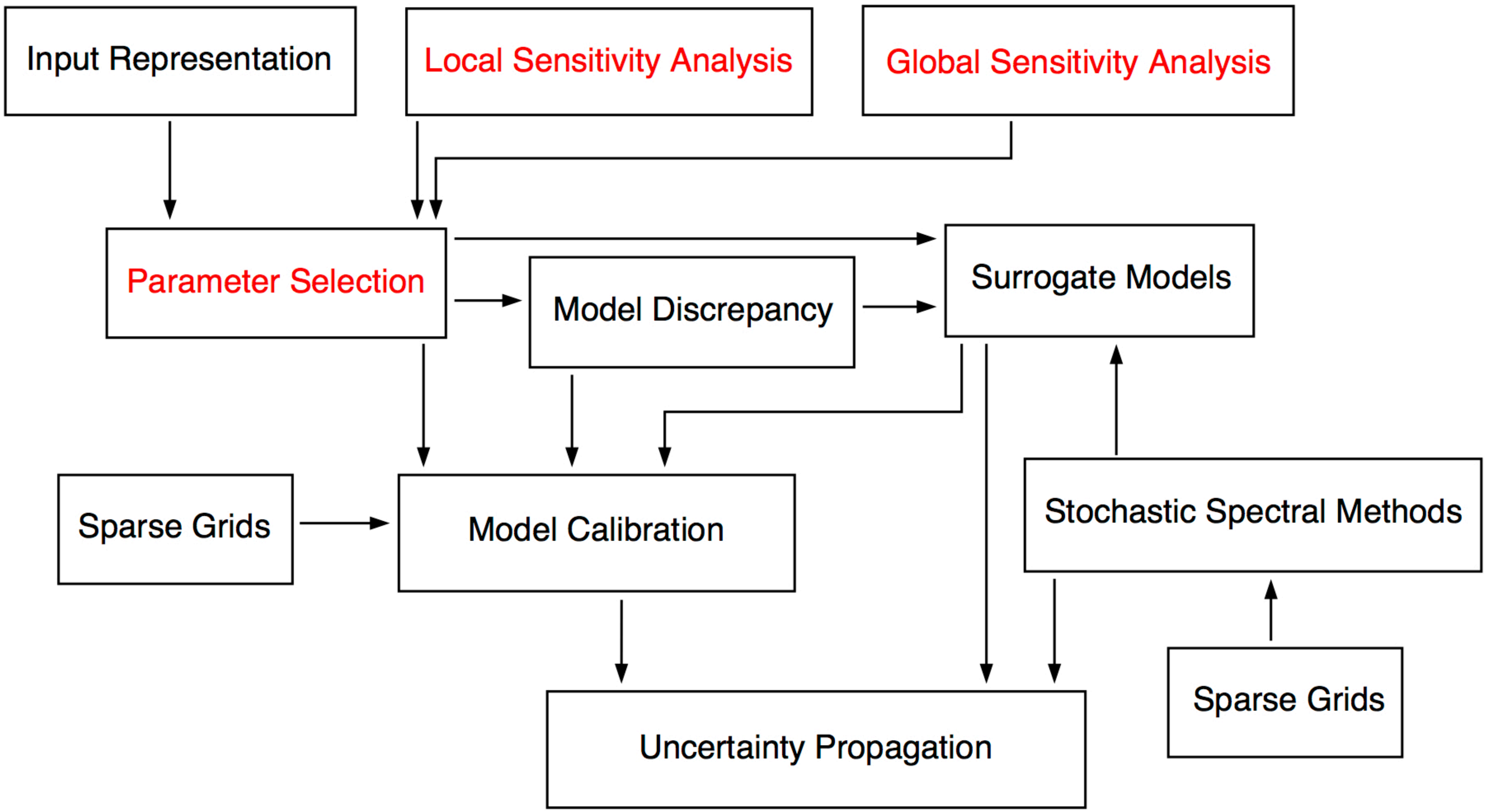
Steps in Uncertainty Quantification



Parameter Selection: Required for models with unidentifiable or noninfluential inputs

- e.g., SIR model

Parameter Selection Techniques and Surrogate Models

Parameter Space Reduction: SIR Model

$$\frac{dS}{dt} = \delta N - \delta S - \underline{\gamma k} IS \quad , \quad S(0) = S_0 \qquad \text{Susceptible}$$

$$\frac{dI}{dt} = \underline{\gamma k} IS - (r + \delta) I \quad , \quad I(0) = I_0 \qquad \text{Infectious}$$

$$\frac{dR}{dt} = rI - \delta R \quad , \quad R(0) = R_0 \qquad \text{Recovered}$$

Parameters:

- γ: Infection coefficient
- k: Interaction coefficient
- r: Recovery rate
- δ: Birth/death rate

Response:

$$y = \int_0^5 R(t, q)dt$$

Note: Parameters $q = [\gamma, k, r, \delta]$ not uniquely determined by data

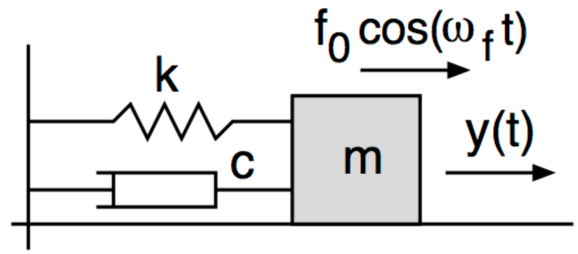
Parameter Selection Techniques

First Issue: Parameters often not *identifiable* in the sense that they are uniquely determined by the data.

Example: Spring model

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

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



Problem: Parameters $q = [m, c, k, f_0]$ and $q = \left[1, \frac{c}{m}, \frac{k}{m}, \frac{f_0}{m}\right]$ yield same displacements

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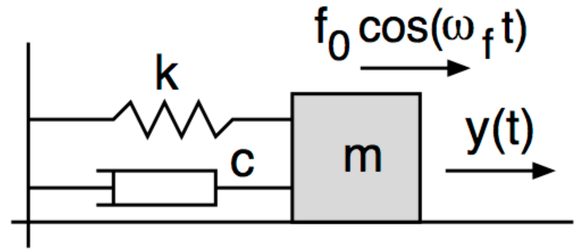

$$m\frac{d^2z}{dt^2} + c\frac{dz}{dt} + kz = f_0\cos(\omega_F t)$$

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Problem: Parameters $q = [m, c, k, f_0]$ and $q = \left[1, \frac{c}{m}, \frac{k}{m}, \frac{f_0}{m}\right]$ yield same displacements

Solution: Reformulate problem as

$$\frac{d^2z}{dt^2} + C\frac{dz}{dt} + Kz = F_0\cos(\omega_F t)$$

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

where $C = \frac{c}{m}$, $K = \frac{k}{m}$ and $F_0 = \frac{f_0}{m}$

Techniques for General Models:

- Linear algebra analysis;
  - e.g., SVD or QR algorithms
- Sensitivity analysis
- Active Subspaces

Parameter Selection Techniques and Surrogate Models

Second Issue: Models can have thousands to millions of parameters

3-D Neutron Transport Equations:

$$\frac{1}{|v|}\frac{\partial \varphi}{\partial t} + \Omega \cdot \nabla \varphi + \Sigma_t(r,E)\varphi(r,E,\Omega,t)$$

$$= \int_{4\pi} d\Omega' \int_0^\infty dE' \Sigma_s(E' \to E, \Omega' \to \Omega)\varphi(r,E',\Omega',t)$$

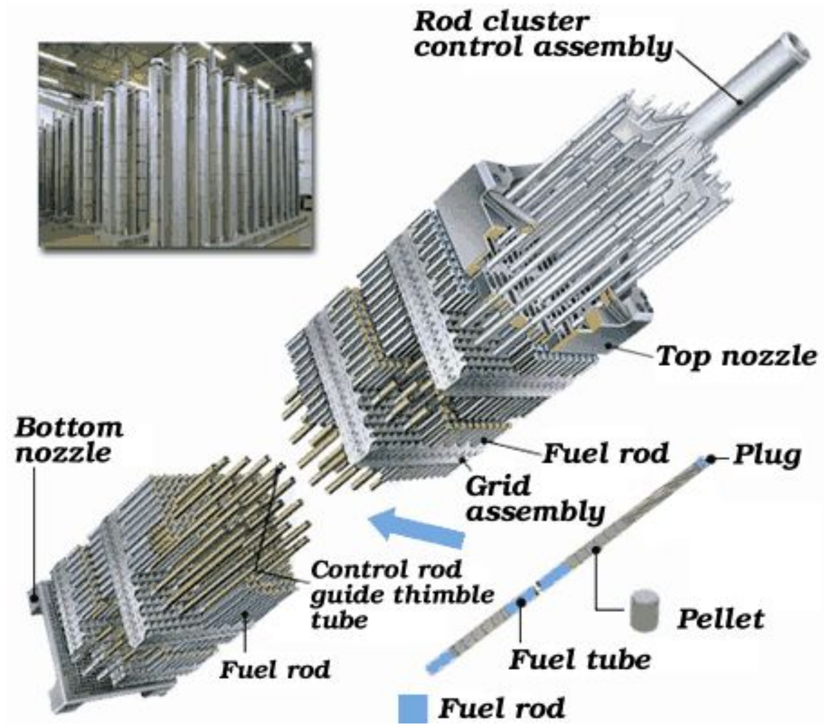
$$+ \underline{\frac{\chi(E)}{4\pi}} \int_{4\pi} d\Omega' \int_0^\infty dE' \underline{\nu(E')}\,\underline{\Sigma_f(E')}\varphi(r,E',\Omega',t)$$

Challenges:

- Very large number of inputs; e.g., 100,000; Active subspace construction critical.
- ORNL Code SCALE: Can take hours to run

Techniques for General Models:

- Identifiability and sensitivity analysis
- Active Subspaces



Global Sensitivity Analysis

Example: Portfolio model

$$Y = c_1 Q_1 + c_2 Q_2$$

Note:

- Q_1 and Q_2 represent hedged portfolios
- c_1 and c_2 amounts invested in each portfolio

Take

$$c_1 = 2 \; , \; c_2 = 1$$

$$Q_1 \sim N(0,1)$$

$$Q_2 \sim N(0,9)$$

Local Sensitivities:

$$\frac{\partial Y}{\partial Q_1} = 2 \quad , \quad \frac{\partial Y}{\partial Q_2} = 1$$

Conclusion: Investment is more sensitive to Portfolio 1 than to Portfolio 2

Limitations:

- Does not accommodate potential uncertainty in parameters.
- Sensitive to units and magnitudes of parameters.

Global Sensitivity Analysis

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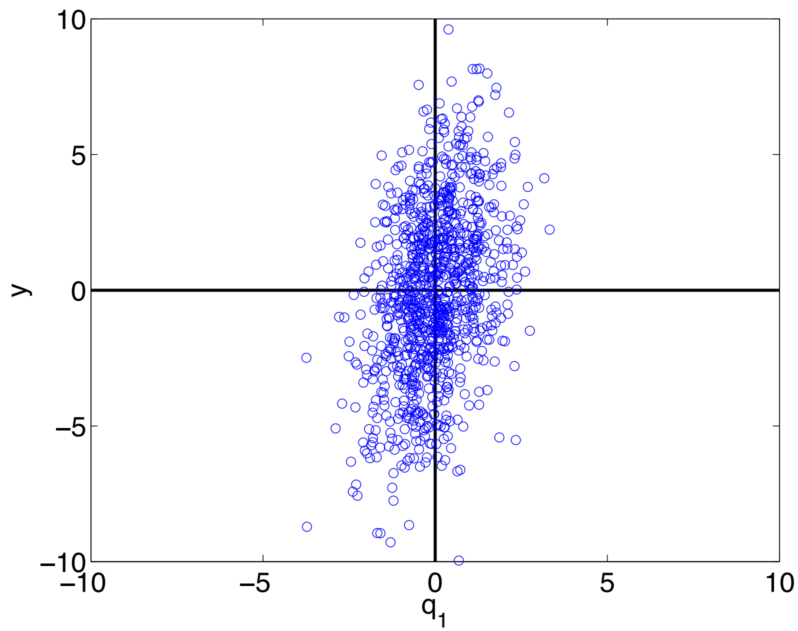
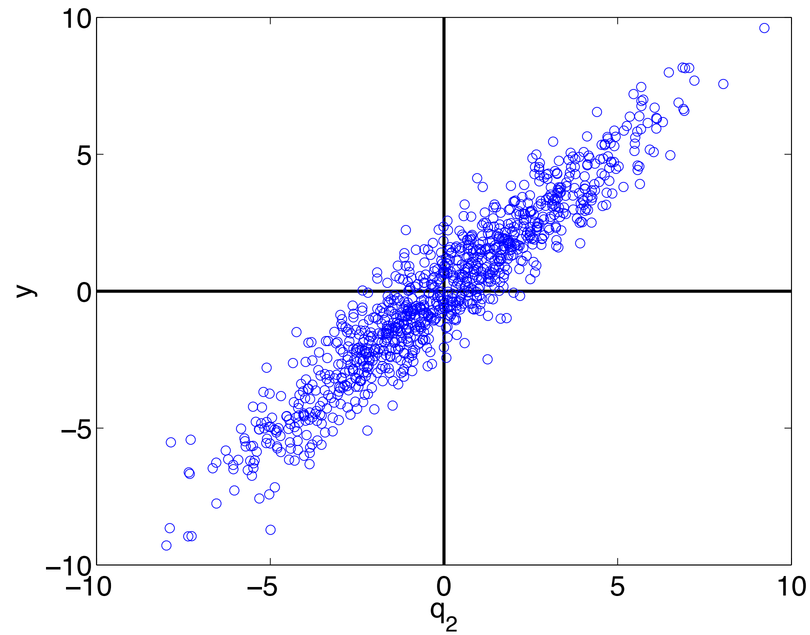




Local Sensitivities:

$$\frac{\partial Y}{\partial Q_1} = 2 \quad , \quad \frac{\partial Y}{\partial Q_2} = 1$$

Solutions:

- Response correlation
- Variance-based methods
- Random sampling of local sensitivities

Global Sensitivity Analysis: Variance-Based Methods

Example: Portfolio model

$$Y = c_1 Q_1 + c_2 Q_2$$

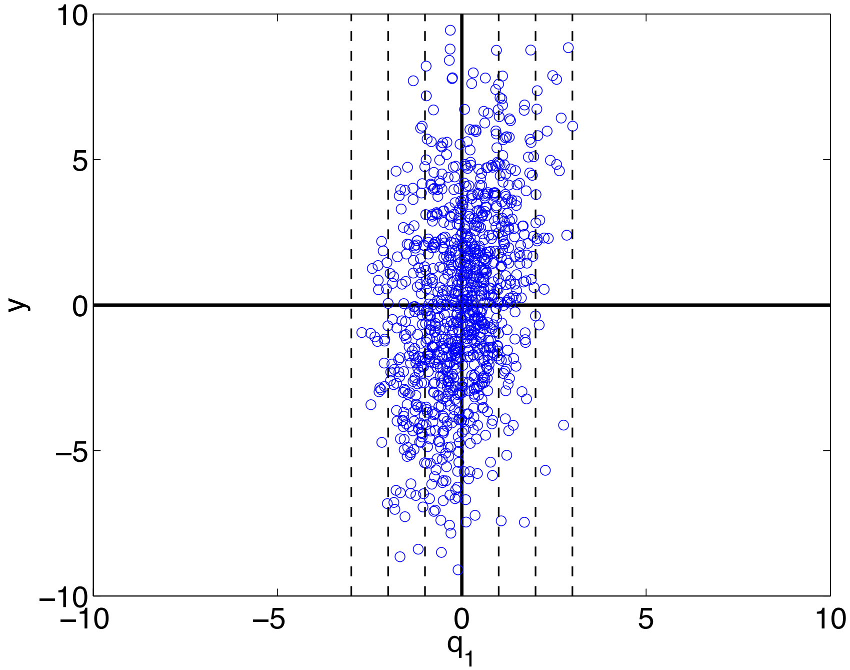
Take $c_1 = 2\ ,\ c_2 = 1$

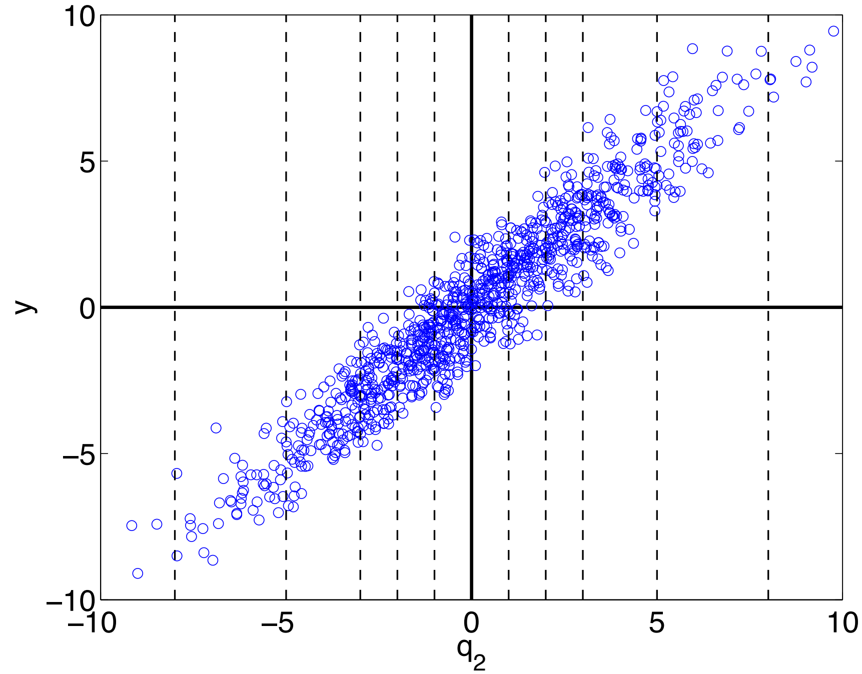
$$Q_1 \sim N(0, 1)$$

$$Q_2 \sim N(0, 9)$$

Statistical Motivation: Consider variability of expected values

$$D_i = \text{var}[\mathbb{E}(Y|q_i)]$$





Note: Here $D_2 > D_1$

Variance-Based Methods

Sobol Representation: For now, take $Q_i \sim \mathcal{U}(0,1)$ and $\Gamma = [0,1]^p$

Take

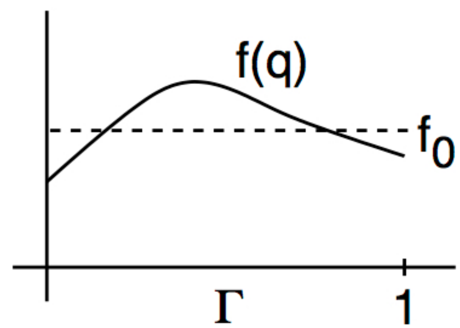
$$f(q) = f_0 + \sum_{i=1}^{p} f_i(q_i) + \sum_{1 \leqslant i < j \leqslant p} f_{ij}(q_i, q_j)$$

Analogy: Taylor or Fourier series

With appropriate assumptions,

$$f_0 = \int_\Gamma f(q)dq$$

$$f_i(q_i) = \int_{\Gamma^{p-1}} f(q)dq_{\sim i} - f_0$$



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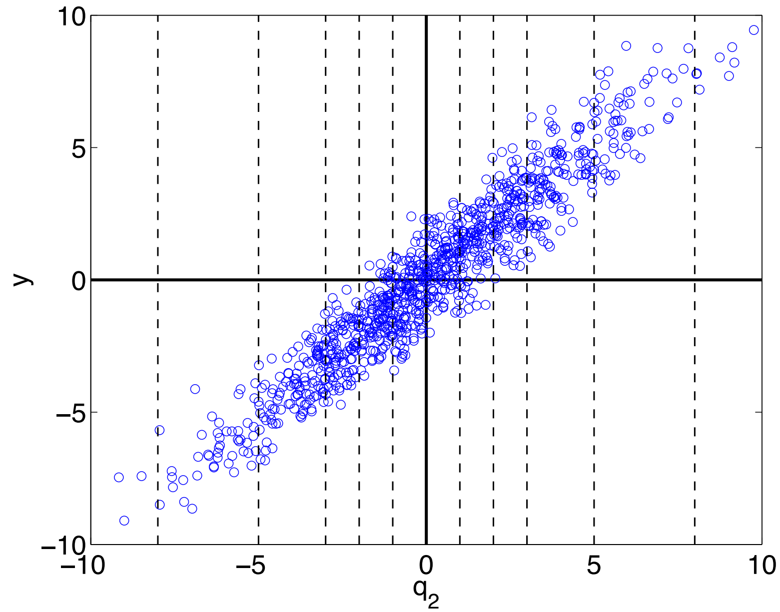
Analogy: Taylor or Fourier series

Assumption: Mutually independent parameters



Variances:

$$D_i = \int_0^1 f_i^2(q_i)dq_i$$

$$D = \text{var}(Y)$$

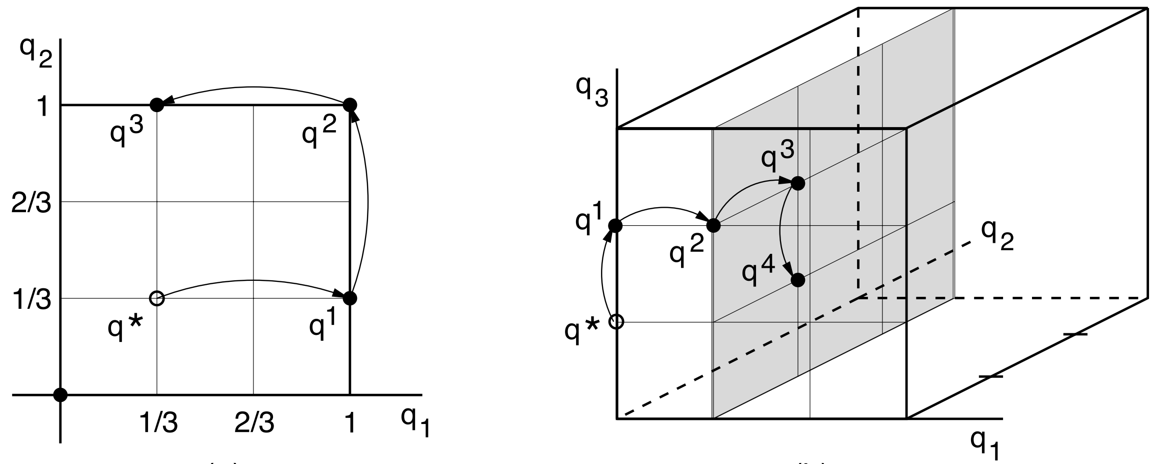
Sobol Indices: $S_i = \frac{D_i}{D}$

Statistical Interpretation:

$$D_i = \text{var}[\mathbb{E}(Y|q_i)] \Rightarrow S_i = \frac{\text{var}[\mathbb{E}(Y|q_i)]}{\text{var}(Y)}$$

Morris Screening: Random Sampling of Approximated Derivatives

Example: Consider uniformly distributed parameters on $\Gamma = [0,1]^p$



(a) (b)

Elementary Effect:

$$d_i^j = \frac{f(q^j + \Delta e_i) - F(q^j)}{\Delta} \quad , i^{th} \text{ parameter }, \; j^{th} \text{ sample}$$

Global Sensitivity Measures: r samples

$$\mu_i^* = \frac{1}{r} \sum_{j=1}^{r} |d_i^j(q)|$$

$$\sigma_i^2 = \frac{1}{r-1} \sum_{j=1}^{r} \left(d_i^j(q) - \mu_i \right)^2 \quad , \quad \mu_i = \frac{1}{r} \sum_{j=1}^{r} d_i^j(q)$$

SIR Disease Example

SIR Model:

$$\frac{dS}{dt} = \delta N - \delta S - \underline{\gamma k} IS \quad , \; S(0) = S_0 \qquad \text{Susceptible}$$

$$\frac{dI}{dt} = \underline{\gamma k} IS - (r + \delta) I \quad , \; I(0) = I_0 \qquad \text{Infectious}$$

$$\frac{dR}{dt} = rI - \delta R \quad , \; R(0) = R_0 \qquad \text{Recovered}$$

Note: Parameter set $q = [\gamma, k, r, \delta]$ is not identifiable

Assumed Parameter Distribution:

$$\gamma \sim \mathcal{U}(0, 1) \; , \; k \sim Beta(\alpha, \beta) \; , \; r \sim \mathcal{U}(0, 1) \; , \; \delta \sim \mathcal{U}(0, 1)$$

Infection Coefficient	Interaction Coefficient	Recovery Rate	Birth/death Rate

Response:

$$y = \int_0^5 R(t, q)dt$$

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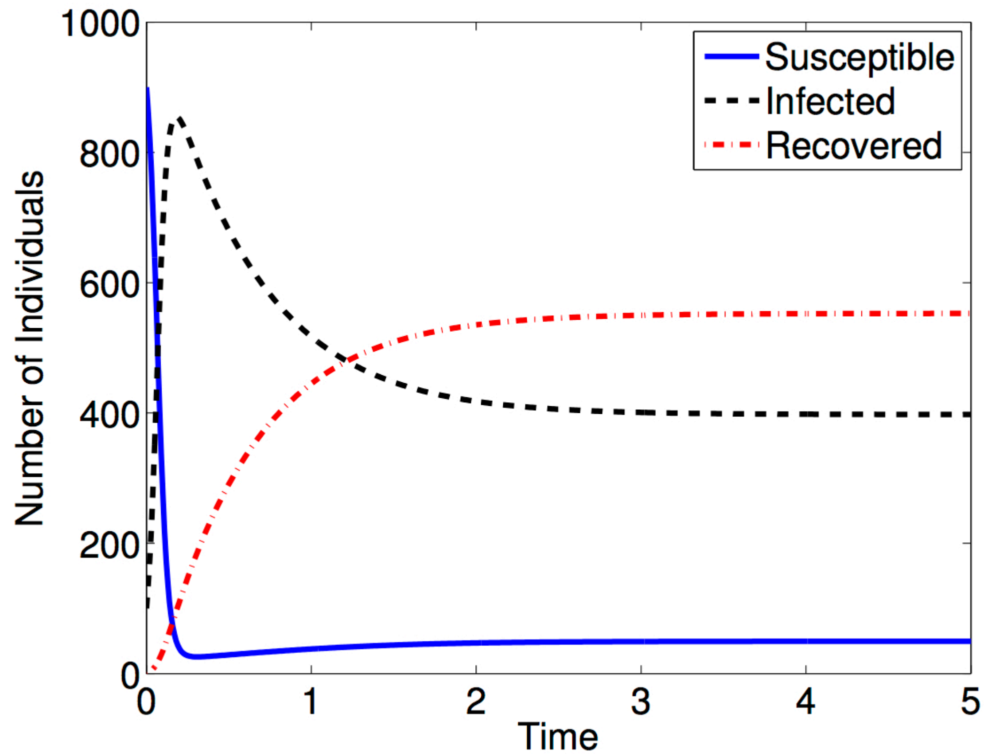
Typical Realization:



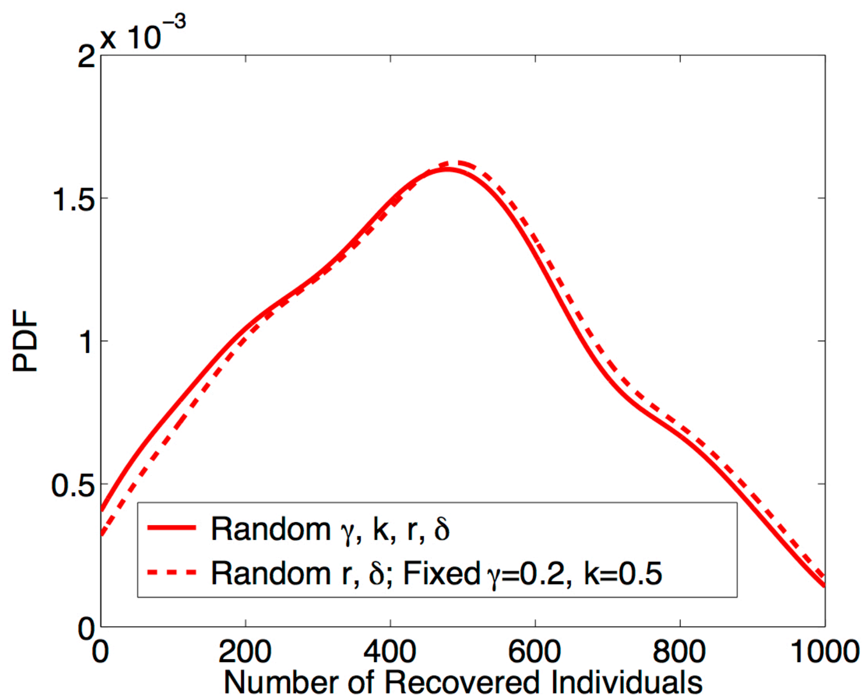
SIR Disease Example

Global Sensitivity Measures:

		γ	k	r	δ
Sobol	S_i	0.0997	0.0312	0.7901	0.1750
	S_{T_i}	-0.0637	-0.0541	0.5634	0.2029
Morris	μ_i^* $(\times 10^3)$	0.2532	0.2812	2.0184	1.2328
	σ_i $(\times 10^3)$	0.9539	1.6245	6.6748	3.9886

Influential Parameters

Result: Densities for $R(t_f)$ at $t_f = 5$



Note: Can fix non-influential parameters γ, k

Parameter Selection: Nuclear Power Plant Design

Subchannel Code (COBRA-TF): numerous closure relation and parameters

parameter	partial correlation	simple correlation	morris main	morris interaction	CPS variation
k_eta	0.07	0.03			
k_gama	-0.03	0.04			
k_sent	-0.03	-0.02			
k_sdent	-0.07	-0.01			
k_tmasv	-0.03	0.00			
k_tmasl	0.11	0.00	6.48E-05	2.28E-05	medium
k_tmasg	-0.19	-0.01			
k_tmomv	-0.12	-0.01			
k_tmome	0.02	0.00			
k_tmoml	0.02	-0.02	2.23E-04	1.30E-04	medium
k_xk	0.08	-0.02			
k_xkes	-0.05	0.00			
k_xkge	-0.07	0.01			
k_xkl	0.04	-0.01			
k_xkle	-0.03	0.00			
k_xkvls	0.11	-0.01			
k_xkwvw	-0.10	0.01			
k_xkwlw	0.14	0.01			
k_xkwew	-0.01	0.03			
k_qvapl	-0.09	-0.01			
k_tnrgv	-0.03	0.00			
k_tnrgl	-0.01	0.03	9.00E-06	9.49E-06	low
k_rodqq	0.02	-0.01			
k_qradd	-0.02	0.00			
k_qradv	-0.01	0.00			
k_qliht	-0.01	0.00			
k_sphts	-0.05	0.03			
k_cond	-0.04	0.00			
k_xkwvx	0.03	-0.02			
k_xkwlx	1.00	0.88	1.80E-01	7.07E-03	high
k_cd	1.00	0.46	9.59E-02	7.88E-03	high
k_cdfb	-0.02	-0.01			
k_wkr	0.02	0.02			

5 Identified Active Inputs:

k_cd: Pressure loss coefficient of space in sub-channel

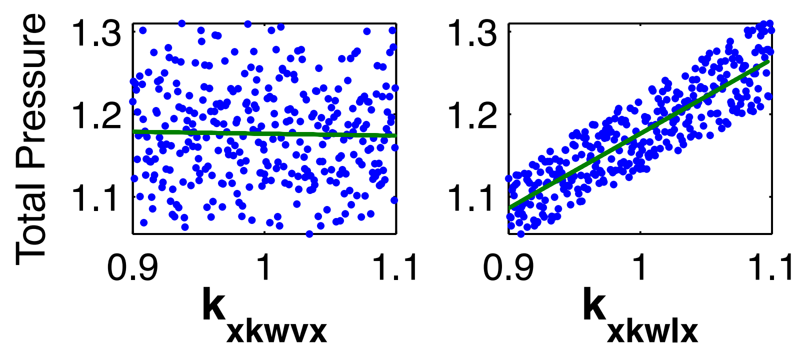
k_xkwlx: Vertical liquid wall drag coefficient

k_tmasl: Loss of liquid mass due to mixing and void drift

k_tmoml: Loss of liquid momentum due to mixing and void drift

k_tnrgl: Loss of liquid enthalpy due to mixing and void drift

Partial Correlation:



Note: 33 initial VUQ parameters reduced to 5 via sensitivity analysis

Global Sensitivity Analysis: Potential Pitfalls

Example: Quantum-informed continuum model

Question: Do we use 4th or 6th-order Landau energy?

$$\psi(P, q) = \alpha_1 P^2 + \alpha_{11} P^4 + \alpha_{111} P^6$$

Parameters:

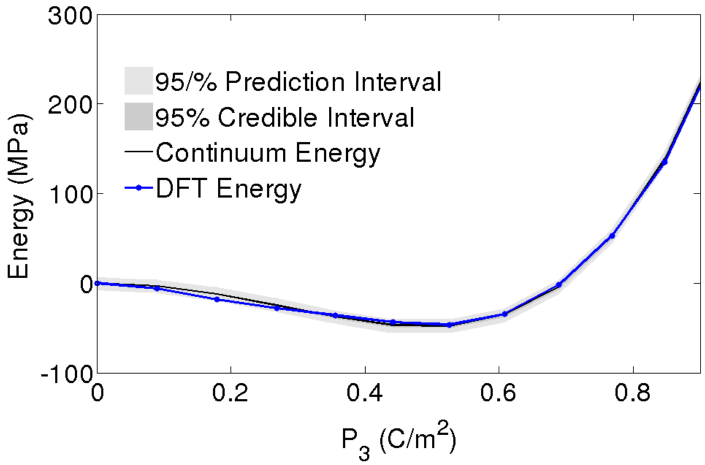
$$q = [\alpha_1, \alpha_{11}, \alpha_{111}]$$

Global Sensitivity Analysis:

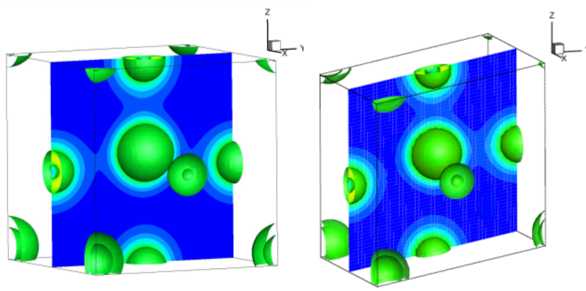
	α_1	α_{11}	α_{111}
S_k	0.62	0.39	0.01
T_k	0.66	0.38	0.06
μ_k^*	0.17	0.07	0.03

Conclusion:

α_{111} insignificant and can be fixed



Landau energy



DFT Electronic Structure Simulation

Global Sensitivity Analysis

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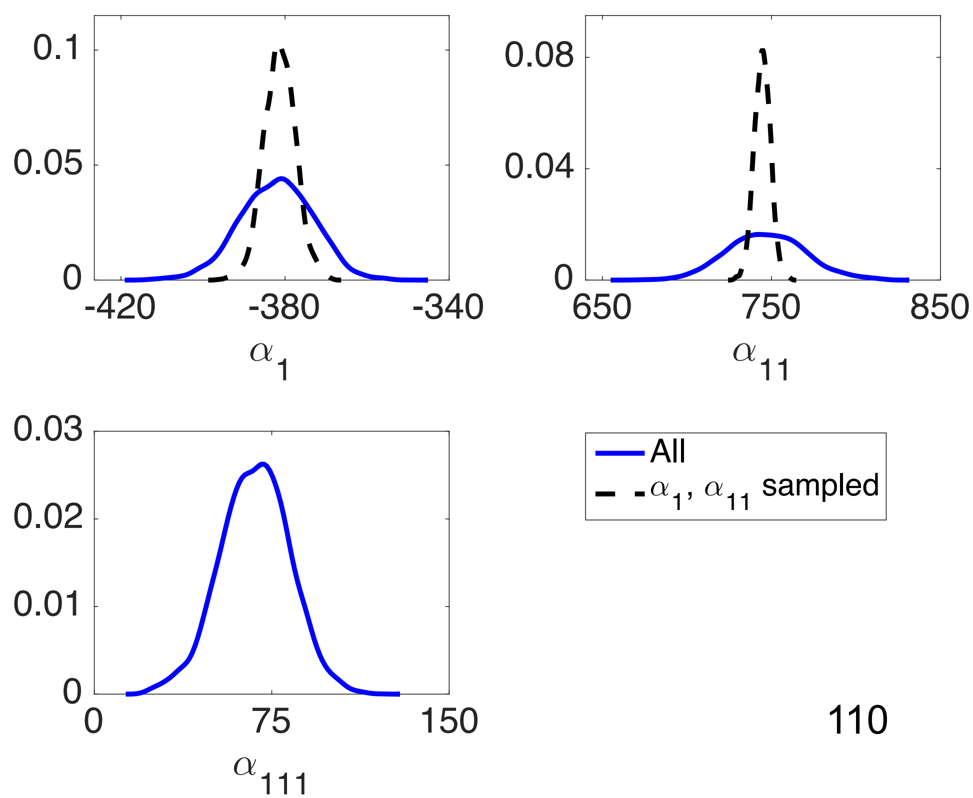
Problem: We obtain different distributions when we perform Bayesian inference with fixed non-influential parameters



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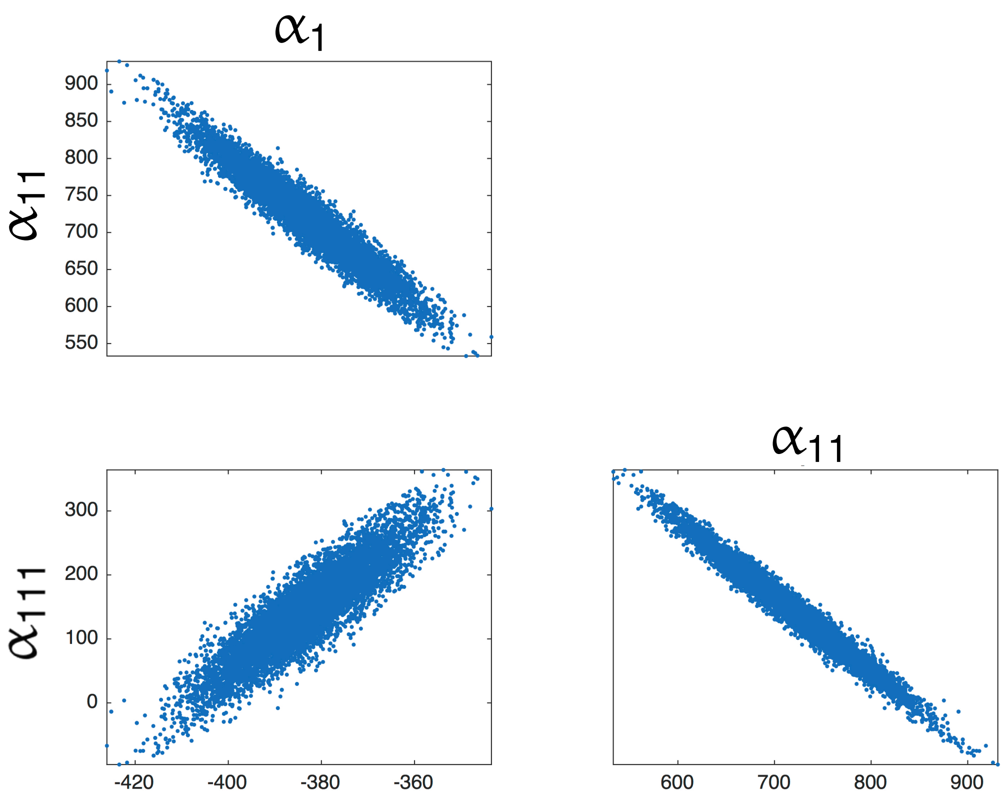
Note: Must accommodate correlation

Problem:

- Parameters correlated
- Cannot fix α_{111}



Global Sensitivity Analysis: Analysis of Variance

Sobol' Representation:

$$f(q) = f_0 + \sum_{i=1}^{p} \sum_{|u|=i} f_u(q_u)$$

One Solution: Take variance to obtain

$$\text{var}[f(q)] = \sum_{i=1}^{p} \sum_{|u|=i} \text{cov}[f_u(q_u), f(q)]$$

Sobol' Indices:

$$S_u = \frac{\text{cov}[f_u(q_u), f(q)]}{\text{var}[f(q)]}$$

Pros:

- Provides variance decomposition that is analogous to independent case

Cons:

- Indices can be negative and difficult to interpret
- Often difficult to determine underlying distribution
- Monte Carlo approximation often prohibitively expensive.

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Alternative: Construct active subspaces

- Can accommodate parameter correlation
- Often effective in high-dimensional space; e.g., p = 7700 for neutronics example

Additional Goal: Use Bayesian analysis on active subspace to construct posterior densities for physical parameters.

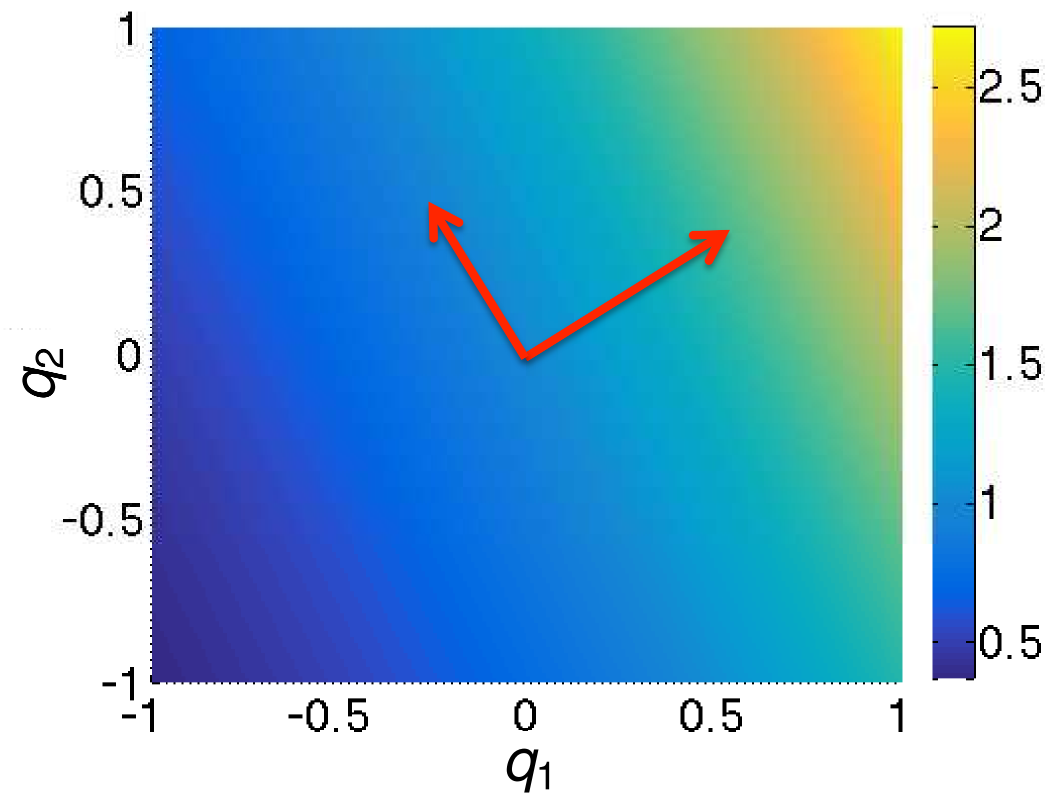
Active Subspaces

Note:

- Functions may vary significantly in only a few directions
- "Active" directions may be linear combination of inputs

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

- Varies most in [0.7, 0.3] direction
- No variation in orthogonal direction



Strategy:

- *Linearly parameterized problems:* Employ SVD or QR decomposition.
- *Nonlinear problems:* Construct approximate gradient matrix and employ SVD or QR.

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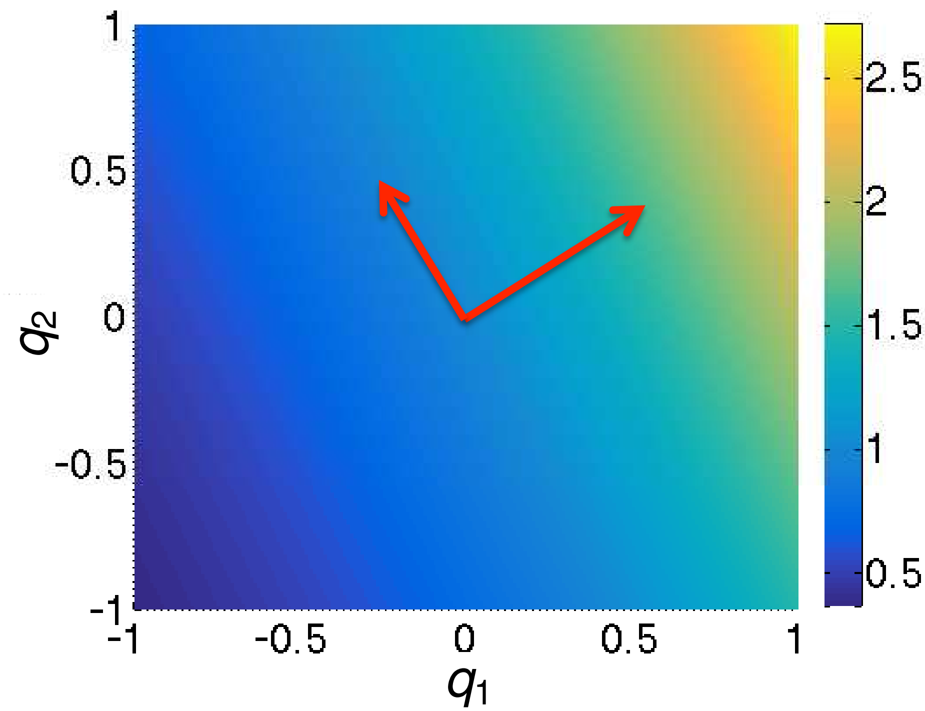


A Bit of History:

• Often attributed to Russi (2010).

• Concept same as *identifiable subspaces* from systems and control; e.g., Reid (1977).

• For linearly parameterized problems, active subspace given by SVD or QR; Beltrami (1873), Jordan (1874), Sylvester (1889), Schmidt (1907), Weyl (1912). See 1993 *SIAM Review* paper by Stewart.

Parameter Space Reduction Techniques: Linear Problems

Second Issue: Models depends on very large number of parameters – e.g., millions – but only a few are "significant".

Linear Algebra Techniques: Linearly parameterized problems

$$y = Aq \ , \ q \in \mathbb{R}^p \ , \ y \in \mathbb{R}^m$$

Singular Value Decomposition (SVD):

$$A = U\Sigma V^T \ , \ \Sigma = [S \quad 0]$$

$$S = \begin{bmatrix} \sigma_1 & & & \\ & \ddots & & \\ & & \sigma_r & \\ & & & 0 \end{bmatrix} \ , \ \sigma_1 \geq \sigma_2 \geq \cdots \geq \sigma_r \geq \varepsilon$$

Rank Revealing QR Decomposition: $A^T P = QR$

Problem: Neither is directly applicable when m or p are very large; e.g., millions.

Solution: Random range finding algorithms.

Random Range Finding Algorithms: Linear Problems

Algorithm: Halko, Martinsson and Tropp, SIAM Review, 2011

1. Choose ℓ random inputs q^i and compute outputs $y^i = Aq^i$ which are compiled in the $m \times \ell$ matrix Y.

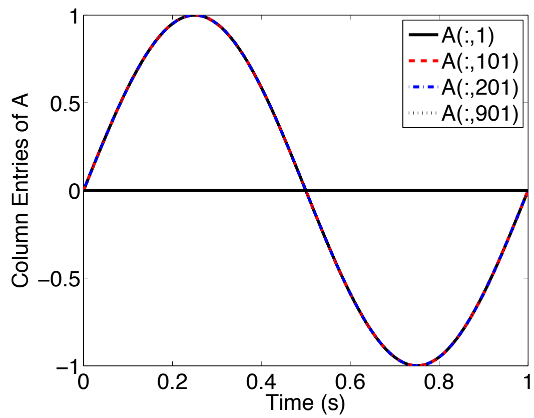
2. Take a pivoted QR factorization $Y = QR$ to construct a matrix Q whose columns form an orthonormal basis for the range of Y.

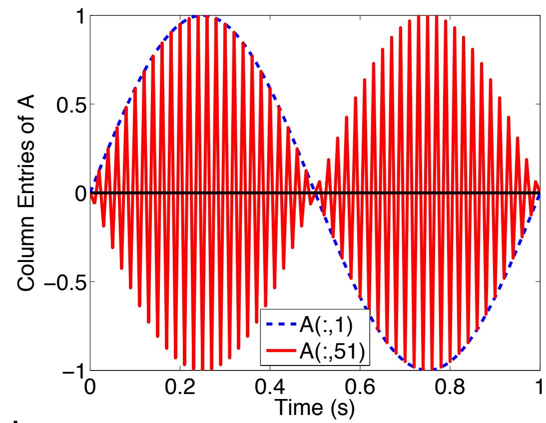
Example: $y_i = \sum_{k=1}^{p} q_k \sin(2\pi k t_i) \ , \ i = 1, \cdots, m$

$$\begin{bmatrix} y_1 \\ \vdots \\ y_m \end{bmatrix} = \begin{bmatrix} \sin(2\pi t_1) & \cdots & \sin(2\pi p t_1) \\ \vdots & & \vdots \\ \sin(2\pi t_m) & \cdots & \sin(2\pi p t_m) \end{bmatrix} \begin{bmatrix} q_1 \\ \vdots \\ q_p \end{bmatrix}$$

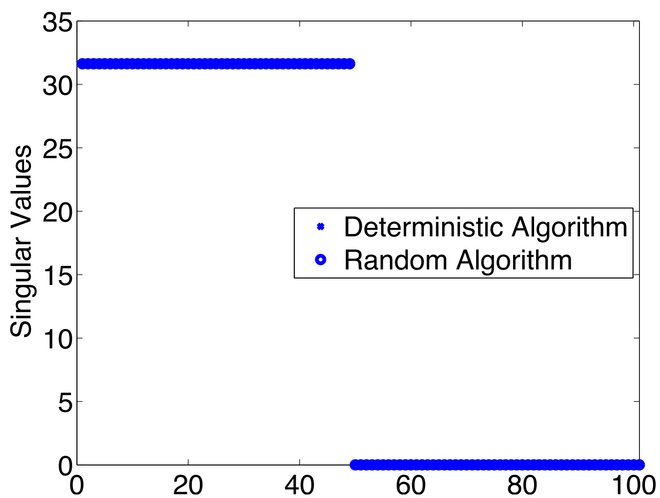
Random Range Finding Algorithms: Linear Problems

Example: m = 101, p = 1000: Analytic value for rank is 49

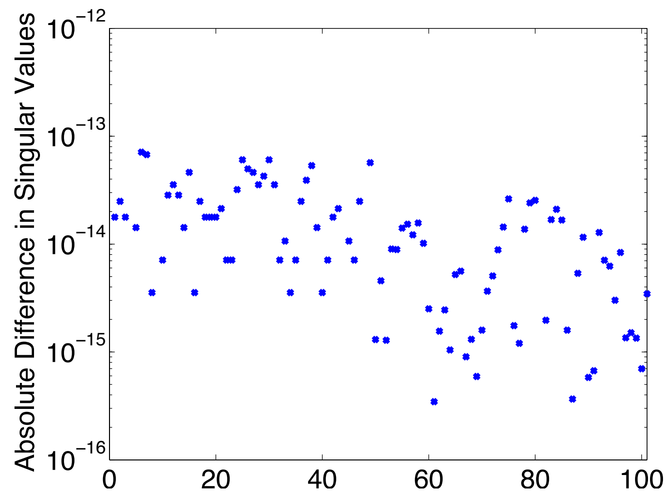




Aliasing



Singular Values



Absolute Difference Between Singular Values

Example: m = 101, p = 1,000,000: Random algorithm still viable

Active Subspaces

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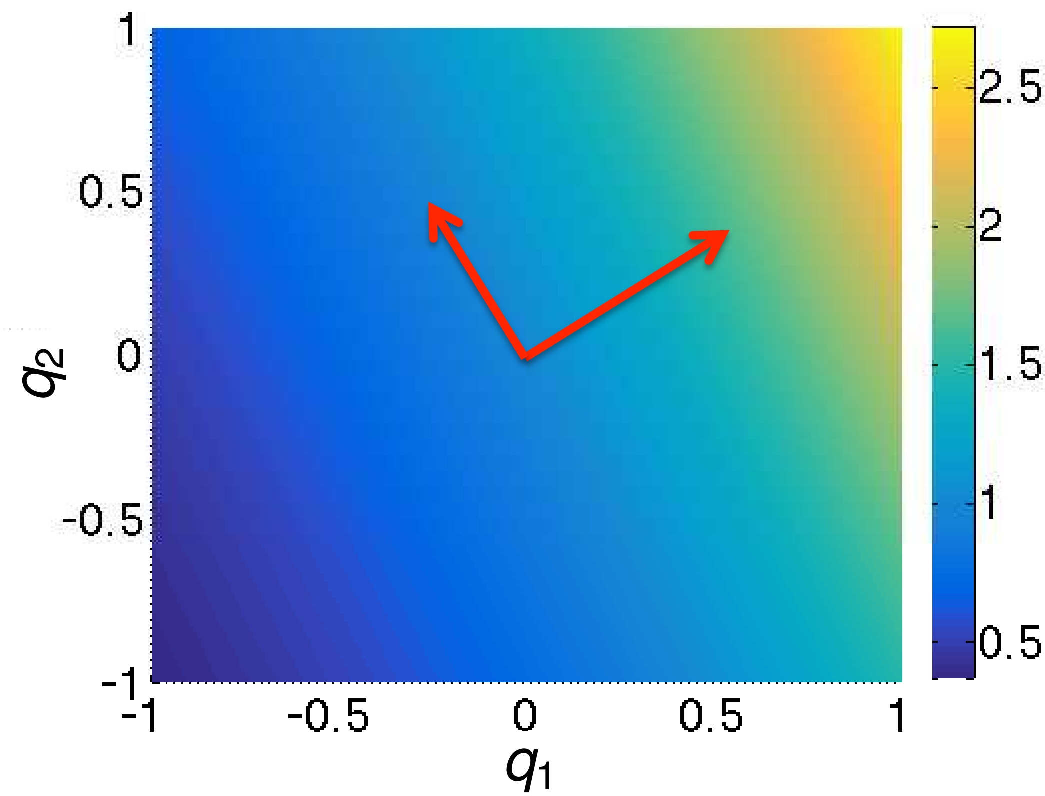
- Varies most in [0.7, 0.3] direction
- No variation in orthogonal direction



Strategy:

- *Linearly parameterized problems:* Employ SVD or QR decomposition.
- *Nonlinear problems:* Construct approximate gradient matrix and employ SVD or QR.

Gradient-Based Active Subspace Construction

Active Subspace: Consider

$$f = f(q)\ ,\ q \in \mathcal{Q} \subseteq \mathbb{R}^p$$

- E.g., see [Constantine, SIAM, 2015; Stoyanov & Webster, *IJUQ*, 2015]

and

$$\nabla_q f(q) = \left[\frac{\partial f}{\partial q_1}, \cdots, \frac{\partial f}{\partial q_p}\right]^T$$

Construct outer product

$$C = \int (\nabla_q f)(\nabla_q f)^T \rho dq$$

$\rho(q)$: Distribution of input parameters q

Question: How sensitive are results to distribution, which is typically not known?

Partition eigenvalues: $C = W \Lambda W^T$

$$\Lambda = \begin{bmatrix} \Lambda_1 & \\ & \Lambda_2 \end{bmatrix}\ ,\ W = [W_1 \quad W_2]$$

Rotated Coordinates:

$$y = W_1^T q \in \mathbb{R}^n \quad \text{and} \quad z = W_2^T q \in \mathbb{R}^{p-n}$$

Active Variables

Active Subspace: Range of eigenvectors in W_1

Gradient-Based Active Subspace Construction

Active Subspace: Construction based on random sampling

1. Draw M independent samples $\{q^j\}$ from ρ

2. Evaluate $\nabla_q f_j = \nabla_q f(q^j)$

3. Approximate outer product

$$C \approx \widetilde{C} = \frac{1}{M} \sum_{j=1}^{M} (\nabla_q f_j)(\nabla_q f_j)^T$$ Monte Carlo Quadrature

   Note: $\widetilde{C} = GG^T$ where $G = \frac{1}{\sqrt{M}}[\nabla_q f_1, \ldots, \nabla_q f_M]$

4. Take SVD of $G = W\sqrt{\Lambda}V^T$

   - Active subspace of dimension n is first n columns of W

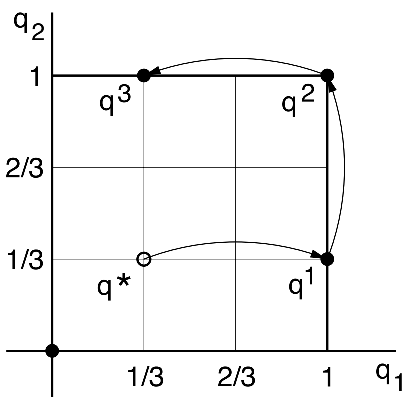
Goal: Develop efficient algorithm for codes that do not have adjoint capabilities

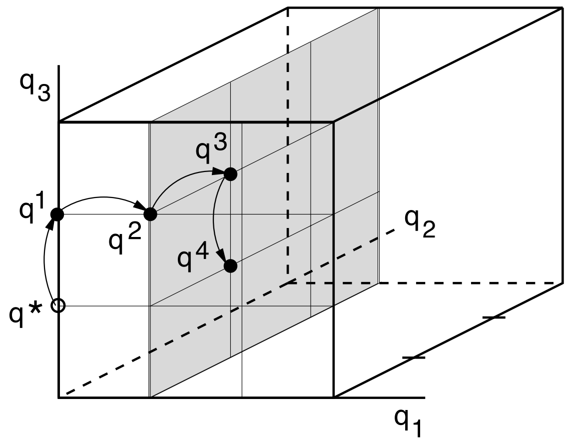
Note: Finite difference approximations tempting but not very effective

Strategy: Algorithm based on initialized adaptive Morris indices

Morris Screening: Random Sampling of Approximated Derivatives

Example: Consider uniformly distributed parameters on $\Gamma = [0,1]^p$





Adaptive Algorithm:

- Use SVD to adapt stepsizes and directions to reflect active subspace.
- Reduce dimension of differencing as active subspace is discovered.

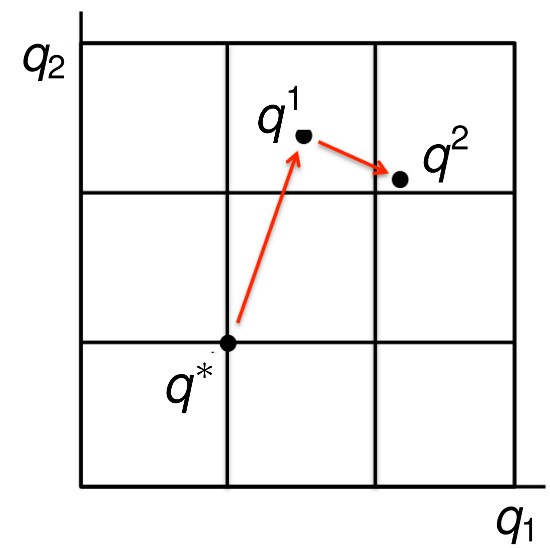
Elementary Effect:

$$d_i = \frac{f(q^j + \Delta e_i) - f(q^j)}{\Delta}$$

Global Sensitivity Measures: r samples

$$\mu_i^* = \frac{1}{r}\sum_{j=1}^{r} |d_i^j(q)|$$

$$\sigma_i^2 = \frac{1}{r-1}\sum_{j=1}^{r}\left(d_i^j(q) - \mu_i\right)^2 \quad , \quad \mu_i = \frac{1}{r}\sum_{j=1}^{r} d_i^j(q)$$



Note: Gets us to moderate-D but initialization required for high-D

Initialization Algorithm

1. Inputs: ℓ iterations, h function evaluations per iteration
2. Sample w^1 from surface of unit sphere where approximately linear

For $j = 1, \ldots, \ell$

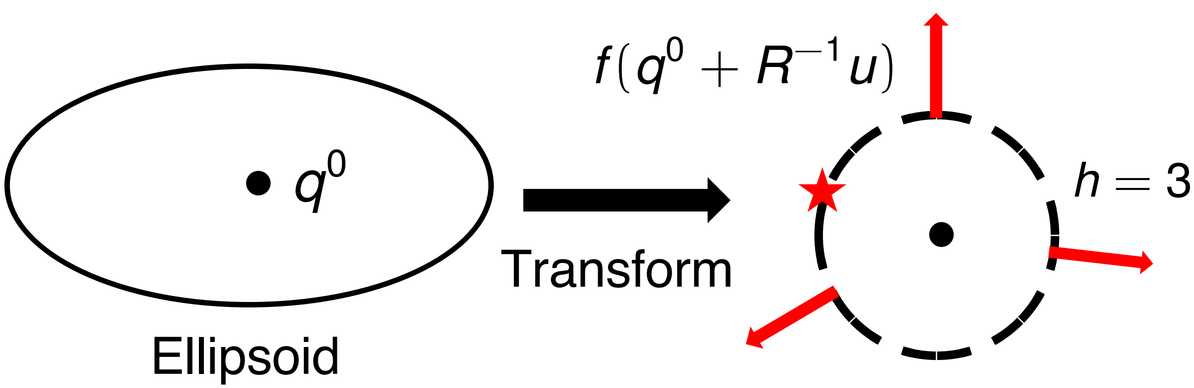
3. Sample $\{\tilde{v}_1^j, \ldots, \tilde{v}_h^j\}$ from surface of sphere
4. Use Lagrange multiplier to determine

$$u_{\max}^j = a_0^+ w^j + \sum_{i=1}^{h} a_i^+ v_i^j \ , \ v_i^1 = \tilde{v}_i^1$$

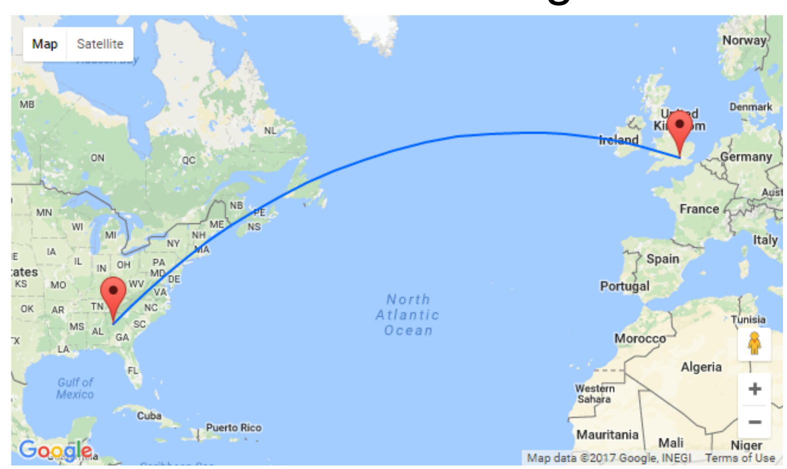
that maximizes $g(u) = f(q^0 + R^{-1}u)$.

Note: For h=1, maximizing great circle through w^1, v^1

Example: Let w^1 = Atlanta, v^1 = London, and g(u) = 'QUIETness' of seatmate on flight



$$(z - q^0)^T S (z - q^0) = 1$$
$$S = R^T R$$



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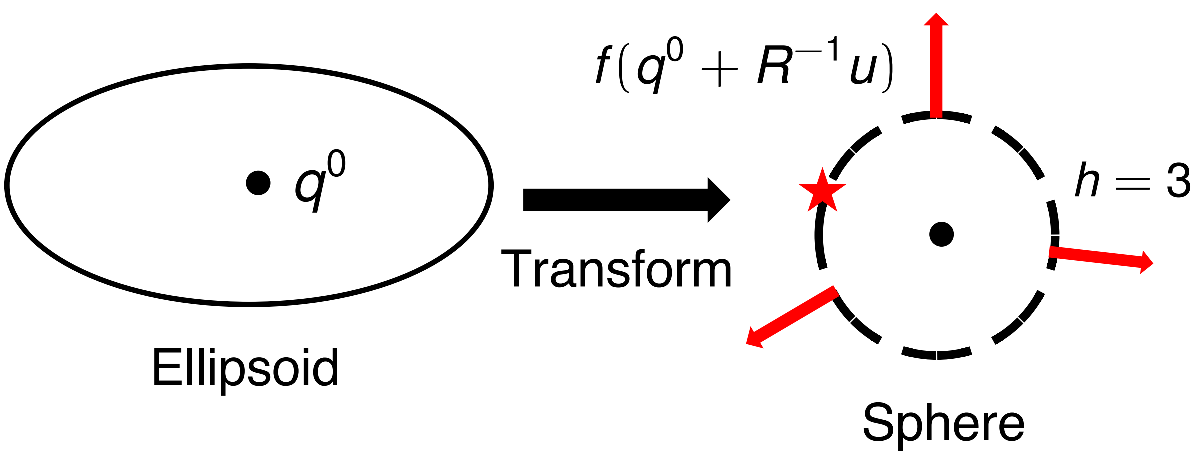

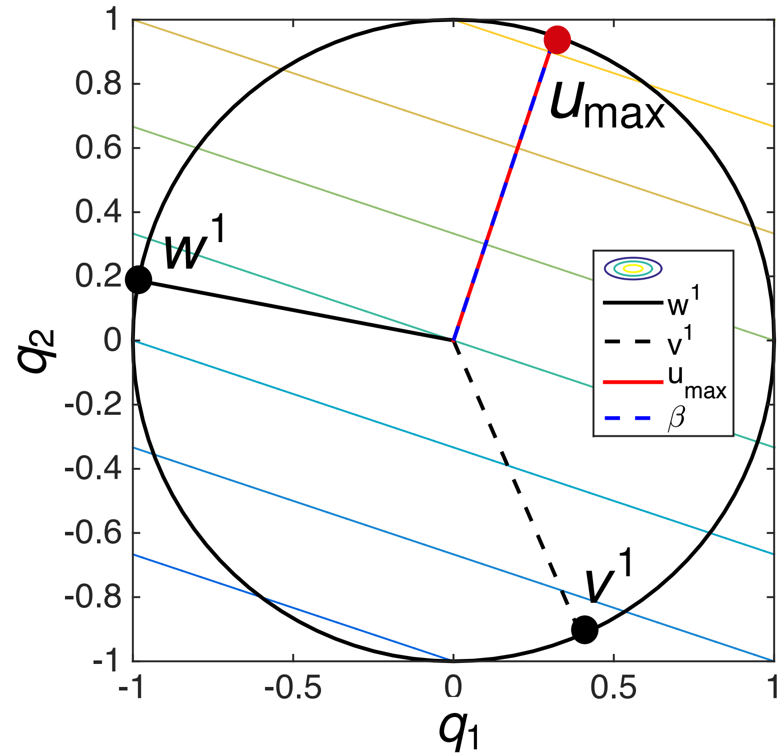

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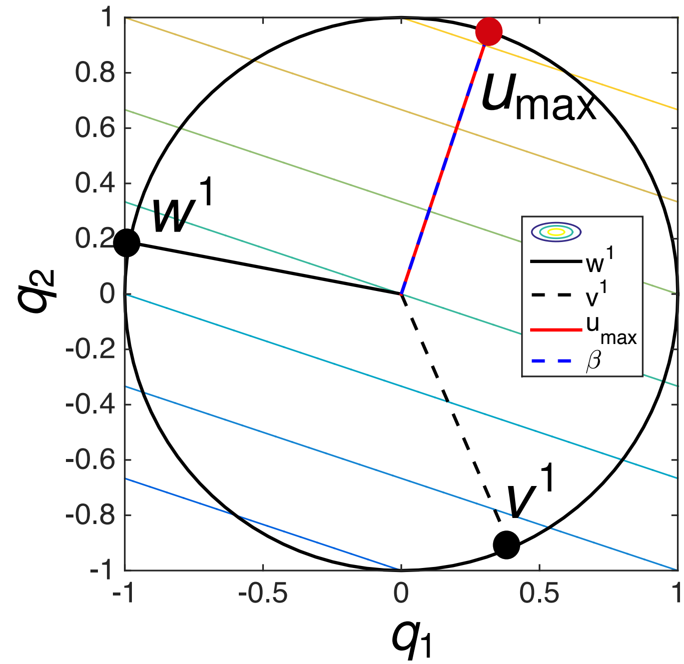
that maximizes $g(u) = f(q^0 + R^{-1}u)$.

Set $w^{j+1} = u_{\max}^j$.



5. Take $C = [w^j, v_1^j, \ldots, v_h^j]$ and set $P_{u_{\max}^j} = u_{\max}^j (u_{\max}^j)^T$
6. Let $C_{j\perp} = \left[\text{span}\left(C_{(j-1)\perp}, (I_m - P_{u_{\max}^j} C\right)\right]$ and set $P_{C_{j\perp}} = C_{j\perp}(C_{j\perp}^T C_{j\perp})^{-1} C_{j\perp}^T$
7. Take $v_i^j = \dfrac{(I_m - P_{C_{j\perp}})\tilde{v}_i^j}{\|(I_m - P_{C_{j\perp}})\tilde{v}_i^j\|}$, $i = 1, \ldots, h$ and repeat

Ortho-complement of $u_{\max}$

Example: Initialization Algorithm to Approximate Gradient

Example: Family of elliptic PDE's

$$-\nabla_s \cdot (a(q,s,\ell)\nabla_s u(s,a(q,s,\ell))) = 1 \ , \ s = [0,1]^2 \ , \ \ell = 1,\cdots,n$$

with the random field representations

$$a(q,s,\ell) = a_{\min} + e^{\overline{a}(s,\ell)+\sum_{i=1}^{p} q_k^\ell \gamma_i \phi_i(s)}$$

Quantity of interest: e.g., strain along edge at n levels

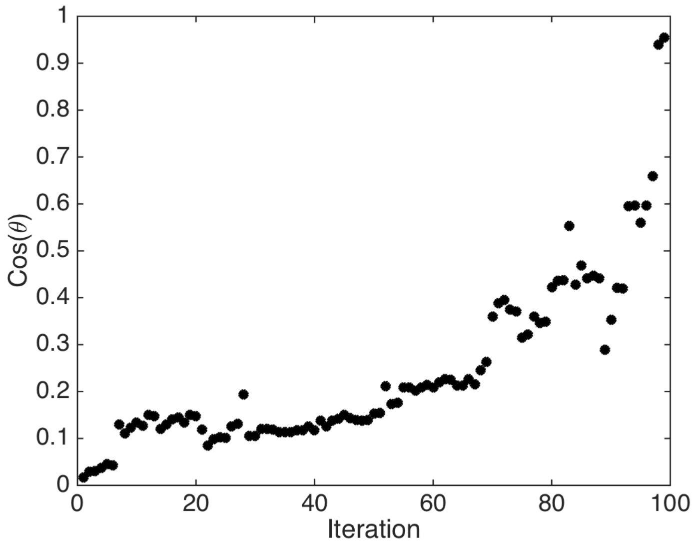
$$f\left(\mathbf{q}^1, \ldots, \mathbf{q}^n\right) \approx \sum_{\ell=1}^{n} \frac{1}{|\Gamma_2|} \int_{\Gamma_2} u(q,s,\ell) ds$$

Problem Dimensions:

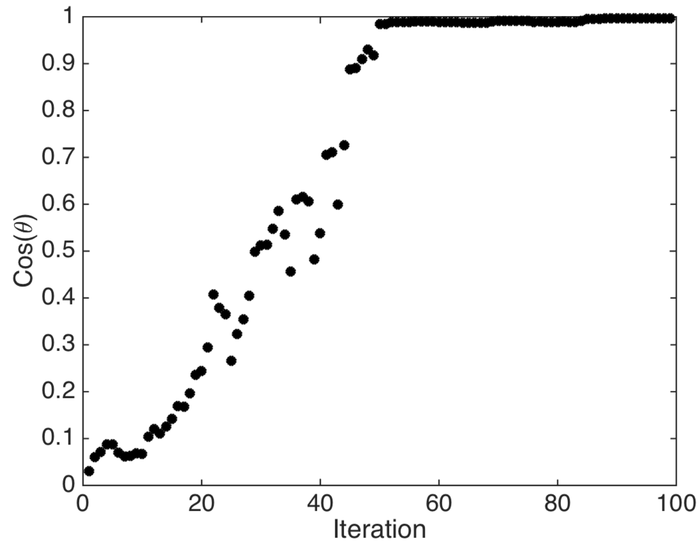
- Parameter dimension: p = 100
- Active subspace dimension: n = 1
- Finite element approximation

Example: Initialization Algorithm to Approximate Gradient

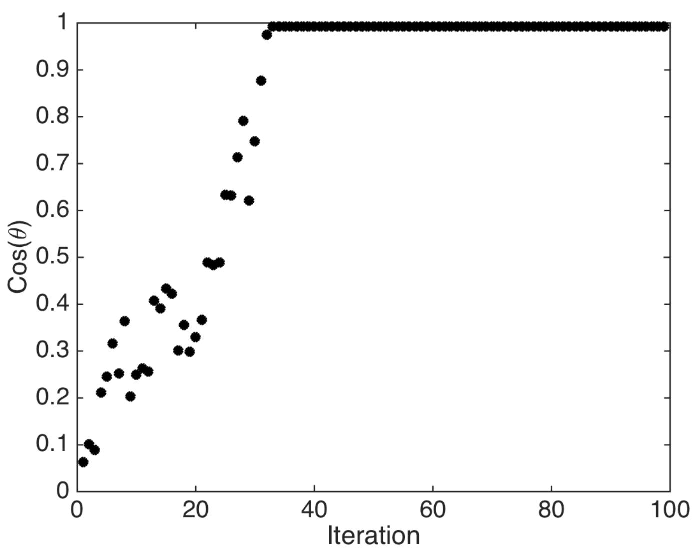
Results: Cosine of angle between ’analytic’ and computed gradient



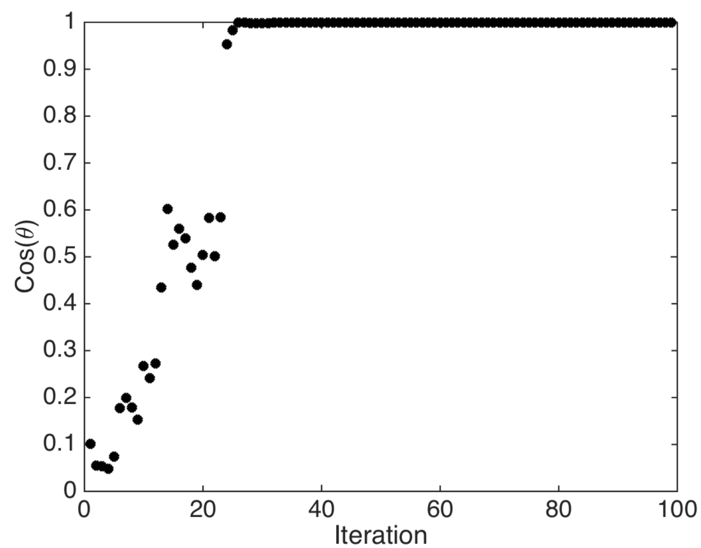
$h = 1$



$h = 2$



$h = 3$



$h = 4$

Recall: p=100

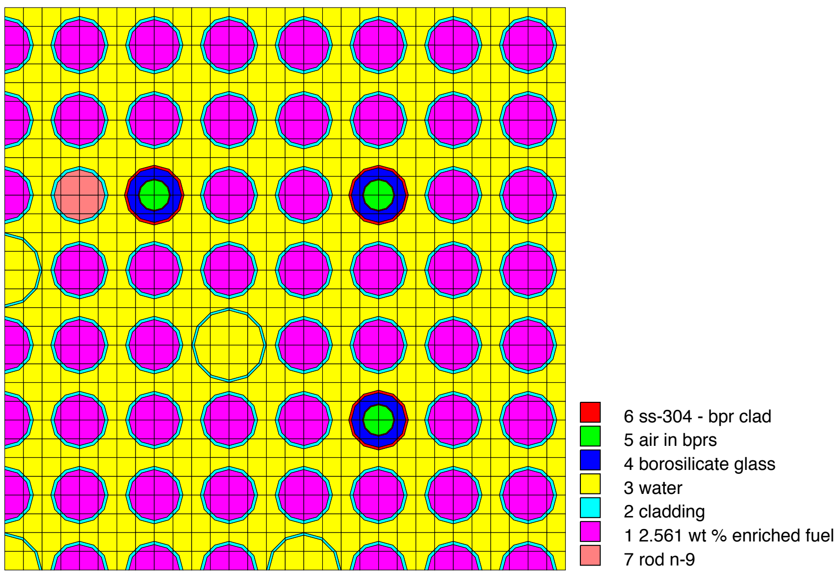
Note: Convergence within $h \cdot \ell$ iterations

SCALE6.1: High-Dimensional Example

Setup: Cross-section computations SCALE6.1

- Input Dimension: 7700
- Output k_{eff}

Materials			Reactions	
$^{234}_{92}U$	$^{10}_{5}B$	$^{31}_{15}P$	Σ_t	$n \to \gamma$
$^{235}_{92}U$	$^{11}_{5}B$	$^{55}_{25}Mn$	Σ_e	$n \to p$
$^{236}_{92}U$	$^{14}_{7}N$	$_{26}Fe$	Σ_f	$n \to d$
$^{238}_{92}U$	$^{15}_{7}N$	$^{116}_{50}Sn$	Σ_c	$n \to t$
$^{1}_{1}H$	$^{23}_{11}Na$	$^{120}_{50}Sn$	$\bar{\nu}$	$n \to {}^3He$
$^{16}_{8}O$	$^{27}_{13}Al$	$_{40}Zr$	χ	$n \to \alpha$
$_{6}C$	$_{14}Si$	$_{19}K$	$n \to n'$	$n \to 2n$



PWR Quarter Fuel Lattice

Note: We cannot efficiently approximate all directional derivatives required to approximate the gradient matrix. Requires efficient initialization algorithm.

SCALE6.1: High-Dimensional Example

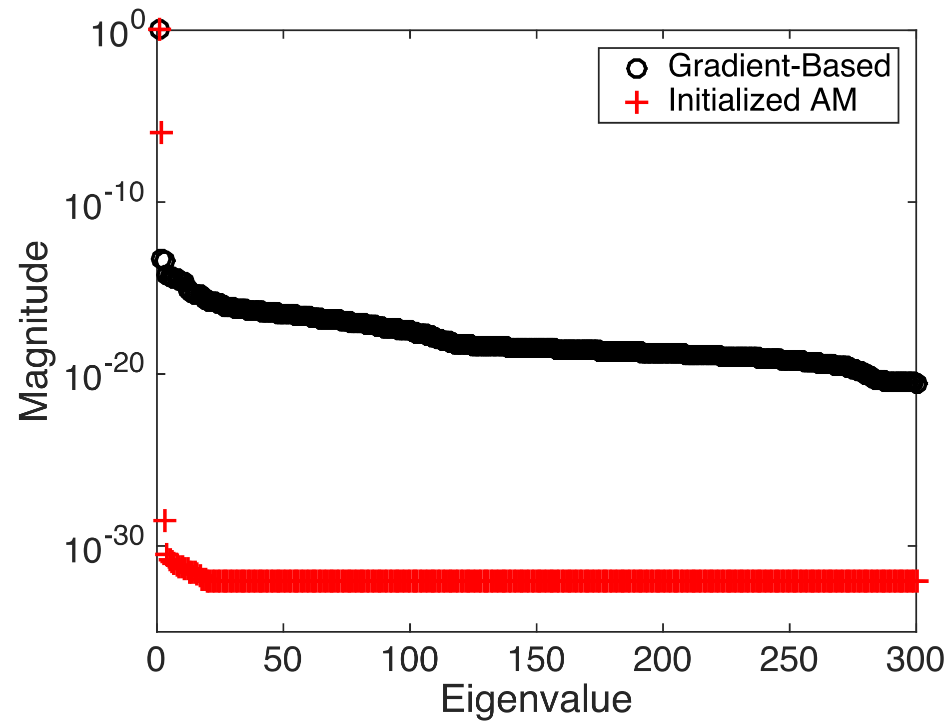
Setup:

- Input Dimension: 7700

SCALE Evaluations:

- Gradient-Based: 1000
- Initialized Adaptive Morris: 18,392
- Projected Finite-Difference: 7,701,000

Note: Analytic eigenvalues: 0, 1



Active Subspace Dimensions:

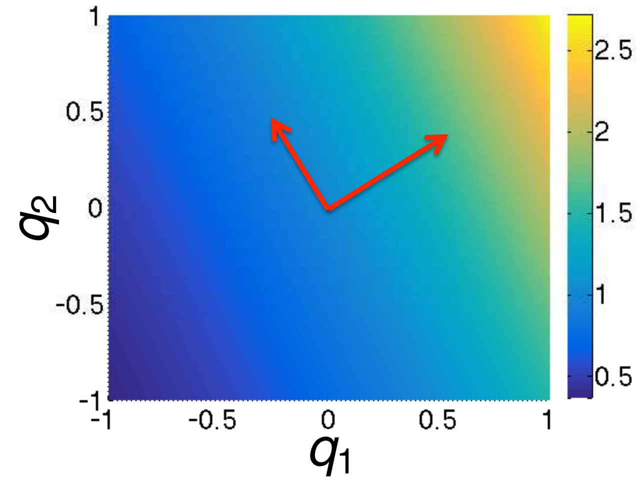
For surrogate sampled off space

	Gap	PCA				Error Tolerance			
Method		0.75	0.90	0.95	0.99	10^{-3}	10^{-4}	10^{-5}	10^{-6}
Gradient-Based	1	2	6	9	24	1	13	90	233
Initialized AM	1	1	1	1	2	1	2	2	2

Notes: Computing *converged* adjoint solution is expensive and *often not achieved*

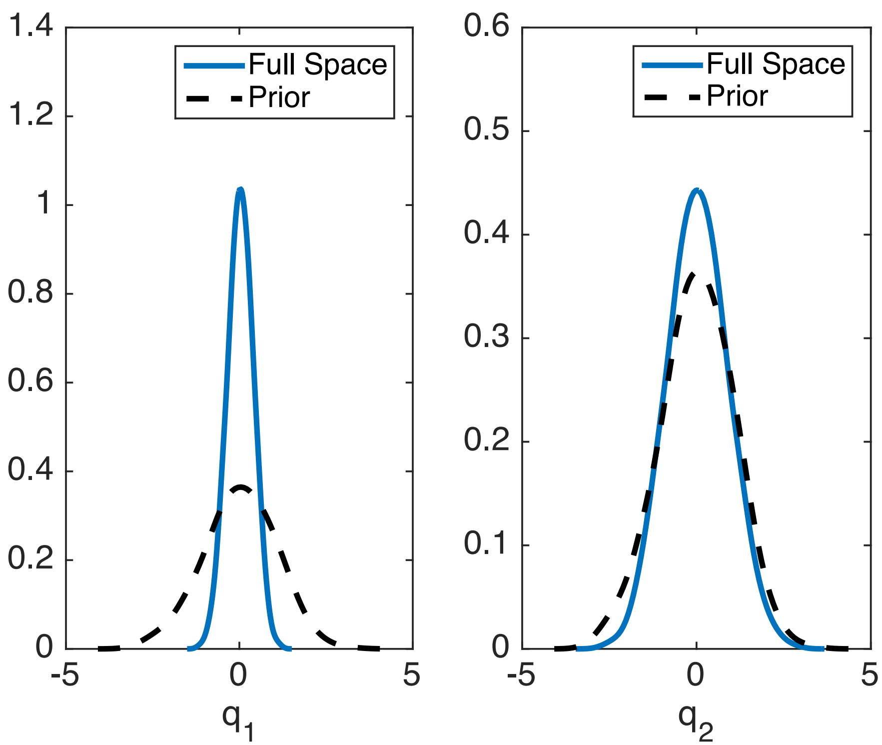
Bayesian Inference on Active Subspaces

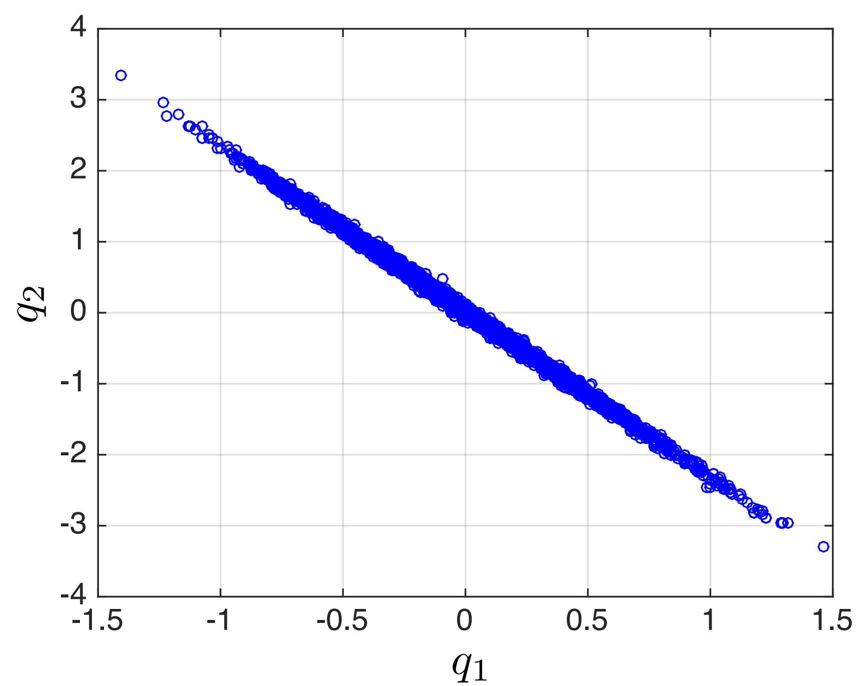
Example: $y = \exp(0.7q_1 + 0.3q_2)$



Full Space Inference:

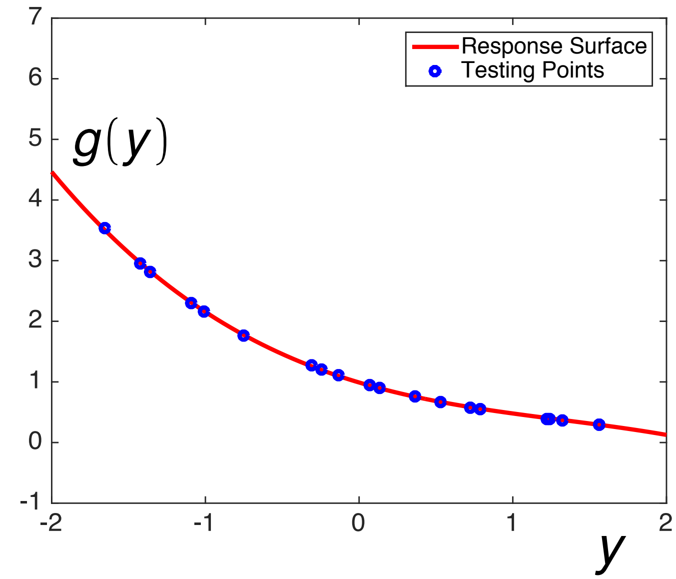
- Parameters not jointly identifiable
- Result: Prior for 2nd parameter is minimally informed.
- Goal: Use active subspace to quantify parameter sensitivity and guide inference.





Bayesian Inference on Active Subspaces

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



Active Subspace: For gradient matrix G, form SVD

$$G = U \Lambda V^T$$

Eigenvalue spectrum indicates 1-D active subspace with basis

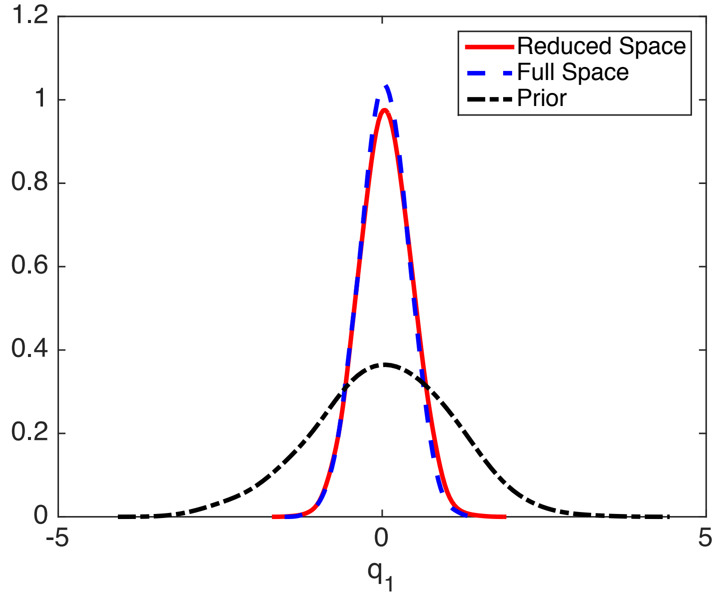
$$U(:,1) = [0.91 \ , \ 0.39]$$

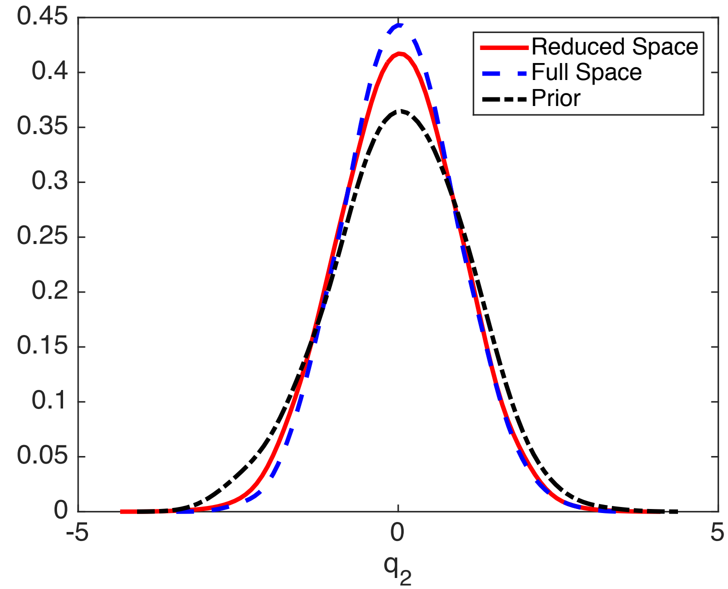
Strategy: Inference based on active subspace

- For values $\{q^j\}_{j=1}^M$, compute $y^j = U(:,1)^T q^j$ and fit response surface $g(y)$
- Use DRAM to calibrate y
- Because model is "invariant" to $z = U(:,2)^T q$, draw $\{z^j\} \sim N(0,1)$
- Transform to $q^j = U(:,1) y^j + U(:,2) z^j$ to obtain posterior densities for physical parameters

Bayesian Inference on Active Subspaces

Results: Inference based on active subspace





Global Sensitivity: For active subspace of dimension N, consider vector of activity scores

$$\alpha(N) = \sum_{j=1}^{N} \lambda_j w_j^2$$

Note: Here N = 1 and $w_j^2 = U(:,1).*U(:,1) = [0.91^2\ ,\ 0.39^2]$

Conclusion: First parameter is more influential and better informed during Bayesian inference.

Bayesian Inference on Active Subspaces

Example: Family of elliptic PDE's

$$-\nabla_s \cdot (a(s,n)\nabla_s u(s,a(s,n))) = 1 \quad , s \in [0,1]^2 \, , n = 1, \ldots , N$$

with the random field representations

$$\log(a(s,n)) = \sum_{i=1}^{p} q_i^n \gamma_i \phi_i(s)$$

Quantity of interest: e.g., strain along edge at N levels

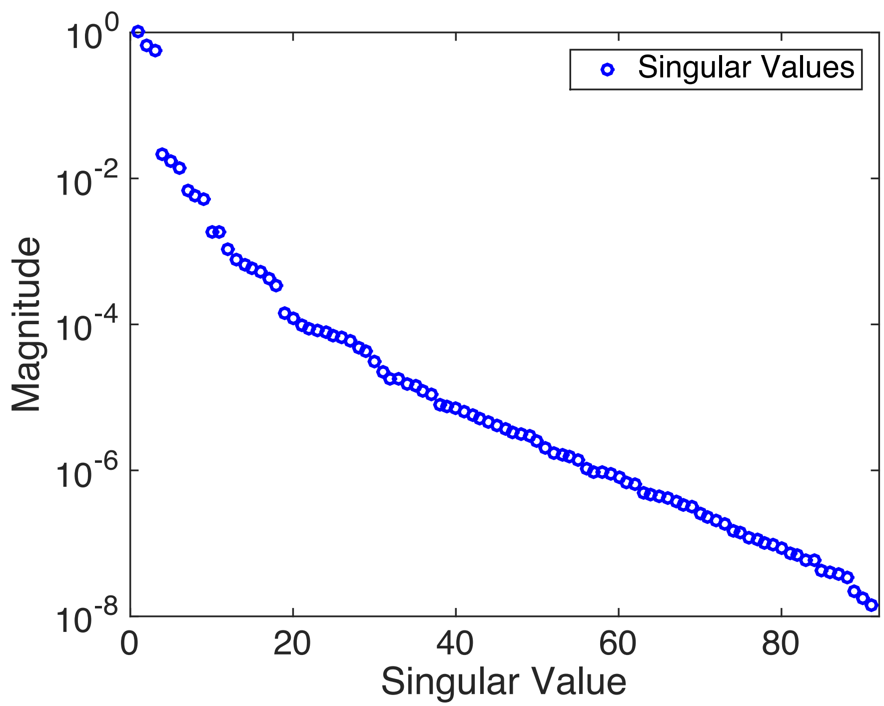
$$f\left(q^1, \ldots , q^N\right) \approx \sum_{n=1}^{N} \frac{1}{|\Gamma_2|} \int_{\Gamma_2} u(a(s,n))ds$$

Problem Dimensions:

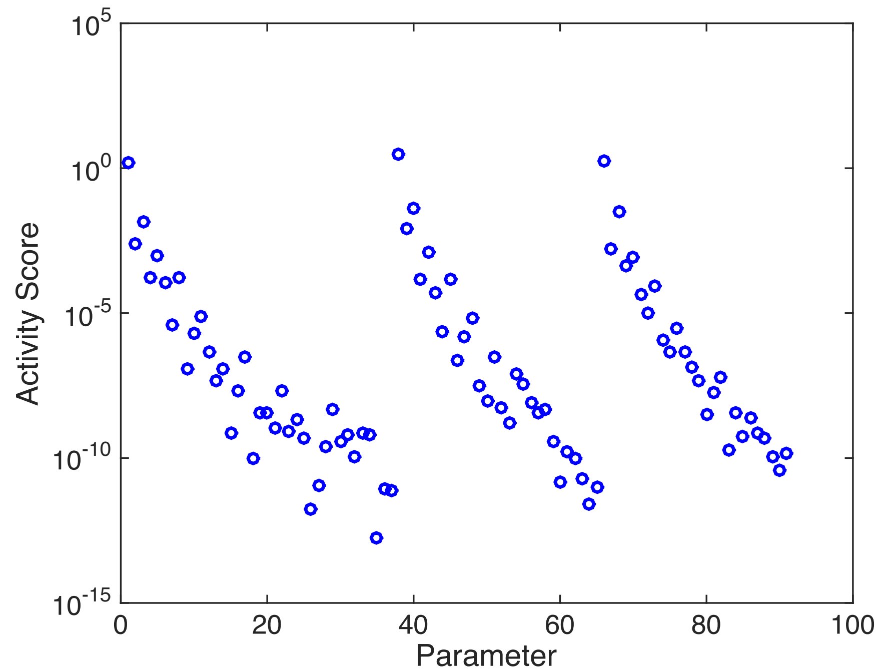
- Parameter dimension: p = 91
- Active subspace dimension: N = 3
- Finite element space: 1372 triangular elements, 727 nodes

Bayesian Inference on Active Subspaces

Singular Values: Recall N = 3



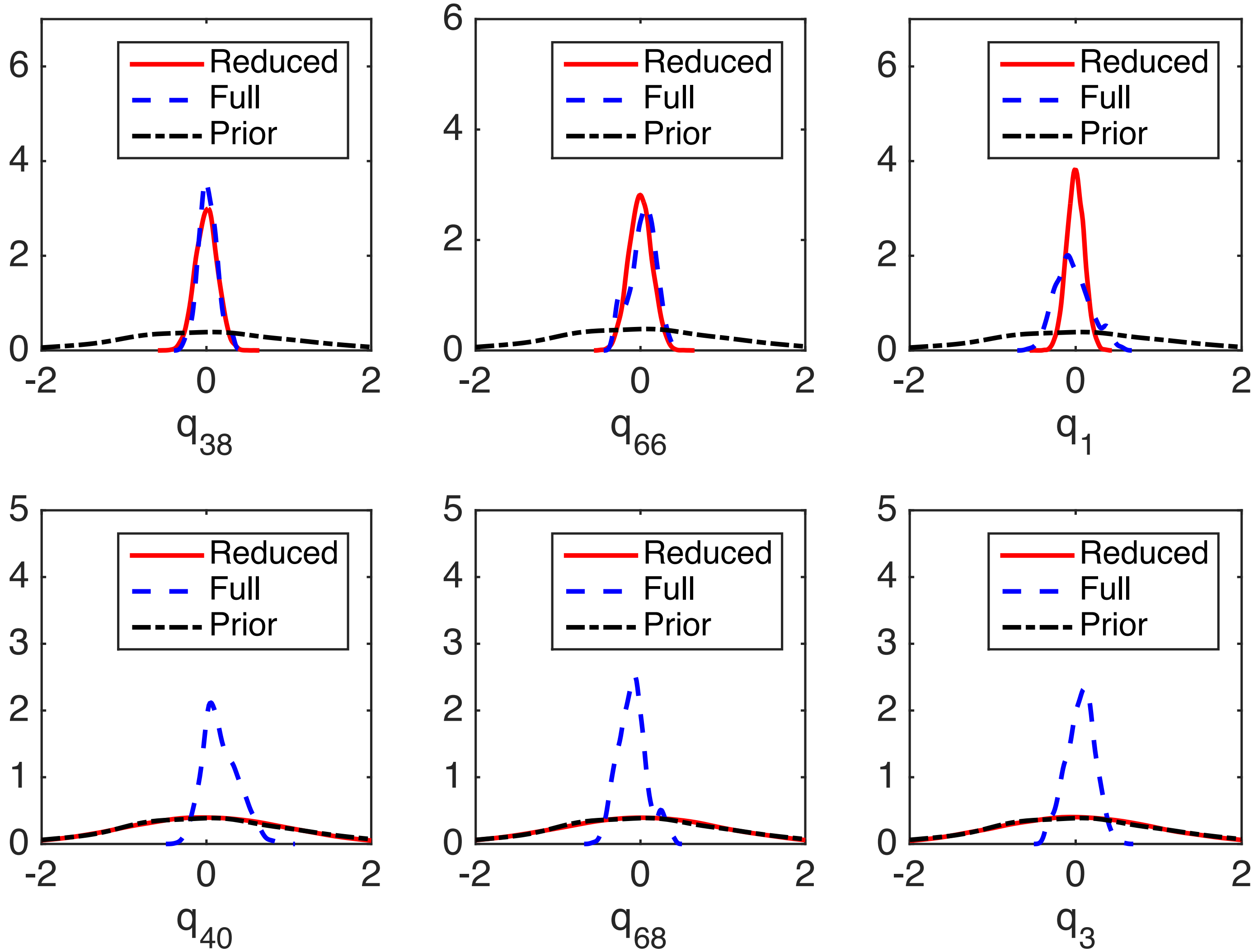
Activity Scores: Quantify global sensitivity



Conclusion: Parameters 1, 38, 66 are most influential and will be primarily informed during Bayesian inference

Bayesian Inference on Active Subspaces

Recall: Parameters 1, 38, 66 are most influential and will be primarily informed during Bayesian inference



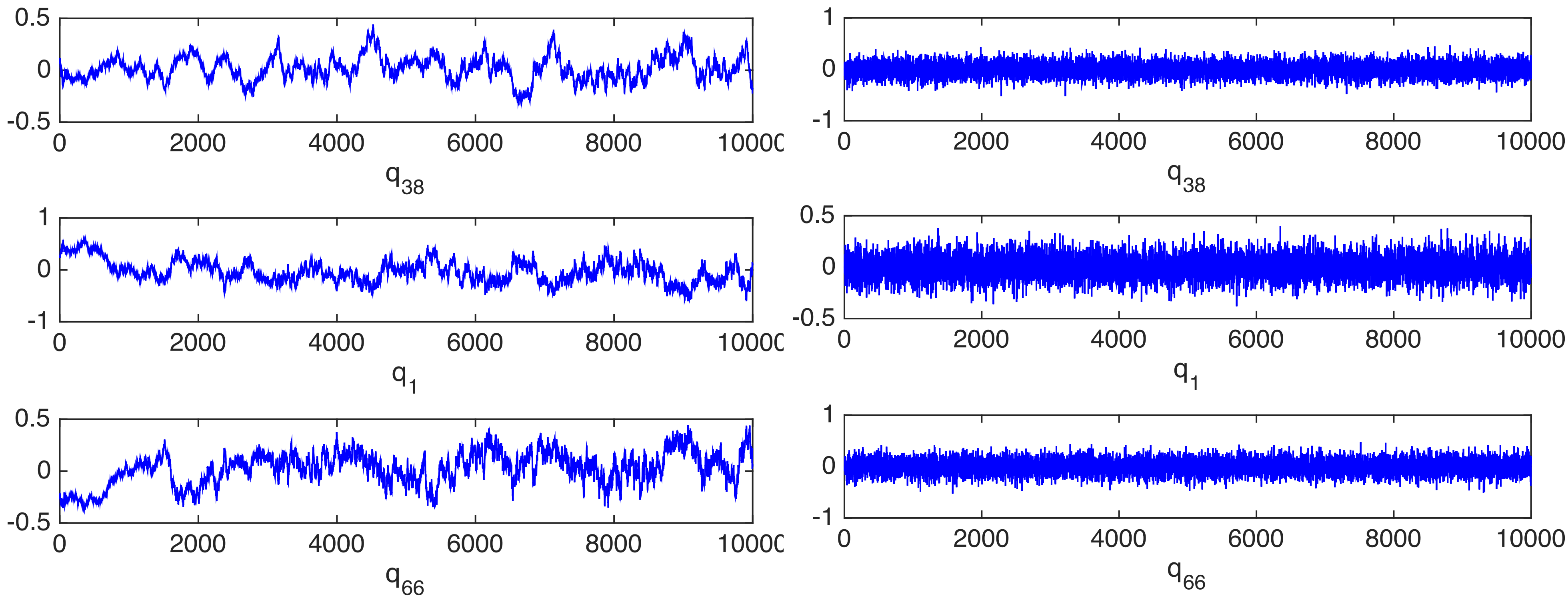
Note:

- Full space: 18 hours
- Reduced: 20 seconds

Bayesian Inference on Active Subspaces

Note:

- Chains for full space not converging well due to parameter nonidentifiability
- Hence full space inference is less reliable



Full Space Active Subspace