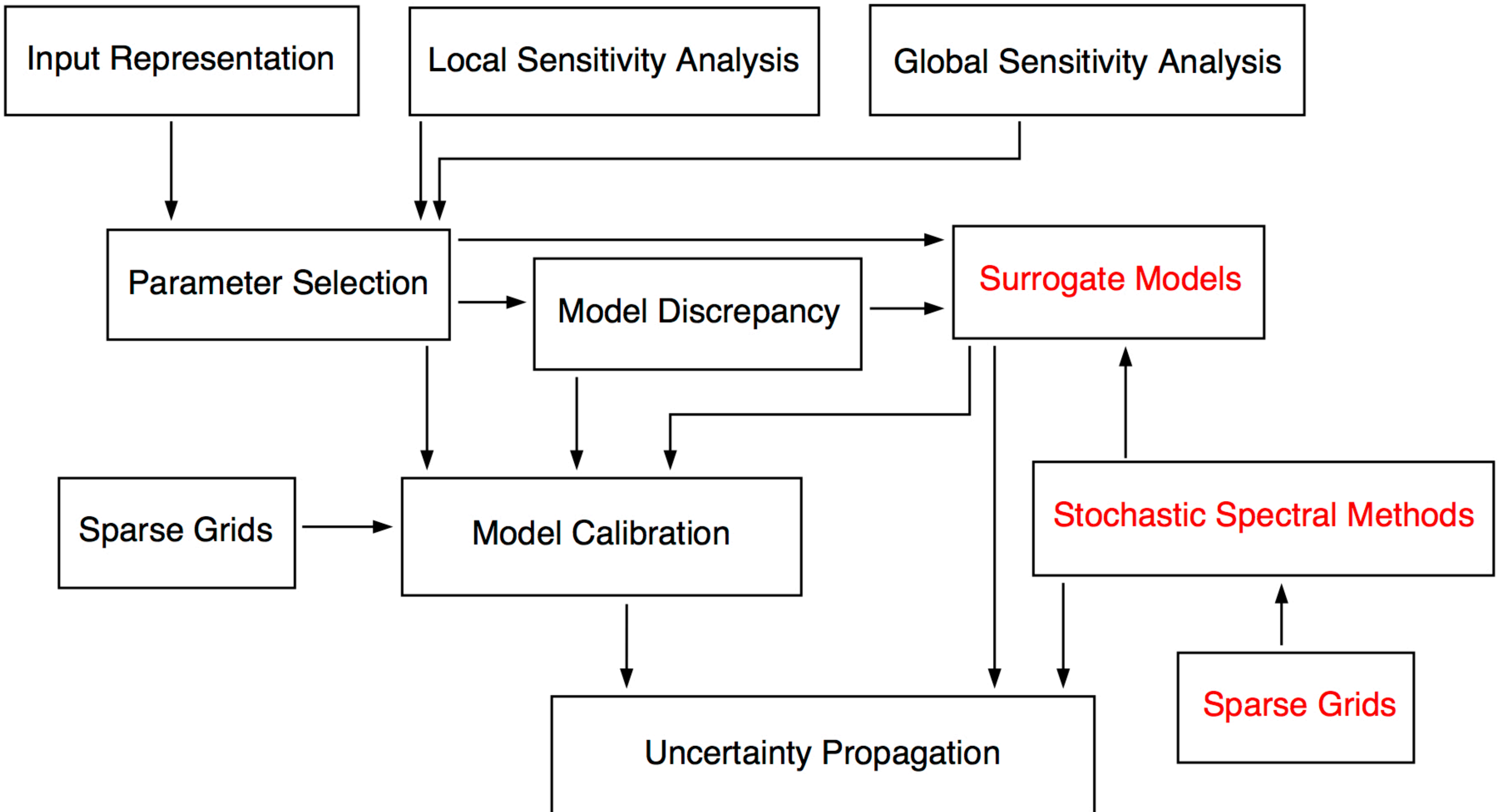
Steps in Uncertainty Quantification



Challenge:

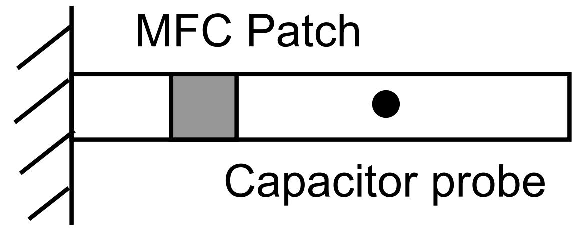
- How do we do uncertainty quantification for computationally expensive models?
- Example:
  - We have a computational budget of 5000 model evaluations.
  - Bayesian inference and uncertainty propagation require 120,000 evaluations.

Uncertainty Quantification Challenges

Example: MFC model – Fourth-order PDE

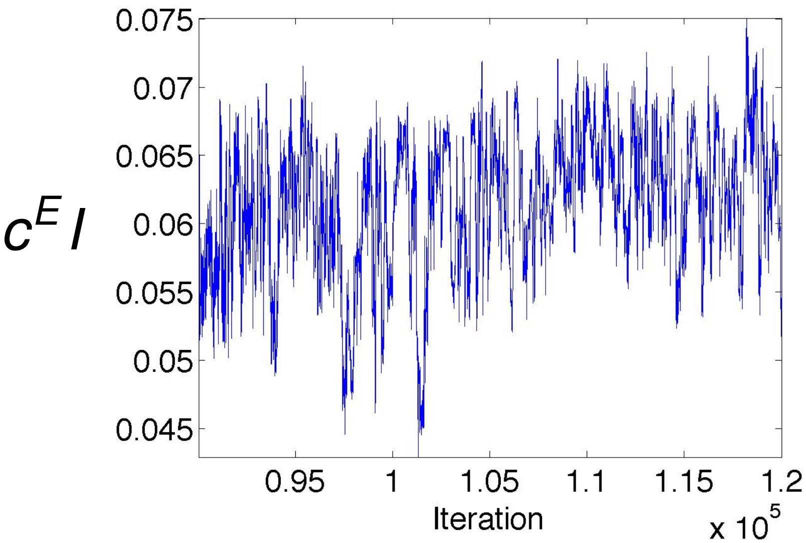
$$\rho \frac{\partial^2 w}{\partial t^2} - \frac{\partial^2 M}{\partial x^2} = f$$

$$M = -\underline{c^E I} \frac{\partial^2 w}{\partial x^2} - c_D I \frac{\partial^3 w}{\partial x^2 \partial t} - \left[k_1 e(E, \sigma_0) E + k_2 \varepsilon_{irr}(E, \sigma_0)\right] \chi_{MFC}(x)$$



Macro-Fiber Composite

Bayesian Inference: Took 6 days!



Problem:

1.2×10^5 PDE solutions

Solution: Highly efficient surrogate models

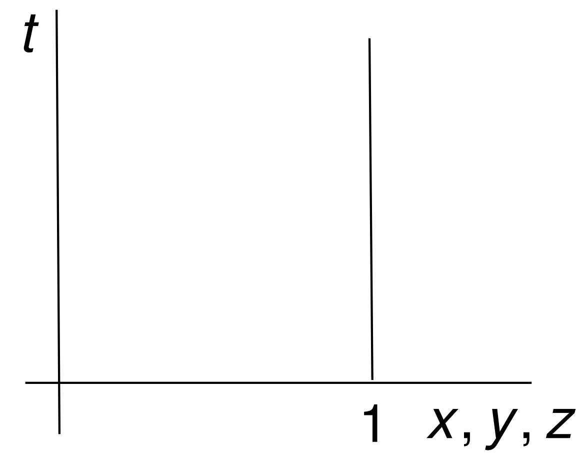
Surrogate Models: Motivation

Example: Consider the heat equation

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

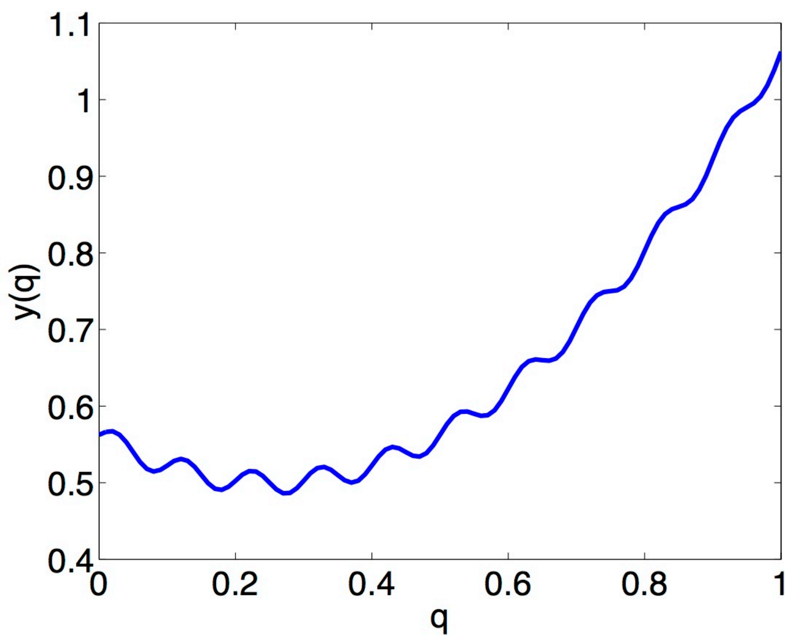
Boundary Conditions

Initial Conditions



with the response

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



Notes:

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

Surrogate Models: Motivation

Example: Consider the heat equation

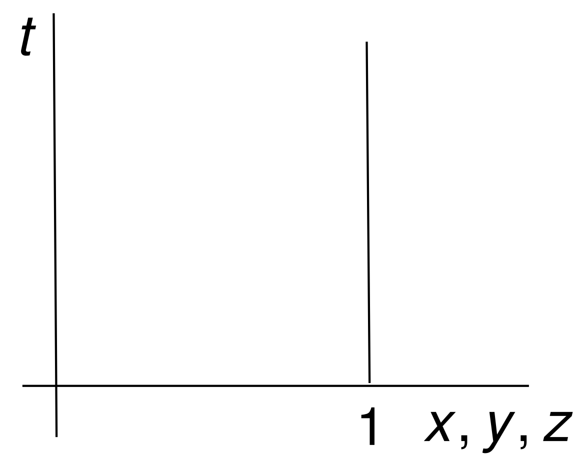
$$\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} + \frac{\partial^2 u}{\partial z^2} + f(q)$$

Boundary Conditions

Initial Conditions

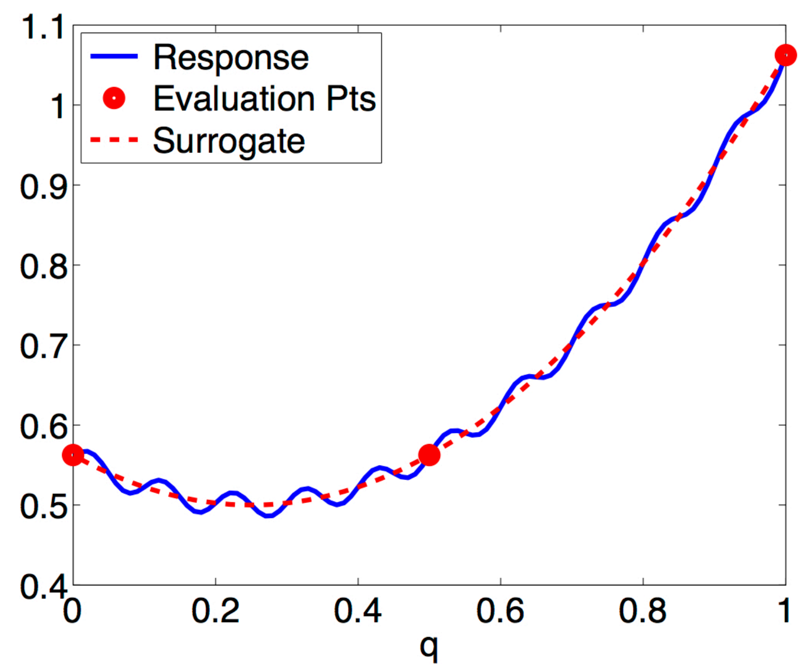
with the response

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



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

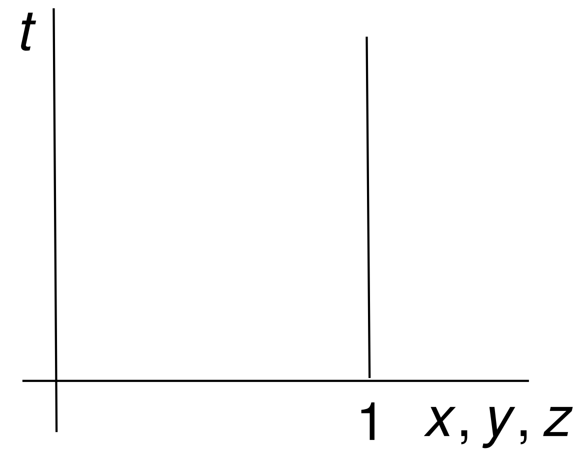
$$\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} + \frac{\partial^2 u}{\partial z^2} + f(q)$$

Boundary Conditions

Initial Conditions

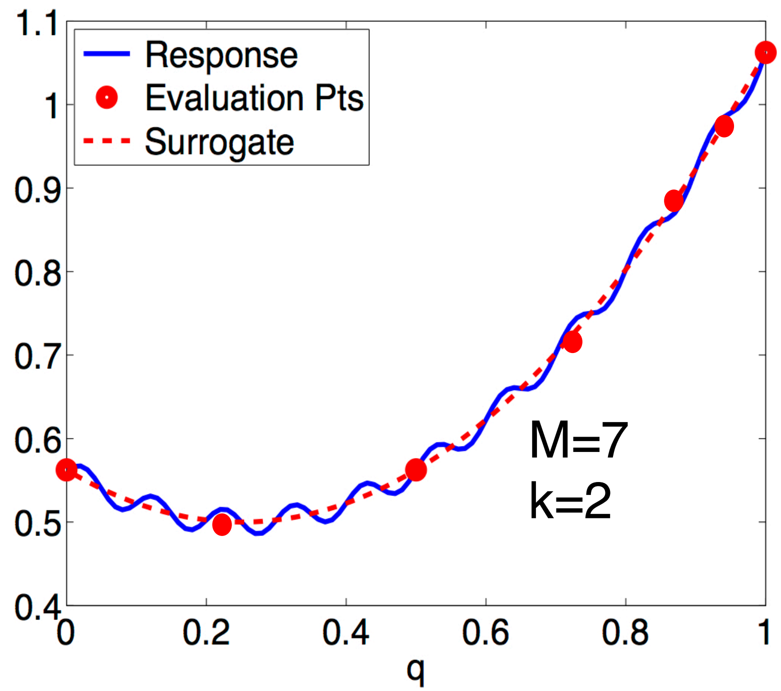
with the response

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



Surrogate: Quadratic

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



Question: How do you construct a polynomial surrogate?

- Interpolation
- Regression

Surrogate Models

Question: How do we keep from fitting noise?

- Akaike Information Criterion (AIC)

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

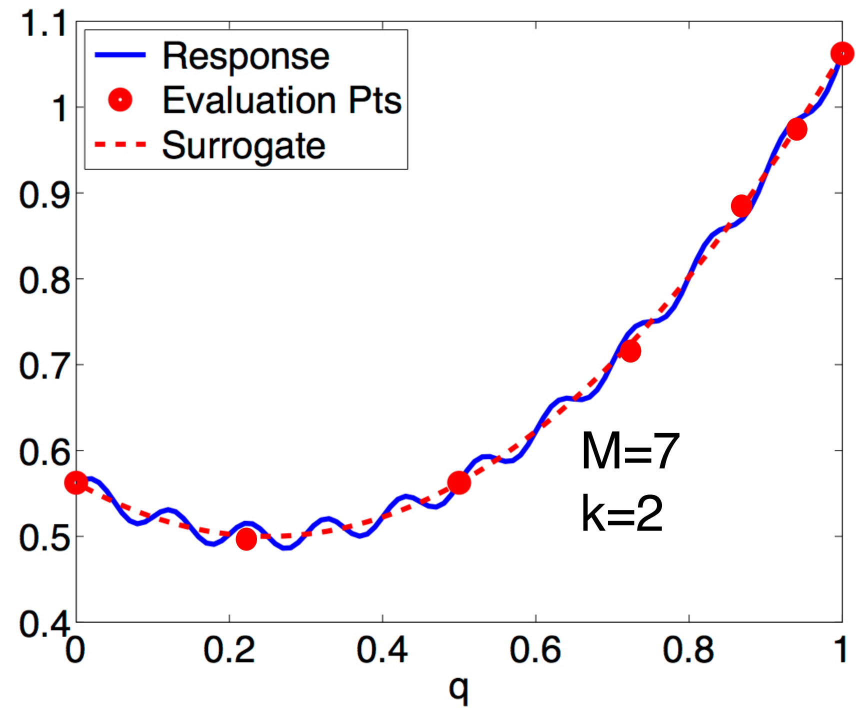
- Bayesian Information Criterion (AIC)

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

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



Surrogate Models

Question: How do we keep from fitting noise?

- Akaike Information Criterion (AIC)

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

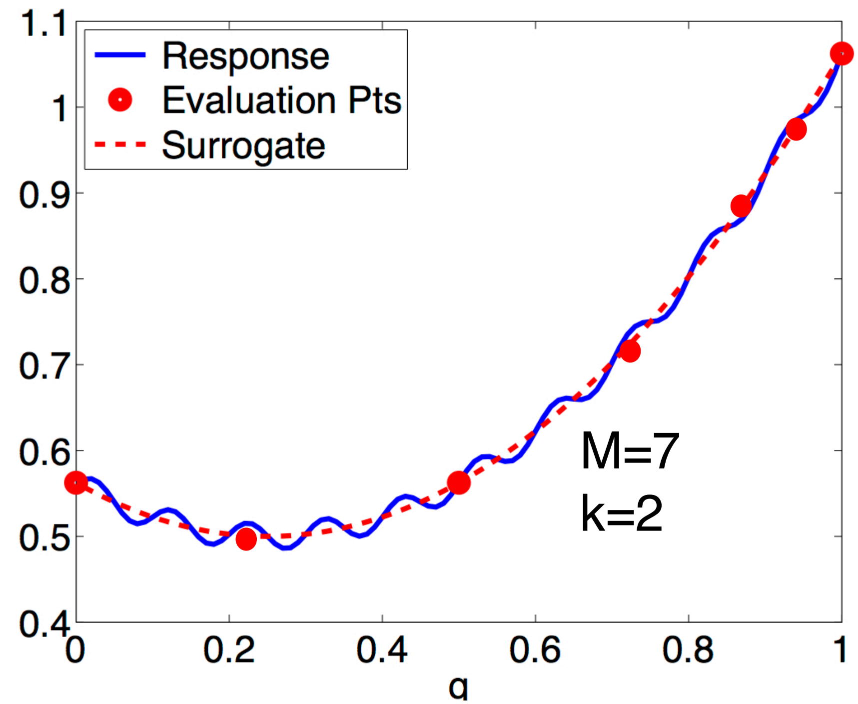
- Bayesian Information Criterion (AIC)

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

Likelihood:

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

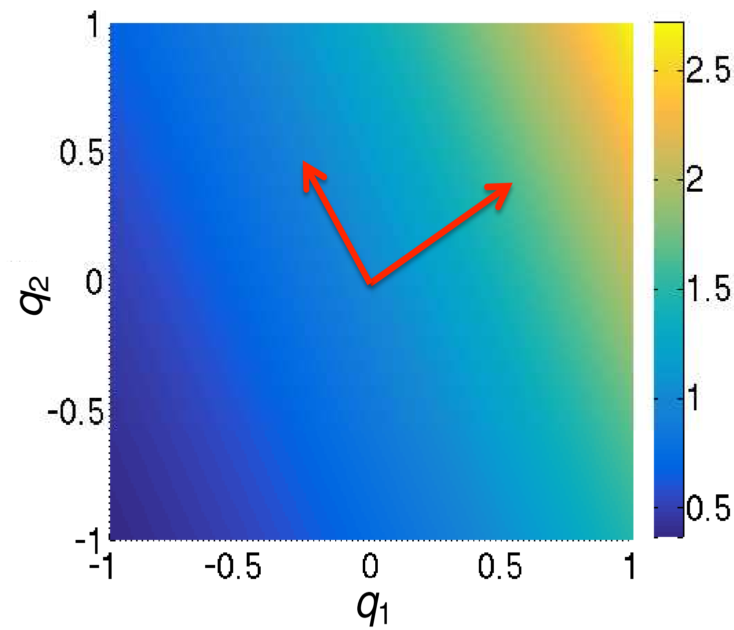
$$SS_q = \sum_{m=1}^{M} [y_m - y_s(q^m)]^2$$ Minimize



Example: $y = \exp(0.7q_1 + 0.3q_2)$

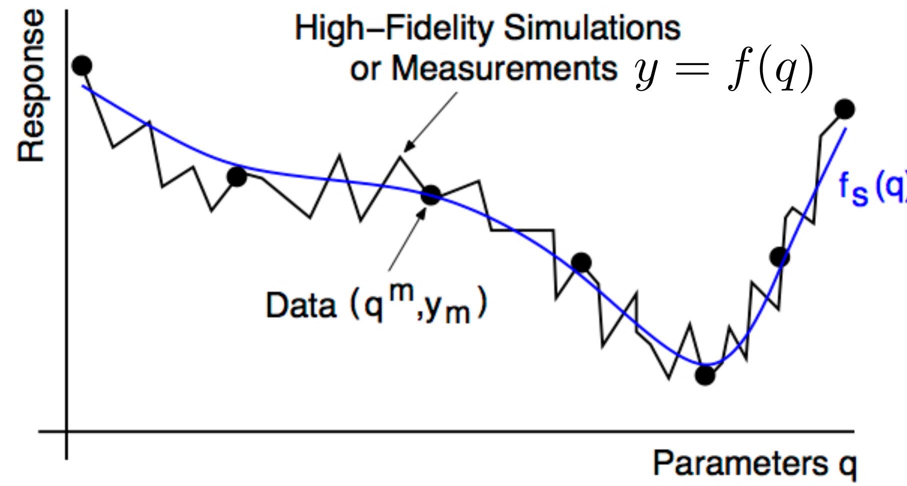
Exercise:

- Construct a polynomial surrogate using the code response_surface.m.
- What order seems appropriate?



Data-Fit Models

Notes:



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

• Constructed via interpolation or regression.

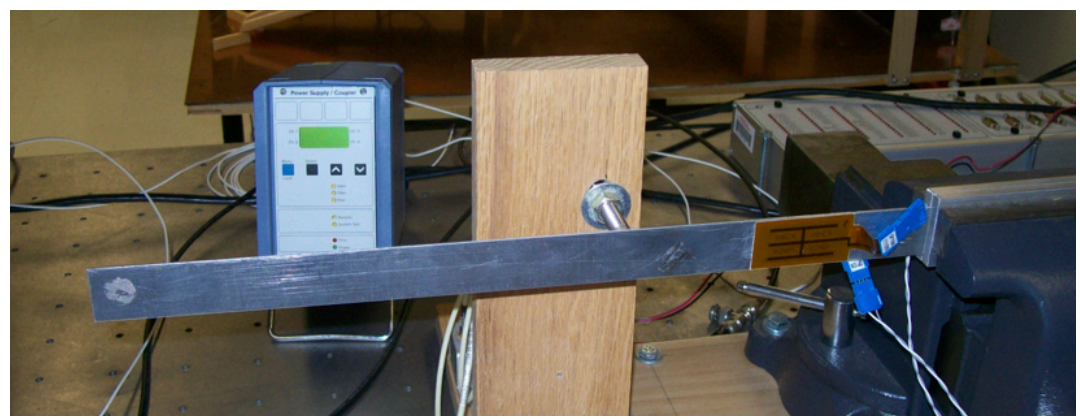
• Data can consist of high-fidelity simulations or experiments.

Example: Steady-state Euler-Bernouilli beam model with PZT patch

$$\underline{YI}\frac{d^4 w}{dx^4}(x) = k_p V \chi_{pzt}(x)$$

Data: Displacement observations

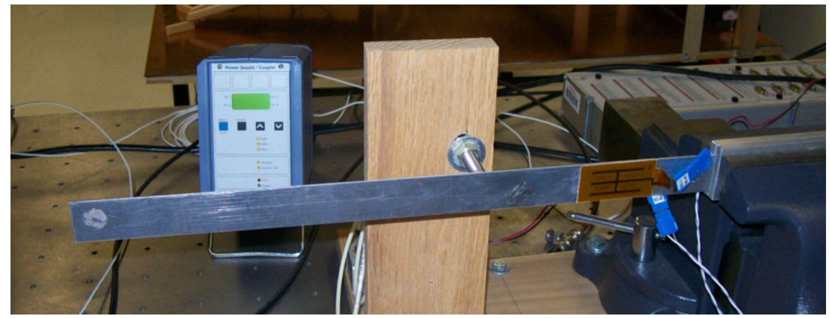
Parameter: YI



Data-Fit Models

Example: Steady-state Euler-Bernouilli beam model with PZT patch

$$\underline{YI}\frac{d^4 w}{dx^4}(x) = k_p V \chi_{pzt}(x)$$

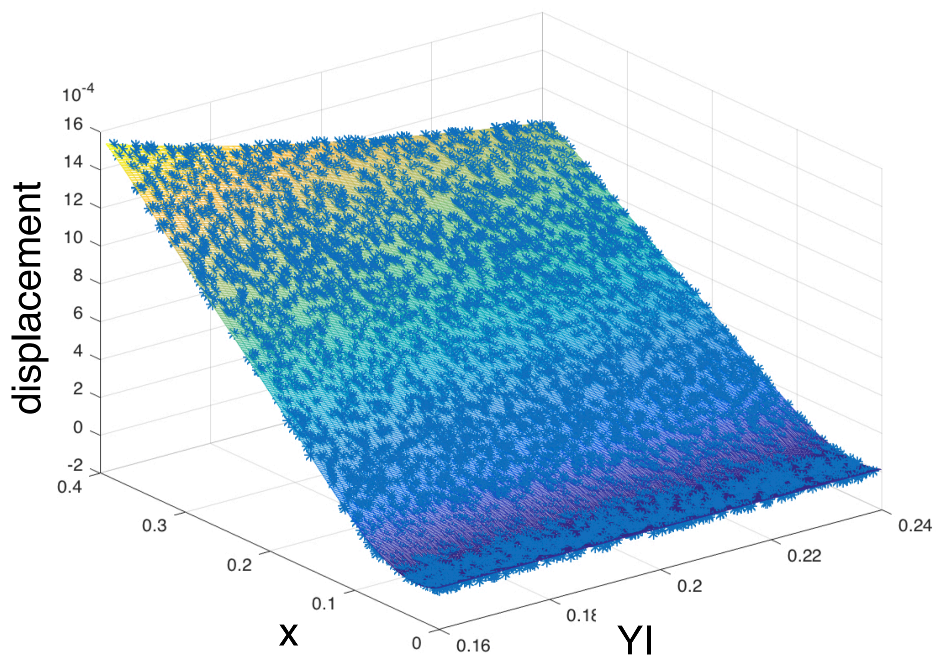


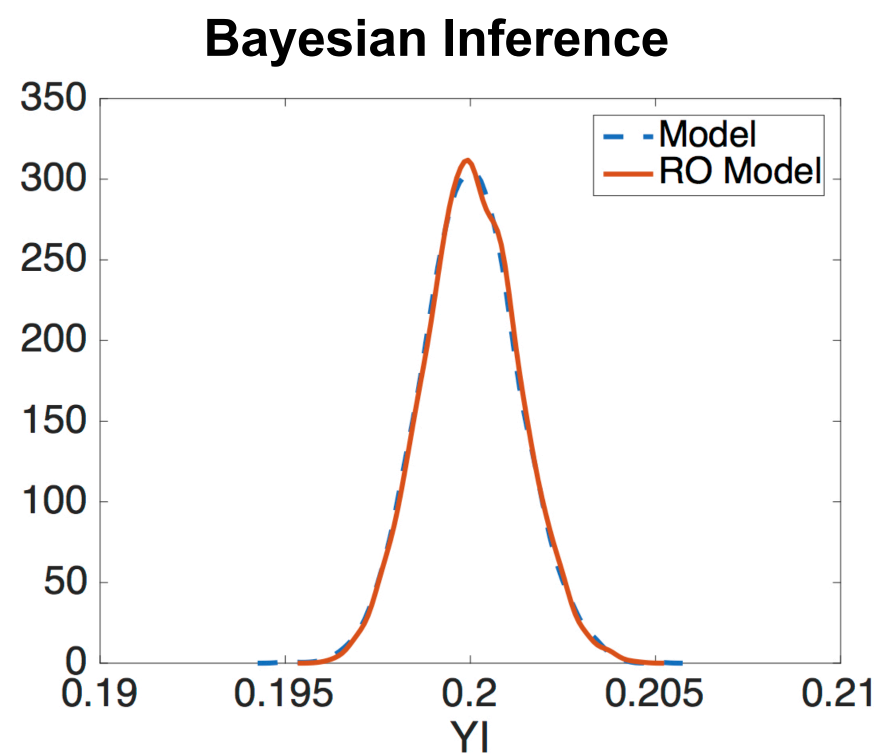
Data: Displacement observations

Parameter: YI

Training points: 5000

Polynomial surrogate: 6th order





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

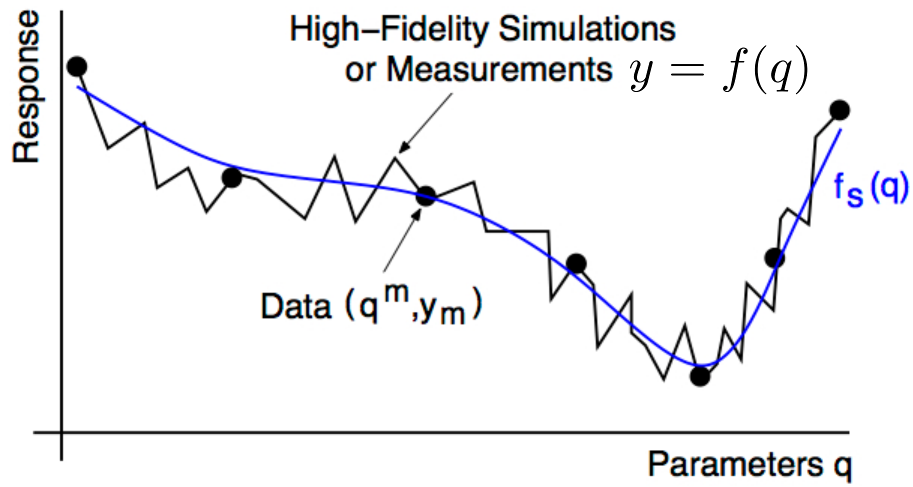
$$y = f(q)$$

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:

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

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

Orthogonal Polynomial Representations

Representation:

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

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

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

$$\mathbb{E}[\Psi_i(Q)\Psi_j(Q)] = \int_\Gamma \Psi_i(q)\Psi_j(q)\rho(q)dq$$

$$= \delta_{ij}\gamma_i$$

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

Properties:

(i) $\mathbb{E}[y^K(Q)] = \alpha_0$

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

Note: Can be used for:

- Uncertainty propagation
- Sobol-based global sensitivity analysis

Issue: How does one compute α_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 $y(q) = \sum_{k=0}^{\infty} \alpha_k \Psi_k(q)$ to obtain

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

Quadrature:

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

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

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

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

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

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

e.g., SPGL1

- MATLAB Solver for large-scale sparse reconstruction

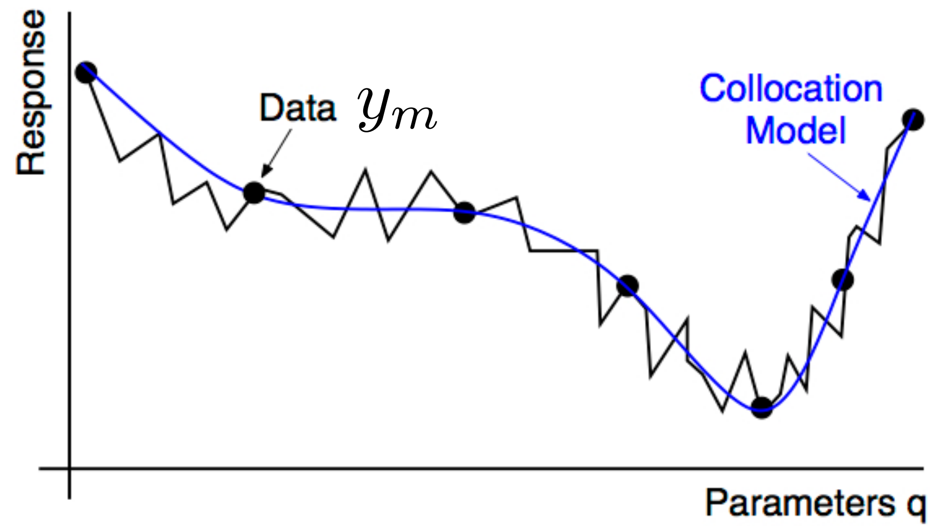
Stochastic Collocation

Strategy: Consider high fidelity model

$$y = f(q)$$

with M model evaluations

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



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: $Y^M(q^m) = y_m$

Orthogonal Polynomial Methods for PDE

Evolution Model: e.g., thermal-hydraulic equations

$$\frac{\partial u}{\partial t} = \mathcal{N}(u, Q) + F(Q) \quad , \; x \in \mathcal{D}, \; t \in [0, \infty)$$

$$B(u, Q) = G(Q) \quad , \; x \in \partial\mathcal{D}, \; t \in [0, \infty)$$

$$u(0, x, Q) = I(Q) \quad , \; x \in \mathcal{D}$$

Weak Formulation: For all $v \in V$

$$\int_{\mathcal{D}} \frac{\partial u}{\partial t} v dx + \int_{\mathcal{D}} N(u, Q) S(v) dx = \int_{\mathcal{D}} F(Q) v dx$$

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

Example: $q = \alpha$

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

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

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

For all $v \in H_0^1(0, L)$

$$\int_0^L \frac{\partial u}{\partial t} v dx + \alpha \int_0^L \frac{\partial u}{\partial x} \frac{dv}{dx} = 0$$

Representation:

$$\begin{aligned} u^K(t, x, Q) &= \sum_{k=0}^{K} u_k(t, x) \Psi_k(Q) \\ &= \sum_{k=0}^{K} \sum_{j=1}^{J} u_{jk}(t) \phi_j(x) \Psi_k(Q) \end{aligned}$$

e.g., Finite elements

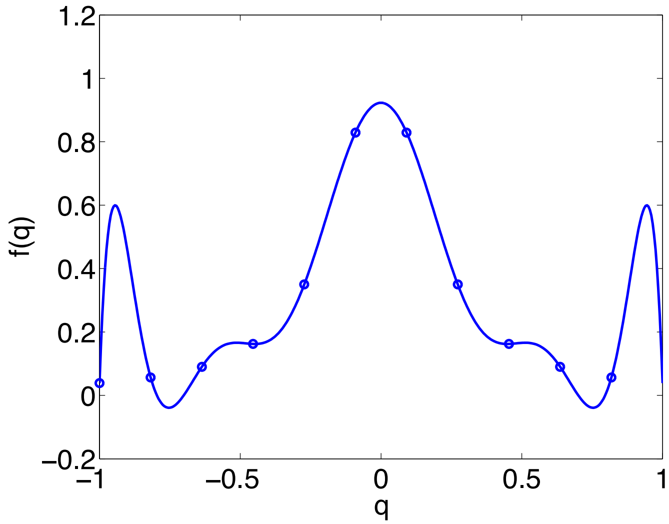
Discrete Projection:

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

Surrogate Models – Grid Choice

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

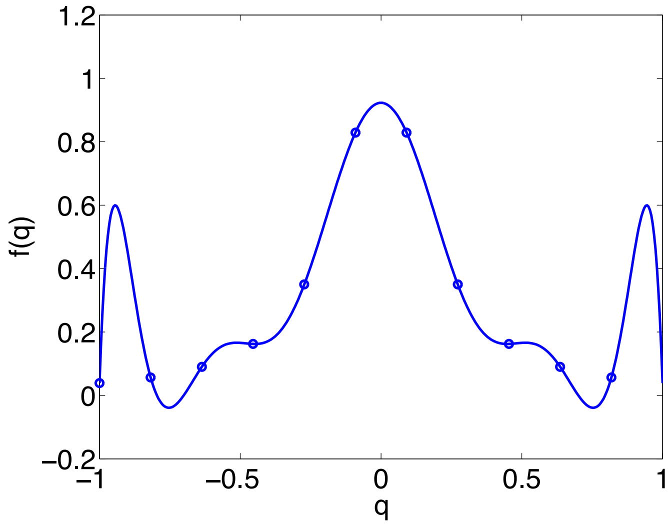
$$q^j = -1 + (j-1)\frac{2}{M} \ , \ j = 1, \ldots, M$$

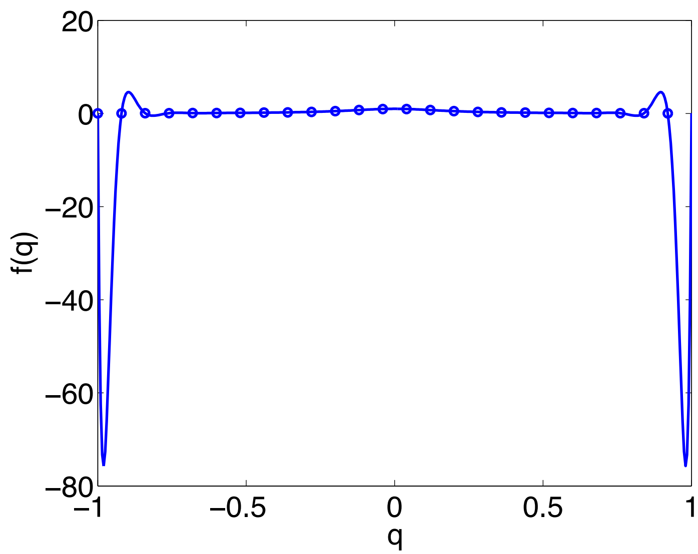


Surrogate Models – Grid Choice

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

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

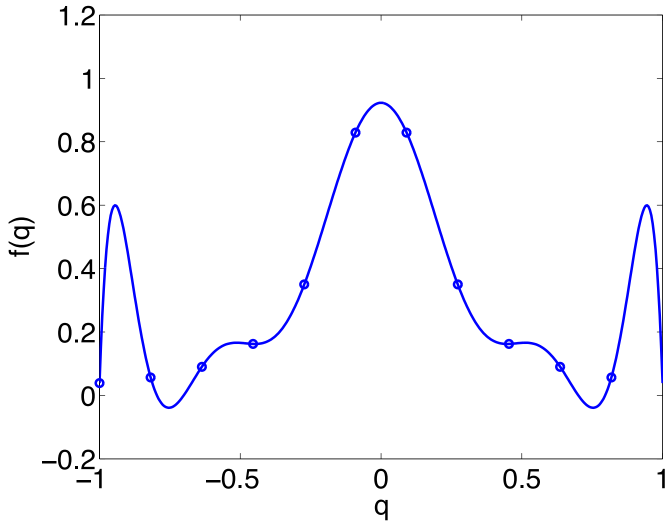


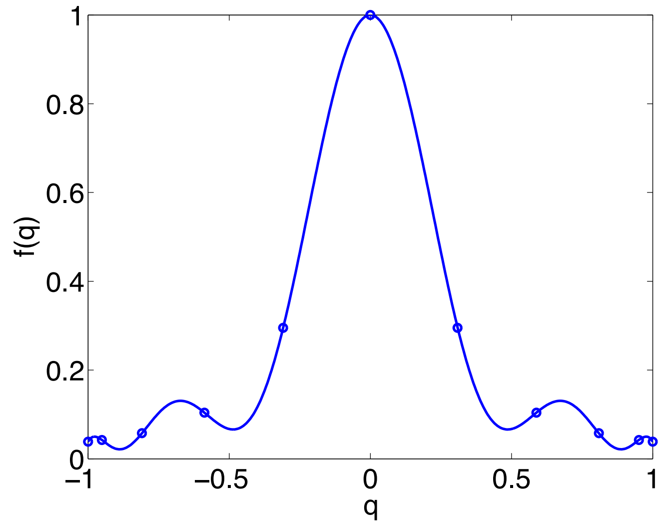


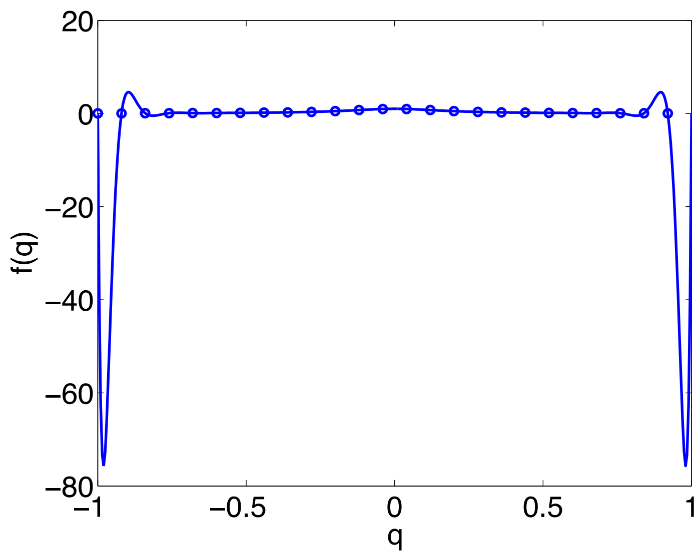
Surrogate Models – Grid Choice

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

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



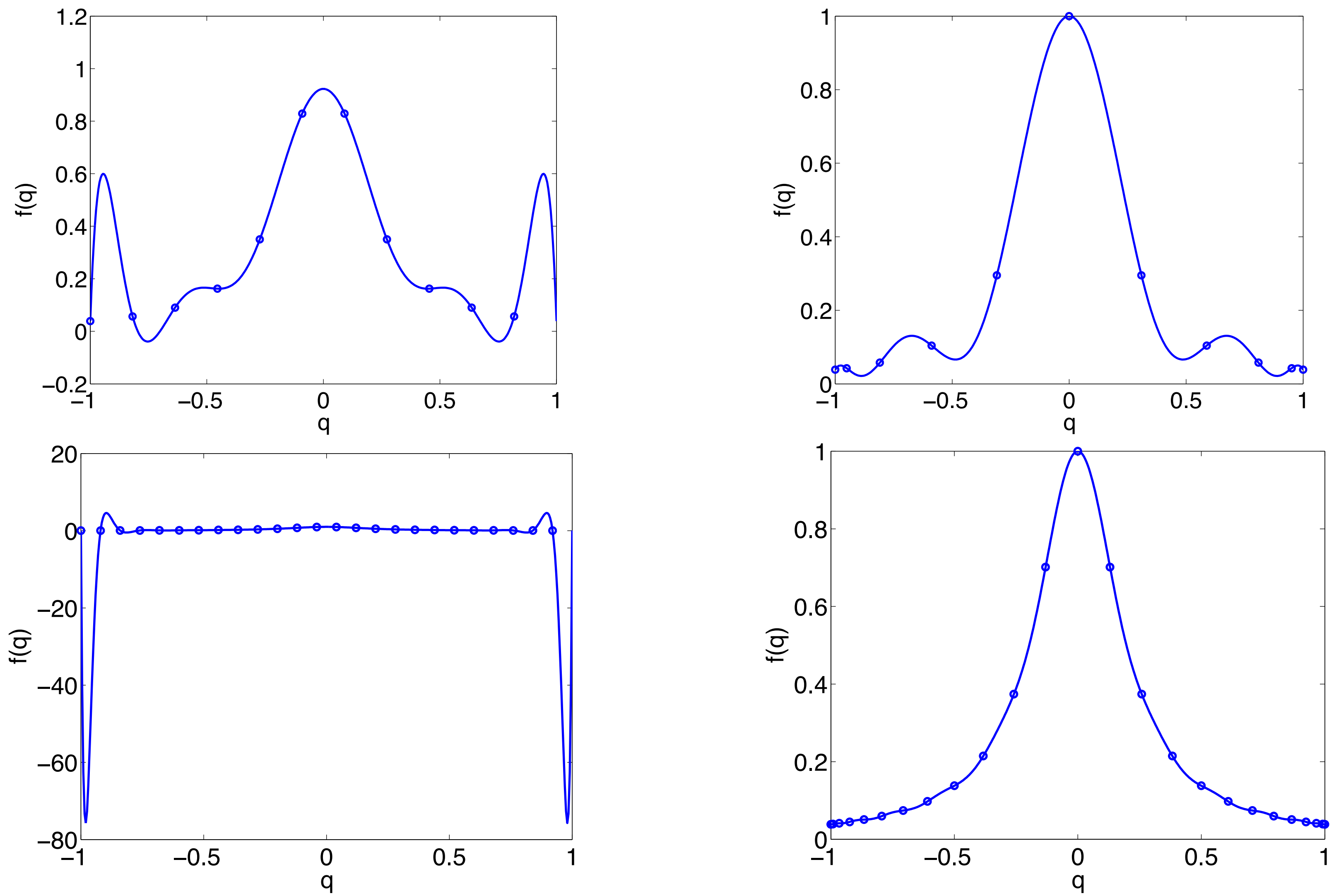




Surrogate Models – Grid Choice

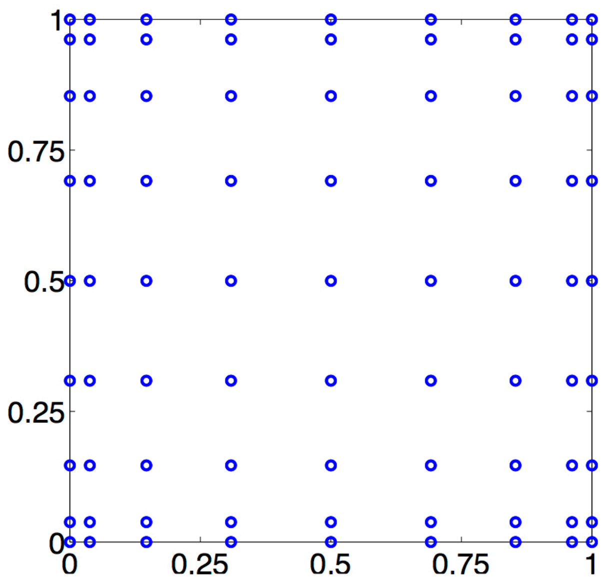
Example: Consider the Runge function $f(q) = \frac{1}{1+25q^2}$ with points

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

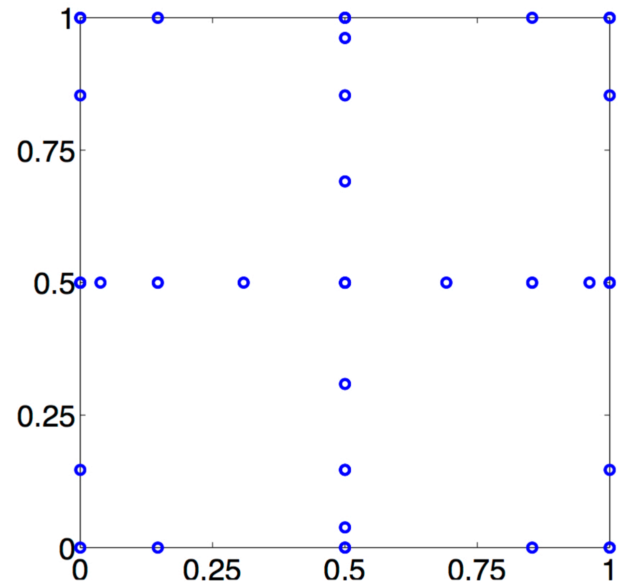


Sparse Grid Techniques

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	$> 2 \times 10^{95}$

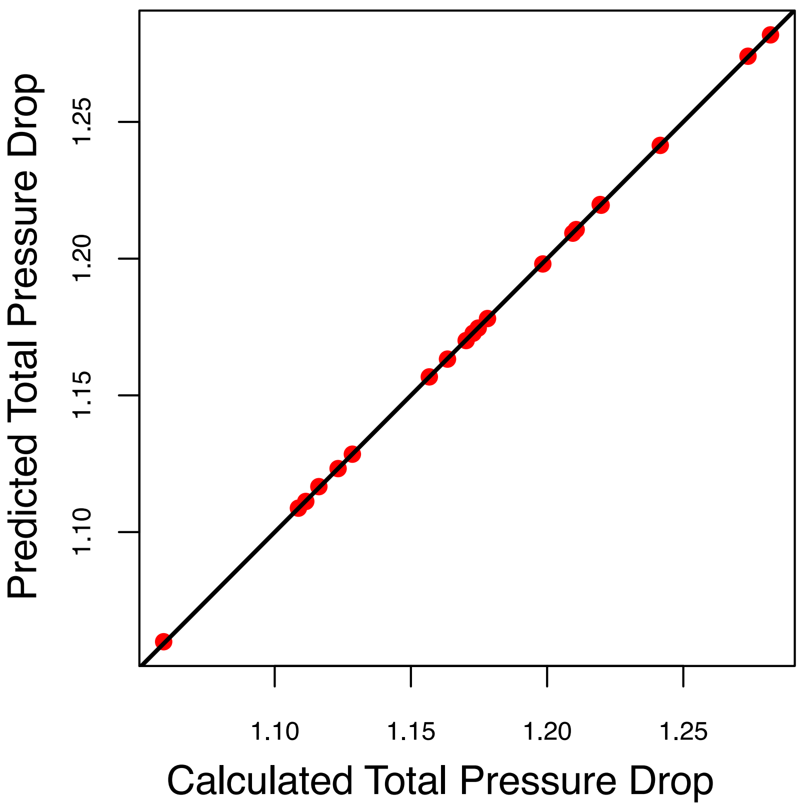
Surrogate Construction: Nuclear Power Plant Design

Subchannel Code (COBRA-TF): 33 VUQ parameters reduced to 5 using SA

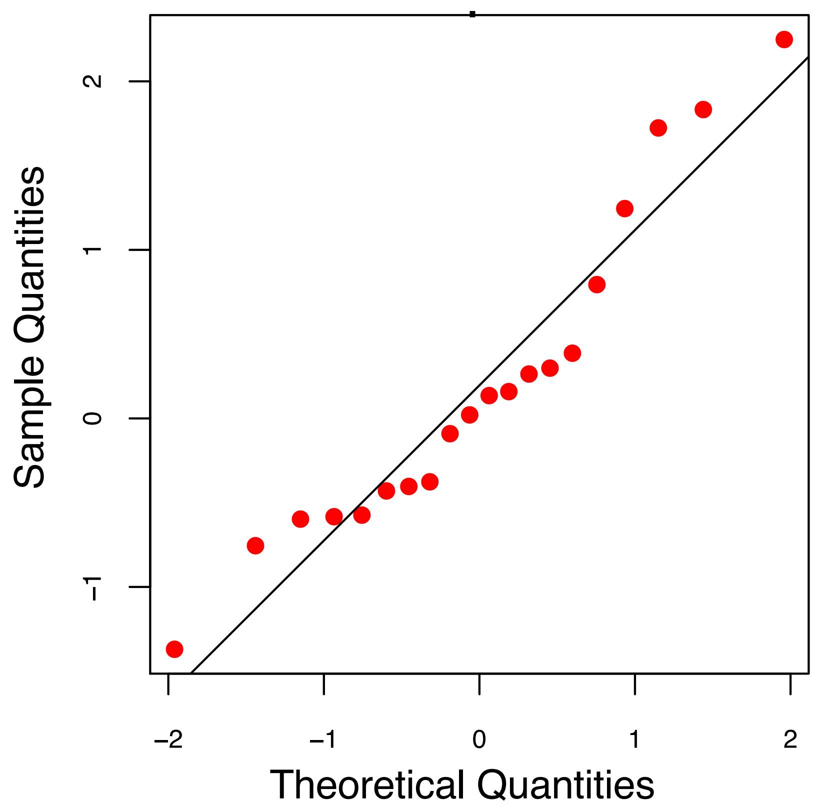
Surrogate: Total pressure drop

• Kriging (GP) emulator constructed using 50 COBRA-TF runs perturbing 5 active inputs.

• Use remaining computational budget to evaluate quality of surrogate using post-processed Dakota outputs.



Out-of-Sample Validation



Example: SIR Cholera Model

Model:

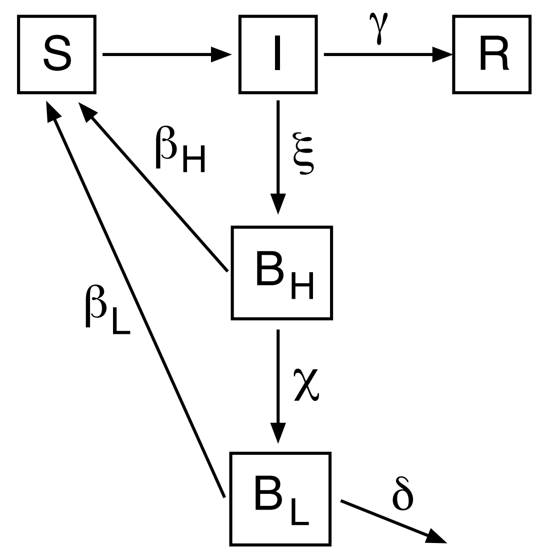
$$\frac{dS}{dt} = bN - \beta_L S \frac{B_L}{\kappa_L + B_L} - \beta_H S \frac{B_H}{\kappa_H + B_H} - bS$$

$$\frac{dI}{dt} = \beta_L S \frac{B_L}{\kappa_L + B_L} + \beta_H S \frac{B_H}{\kappa_H + B_H} - (\gamma + b) I$$

$$\frac{dR}{dt} = \gamma I - bR$$

$$\frac{dB_H}{dt} = \xi I - \chi B_H$$

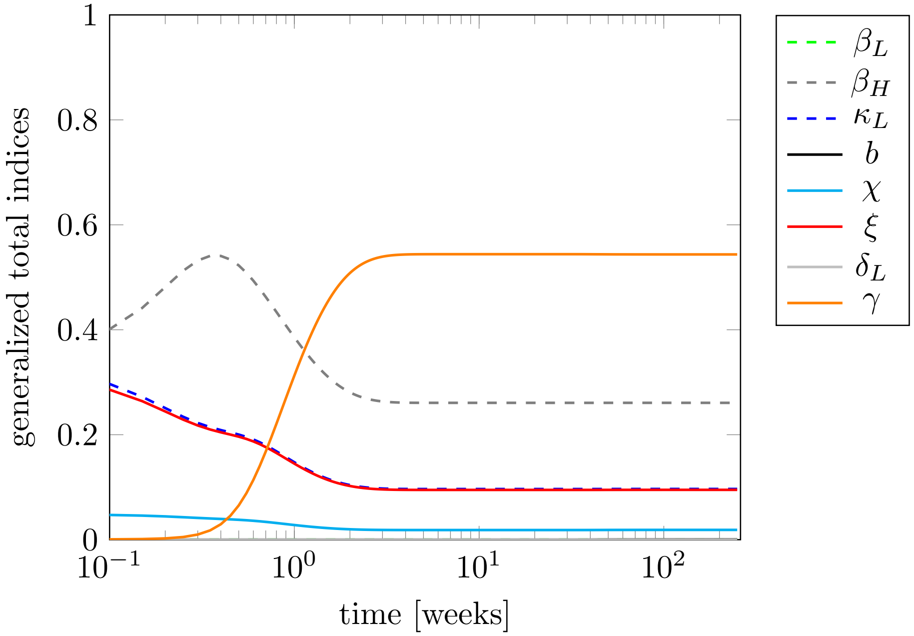
$$\frac{dB_L}{dt} = \chi B_H - \delta B_L$$



Model Parameter	Symbol	Units	Values
Rate of drinking B_L cholera	β_L	$\frac{1}{\text{week}}$	1.5
Rate of drinking B_H cholera	β_H	$\frac{1}{\text{week}}$	7.5 ($*$)
B_L cholera carrying capacity	κ_L	$\frac{\#\ \text{bacteria}}{m\ell}$	10^6
B_H cholera carrying capacity	κ_H	$\frac{\#\ \text{bacteria}}{m\ell}$	$\frac{\kappa_L}{700}$
Human birth and death rate	b	$\frac{1}{\text{week}}$	$\frac{1}{1560}$
Rate of decay from B_H to B_L	χ	$\frac{1}{\text{week}}$	$\frac{168}{5}$
Rate at which infectious individuals spread B_H bacteria to water	ξ	$\frac{\#\ \text{bacteria}}{\#\ \text{individuals}\cdot m\ell\cdot\text{week}}$	70
Death rate of B_L cholera	δ	$\frac{1}{\text{week}}$	$\frac{7}{30}$
Rate of recovery from cholera	γ	$\frac{1}{\text{week}}$	$\frac{7}{5}$

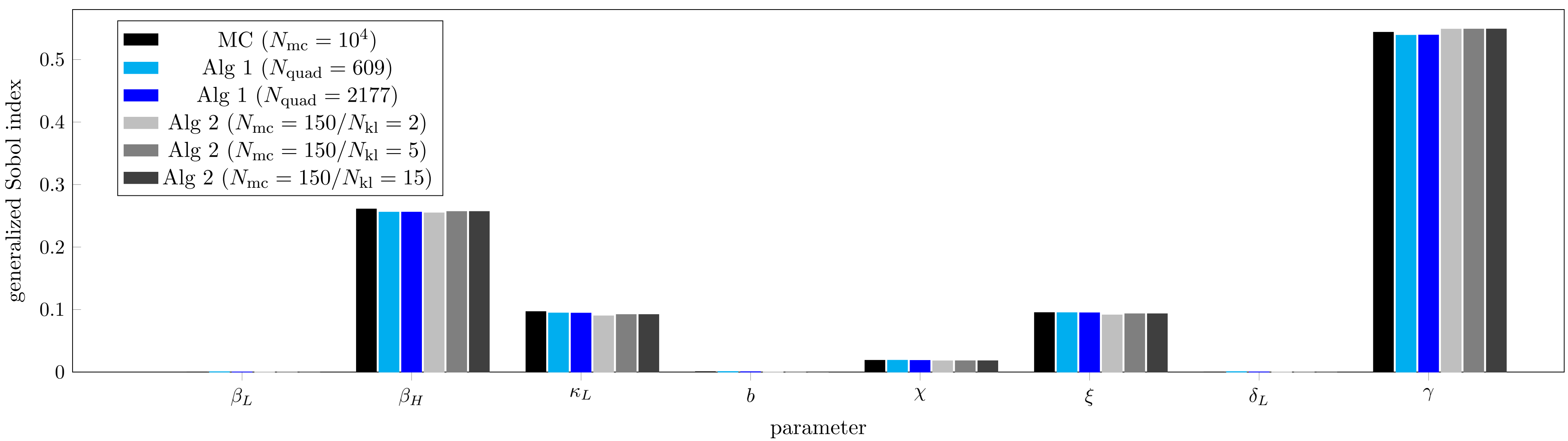
Example: SIR Cholera Model

Strategy: Employed collocation and discrete projection with sparse grids to compute time-dependent global sensitivity indices.



Conclusion: Sensitive indices

- γ: Recovery rate
- β_H: Rate of drinking B_H cholera
- κ_L: B_L carrying capacity; Note $\kappa_H = \kappa_L/700$
- ξ: Rate at which B_H bacteria spread



Example: SIR Cholera Model

Model:

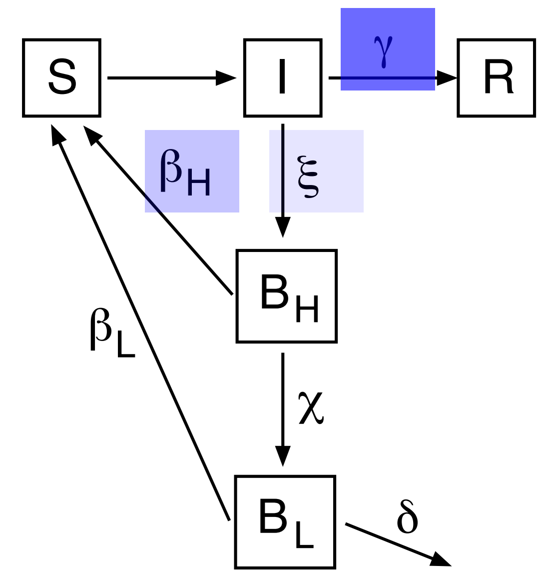
$$\frac{dS}{dt} = bN - \beta_L S \frac{B_L}{\kappa_L + B_L} - \beta_H S \frac{B_H}{\kappa_H + B_H} - bS$$

$$\frac{dI}{dt} = \beta_L S \frac{B_L}{\kappa_L + B_L} + \beta_H S \frac{B_H}{\kappa_H + B_H} - (\gamma + b)I$$

$$\frac{dR}{dt} = \gamma I - bR$$

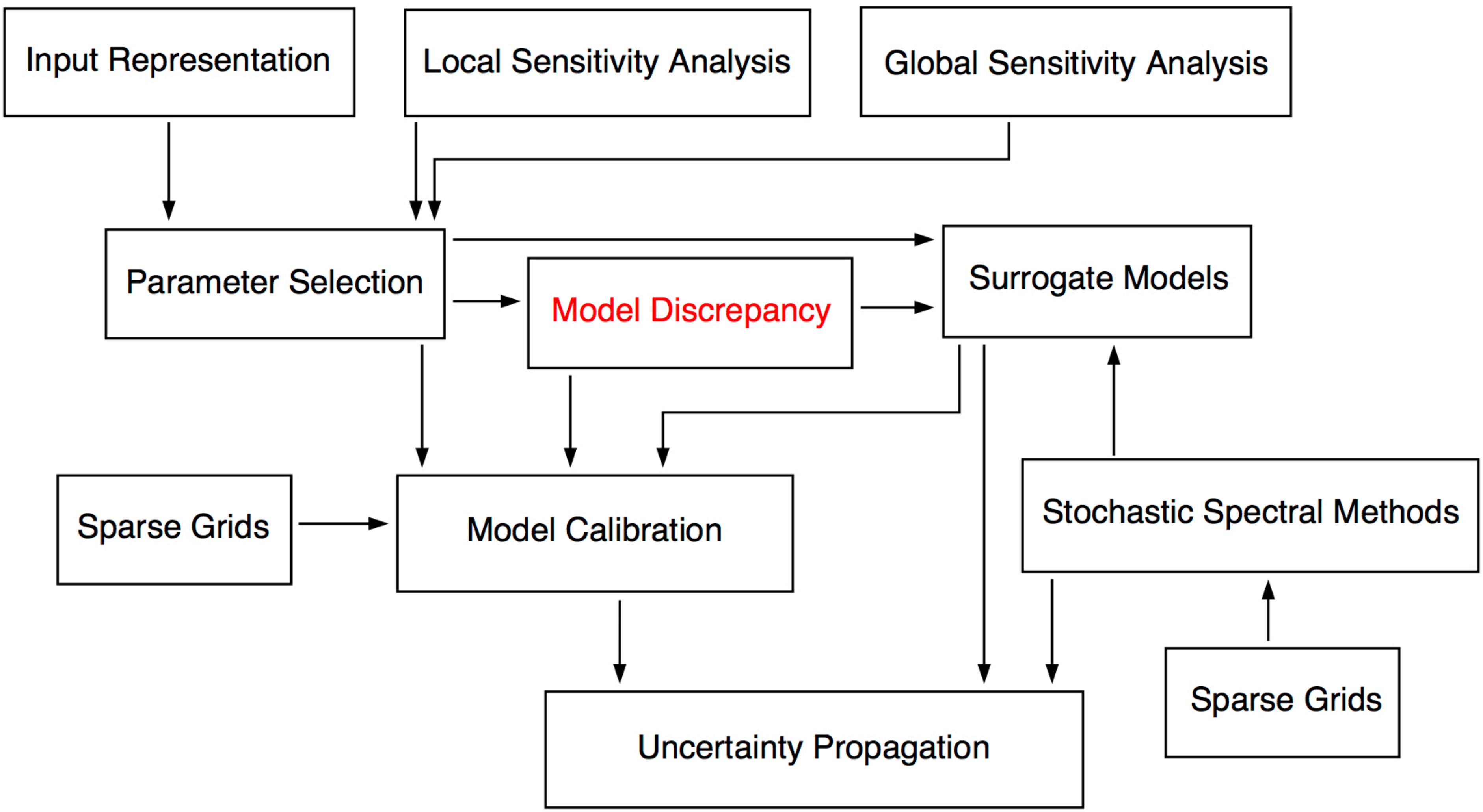
$$\frac{dB_H}{dt} = \xi I - \chi B_H$$

$$\frac{dB_L}{dt} = \chi B_H - \delta B_L$$



Model Parameter	Symbol	Units	Values
Rate of drinking B_L cholera	β_L	$\frac{1}{\text{week}}$	1.5
Rate of drinking B_H cholera	β_H	$\frac{1}{\text{week}}$	7.5 $(*)$
B_L cholera carrying capacity	κ_L	$\frac{\#\ \text{bacteria}}{m\ell}$	10^6
B_H cholera carrying capacity	κ_H	$\frac{\#\ \text{bacteria}}{m\ell}$	$\frac{\kappa_L}{700}$
Human birth and death rate	b	$\frac{1}{\text{week}}$	$\frac{1}{1560}$
Rate of decay from B_H to B_L	χ	$\frac{1}{\text{week}}$	$\frac{168}{5}$
Rate at which infectious individuals spread B_H bacteria to water	ξ	$\frac{\#\ \text{bacteria}}{\#\ \text{individuals}\cdot m\ell\cdot\text{week}}$	70
Death rate of B_L cholera	δ	$\frac{1}{\text{week}}$	$\frac{7}{30}$
Rate of recovery from cholera	γ	$\frac{1}{\text{week}}$	$\frac{7}{5}$

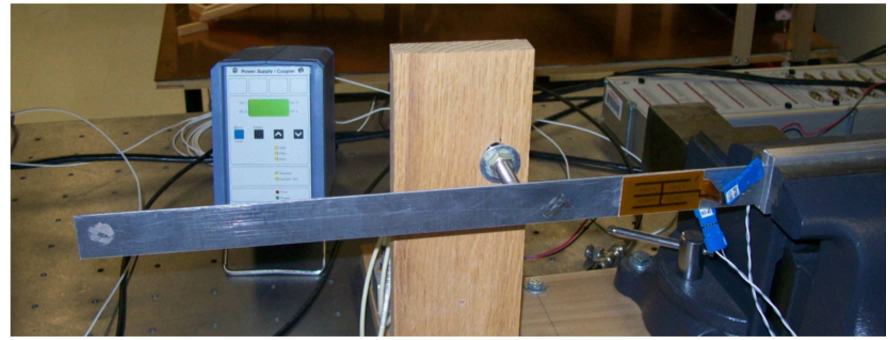
Steps in Uncertainty Quantification



6. Quantification of Model Discrepancy – Thin Beam

"Essentially all models are wrong, but some are useful" George E.P. Box

Example: Thin beam driven by PZT patches



Euler-Bernoulli Model: For all $\phi \in V$

$$\int_0^L \left[\rho(x)\frac{\partial^2 w}{\partial t^2} + \gamma\frac{\partial w}{dt}\right]\phi dx + \int_0^L \left[YI(x)\frac{\partial^2 w}{\partial x^2} + cI(x)\frac{\partial^3 w}{\partial x^2 \partial t}\right]\phi'' dx$$

$$= k_p V(t)\int_{x_1}^{x_2}\phi'' dx$$

with

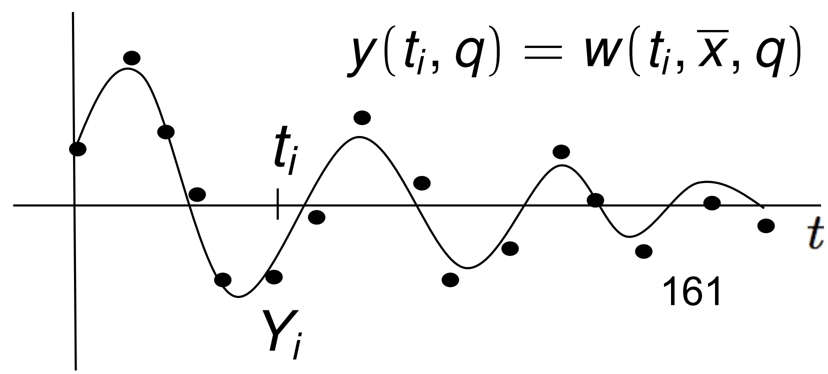
$$\rho(x) = \rho hb + \rho_p h_p b_p \chi_p(x)\ , \ \ YI(x) = YI + Y_p I_p \chi_p(x)$$

$$cI(x) = cI + c_p I_p \chi_p(x)$$

Note: 7 parameters, 32 states

Statistical Model:

$$Y_i = y(t_i, q) + \varepsilon_i$$

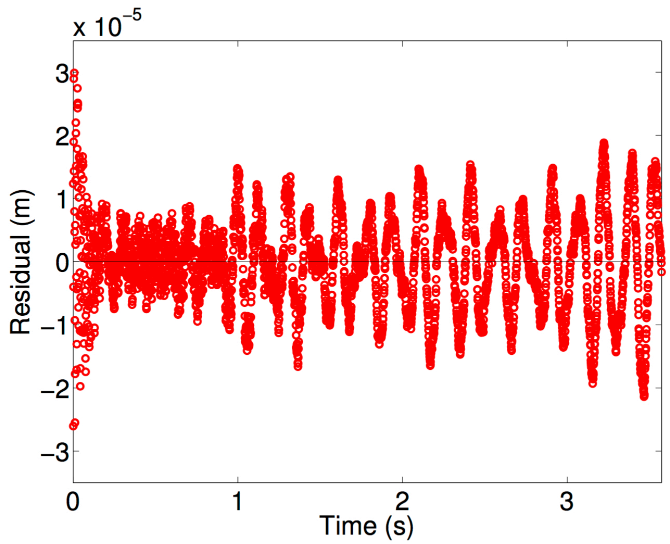


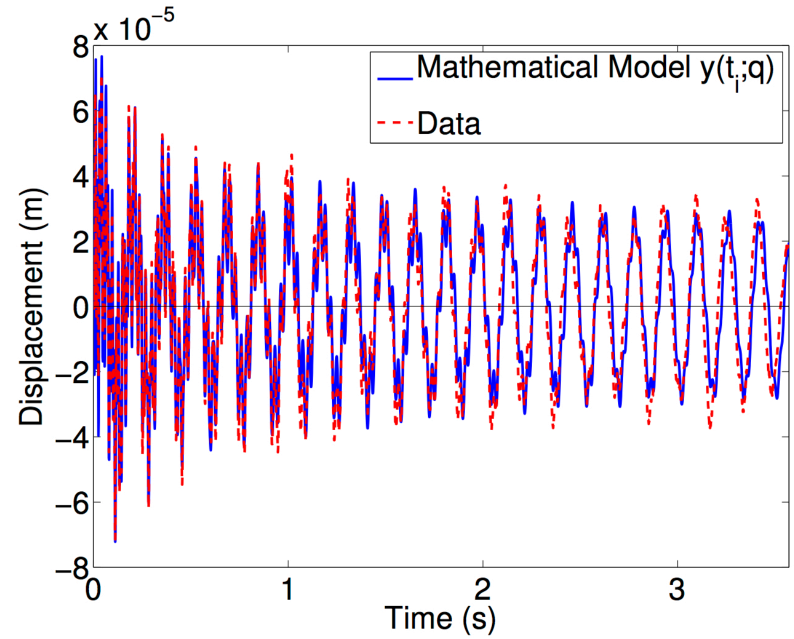
Quantification of Model Discrepancy – Thin Beam

Example: Good model fit

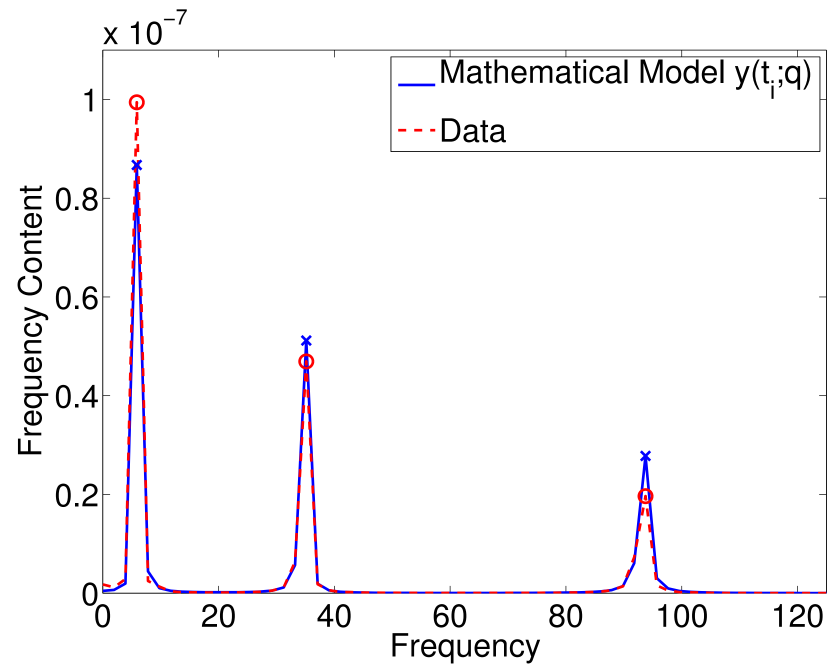
$$Y_i = y(t_i, q) + \varepsilon_i$$

Note: Observation errors not iid





Model Fit to Data



Reference: Additive observation errors

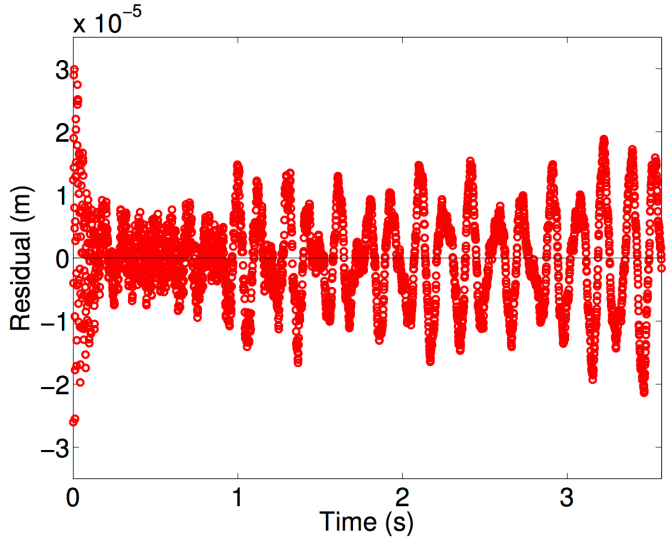
$$Y_i = y(t_i, q) + \delta(t_i, \widetilde{q}) + \varepsilon_i$$

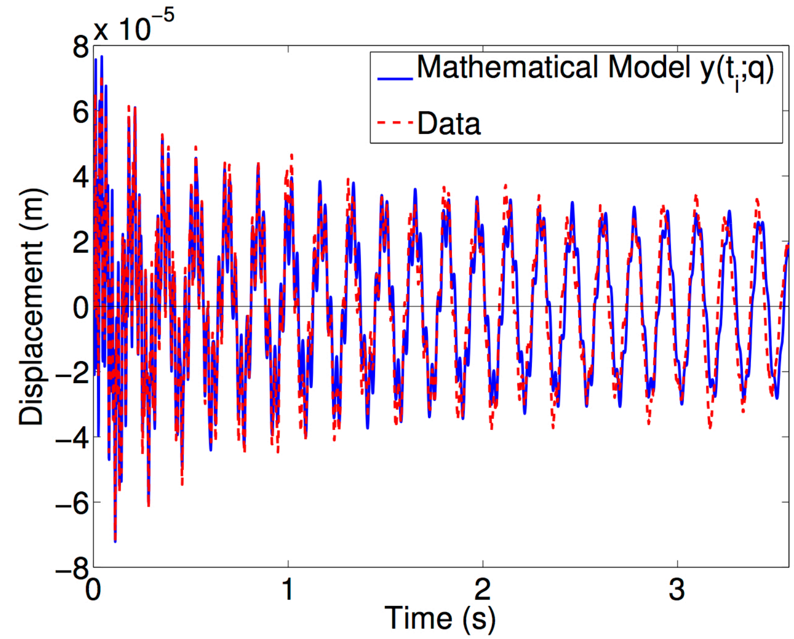
- M.C. Kennedy and A. O'Hagan, *Journal of the Royal Statistical Society, Series B*, 2001.

Quantification of Model Discrepancy – Thin Beam

Example: Good model fit

Problem: Observation errors not iid





Model Fit to Data

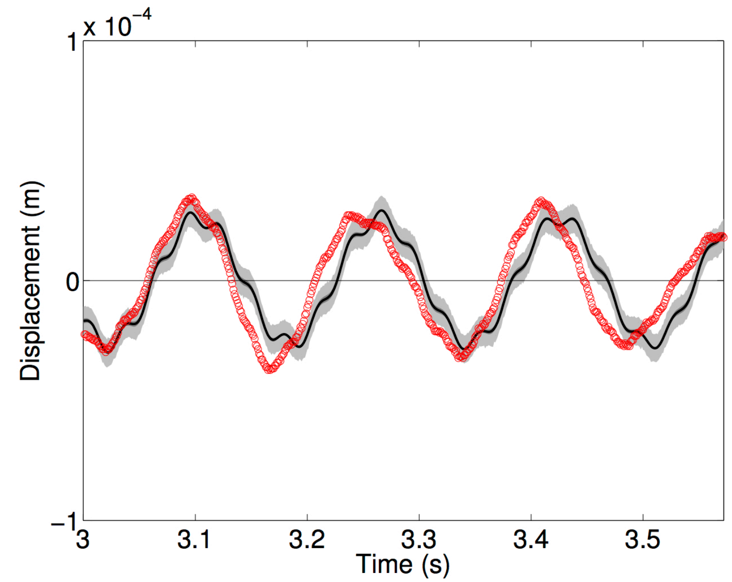
Result: Prediction intervals wrong

Approaches:

• GP Model: Inaccurate for extrapolation

• Control-based approaches: difficult to extrapolate.

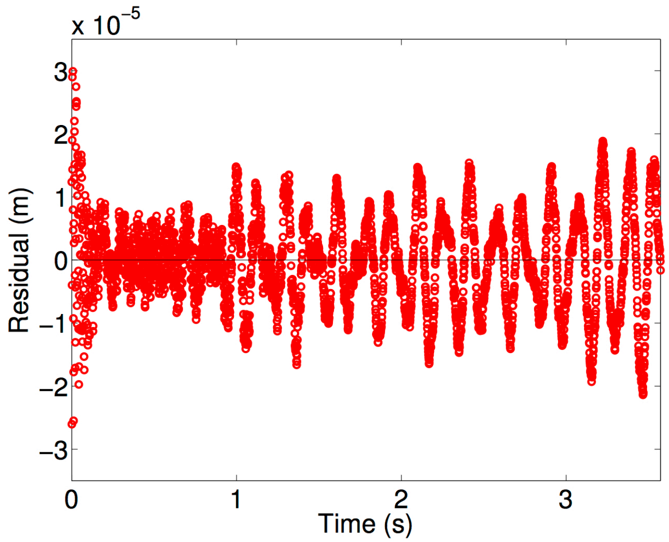
• Problem: correct physics or biology required for extrapolation!

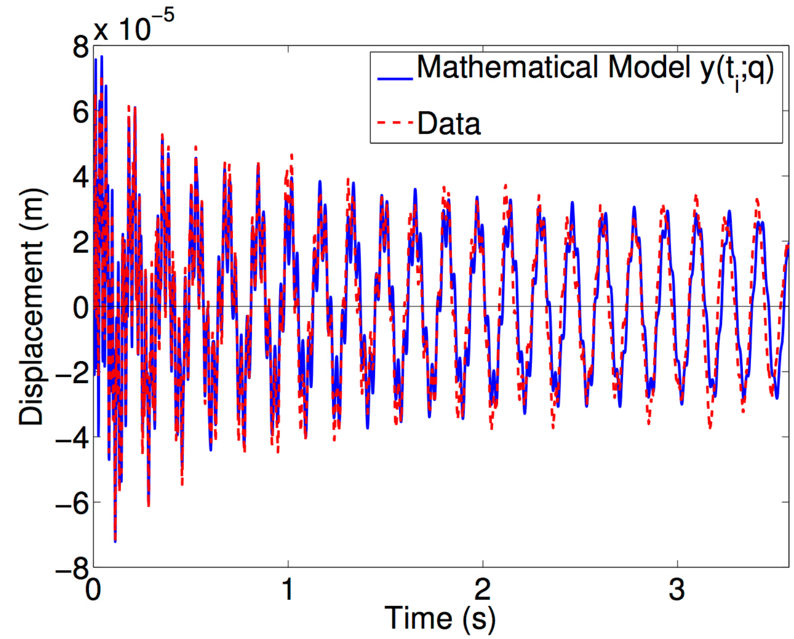


Prediction Intervals and Data

Quantification of Model Discrepancy – Thin Beam

Problem: Measurement errors not iid



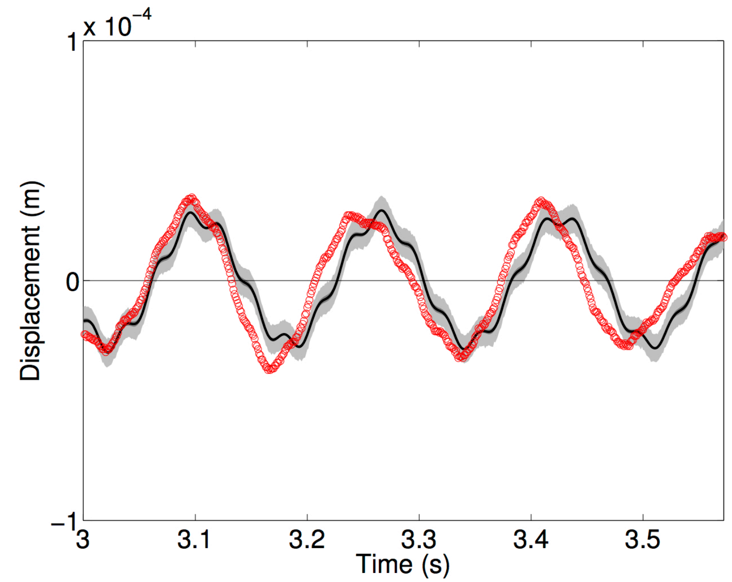


Model Fit to Data

Result: Prediction intervals wrong

One Approach:

- Determine components of model you trust (e.g., conservation laws) and don't trust (e.g., closure relations). Embed uncertainty into latter.
- T. Oliver, G. Terejanu, C.S. Simmons, R.D. Moser, *Comput Meth Appl Mech Eng*, 2015.



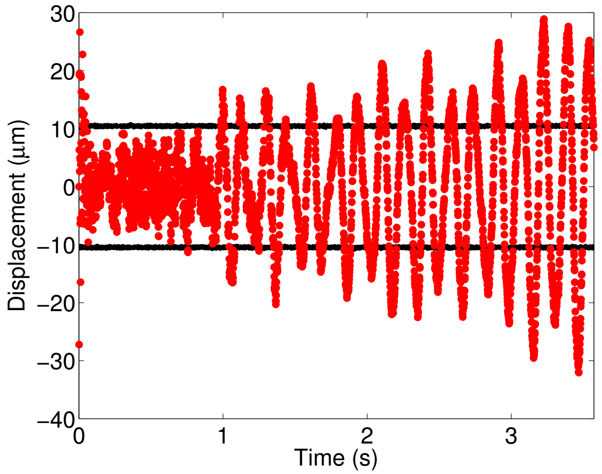
Prediction Intervals and Data

2018-19 SAMSI Program: Model Uncertainty: Mathematical and Statistical (MUMS)

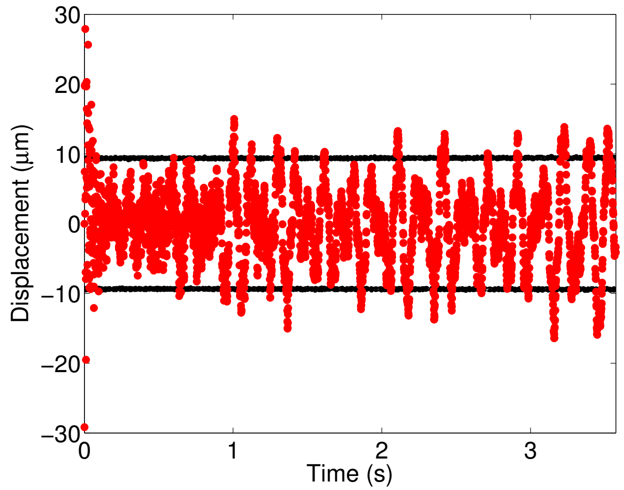
Quantification of Model Discrepancy – Thin Beam

Our Solution: “Optimize” calibration interval

- Use damping/frequency domain results to guide.

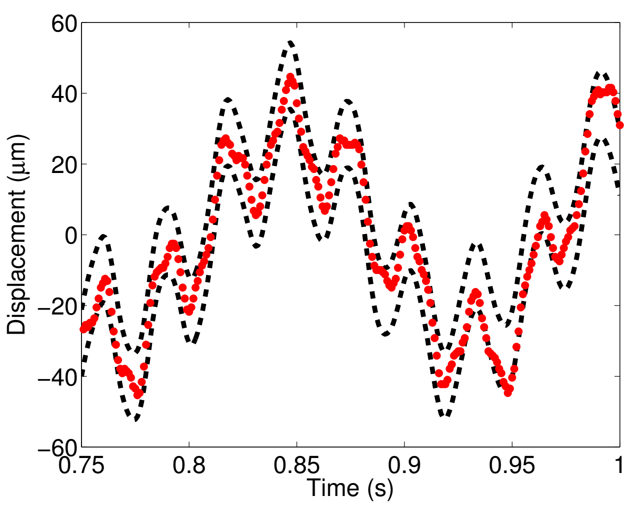


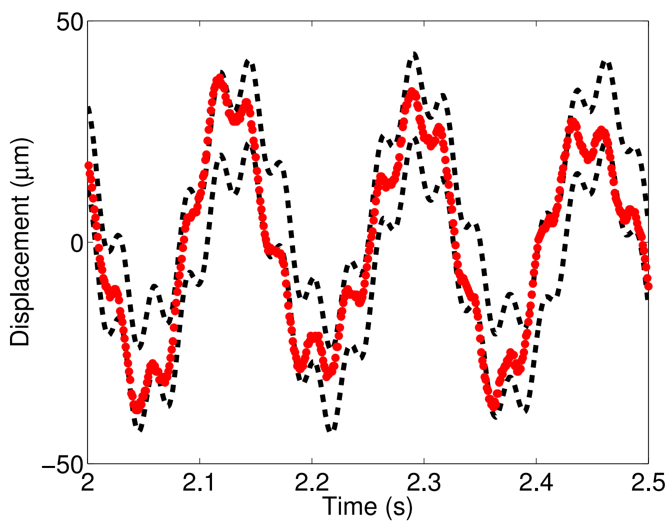
Calibrate on [0,1]

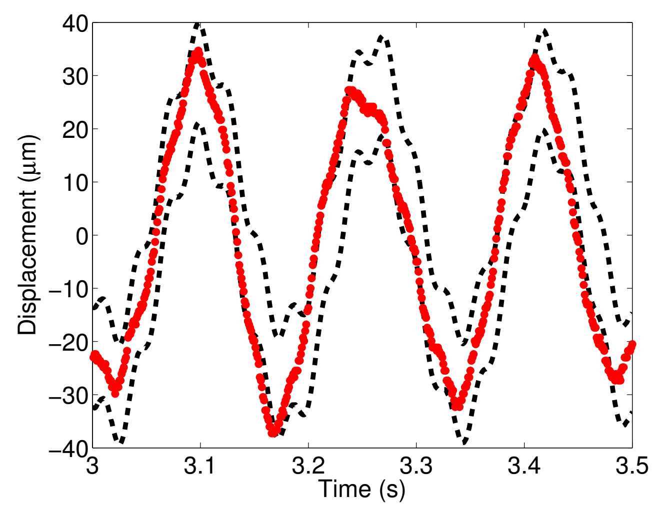


Calibrate on [0.25,1.25]

Note: We have substantially extended calibration regime.







Concluding Remarks

Notes:

• UQ requires a synergy between engineering, statistics, and applied mathematics.

• Model calibration, model selection, uncertainty propagation and experimental design are natural in a Bayesian framework.

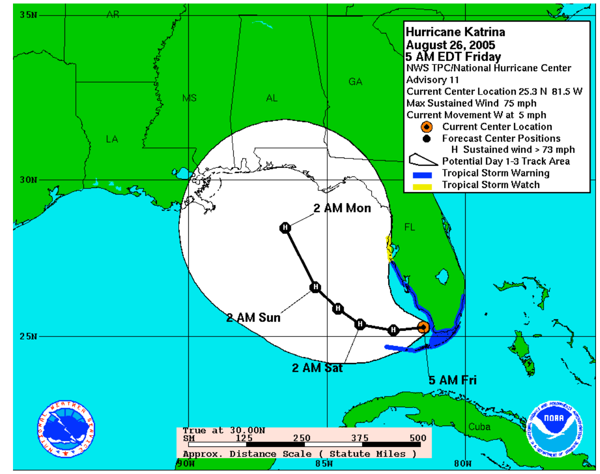
• Goal is to predict model responses with quantified and reduced uncertainties.

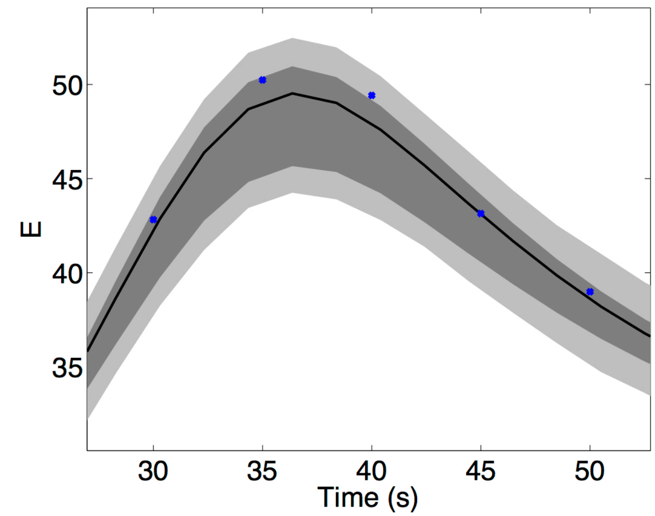
• Parameter selection is critical to isolate identifiable and influential parameters.

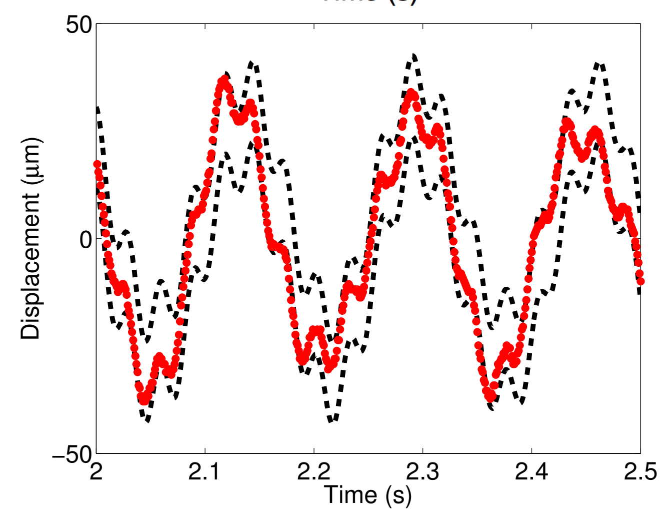
• Surrogate models critical for computationally intensive simulation codes.

• Codes and packages: Sandia Dakota, R, MATLAB, Python, nanoHUB.

• *Prediction is very difficult, especially if it's about the future*, Niels Bohr.







References

Books:

• R.C. Smith, *Uncertainty Quantification: Theory, Implementation, and Applications*, SIAM, Philadelphia, 2014.

Incomplete References:

Orthogonal Polynomial Methods and High-Dimensional Approximation Theory:

- M. Babuška, F. Nobile and R. Tempone, *Numer. Math*., 2005
- A. Cohen, R. De Vore and C. Schwab, *Analysis and Applications*, 2011
- M. Gunzburger, C.G. Webster and G. Zhang, *Acta Numerica*, 2014.
- O.P. Le Maître and O.M. Knio, *Spectral Methods for Uncertainty Quantification*, 2010
- S., *Uncertainty Quantification: Theory, Implementation, and Applications*, 2014.
- A.L. Teckentrup, P. Jantsch, M. Gunzburger and C.G. Webster, *SIAM/ASA J. Uncert. Quant., 2015*
- D. Xiu, *Numerical Methods for Stochastic Computations: A Spectral Method Approach*, 2010.

References

Incomplete References:

Sparse Grids:

- H-J. Bungartz and M. Griebel, *Acta Numerica*, 2004
- M. Gunzburger et al., *Water Resources Research*, 2013.
- F. Nobile, R. Tempone and C.G. Webster, *SIAM J. Num. Anal.*, 2008

Compressed Sensing:

- A. Chkifra, N. Dexter, H. Tran and C.G. Webster, *Mathematics of Computation, Submitted*

Infinite-Dimensional Bayesian Inference:

- A.M. Stuart, *Acta Numerica* 2010
- T. Bui-Thanh et al., *SIAM J. Sci. Comput.*, 2013
- S.J. Vollmer, SIAM/ASA J. Uncertainty Quantification, 2015.
- T. Bui-Thanh and Q. Nguyen, *Inverse Problems and Imaging*, 2016,