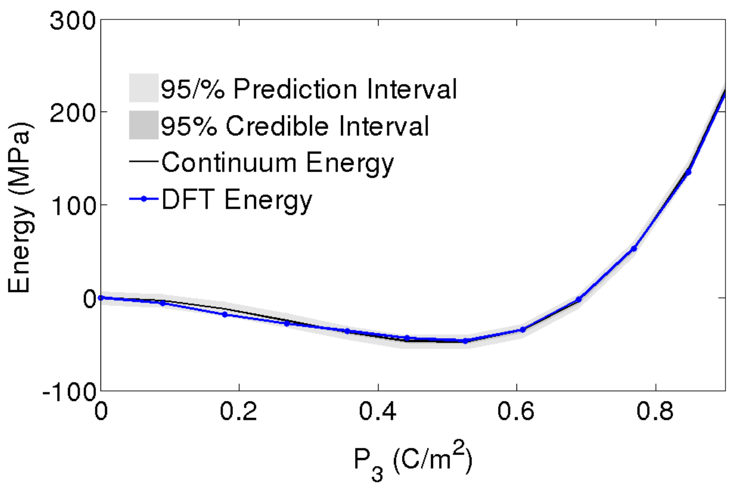
Quantum-Informed Continuum Models

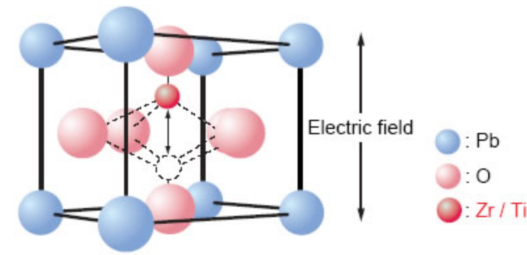
Objectives:

- Employ density function theory (DFT) to construct/calibrate continuum energy relations.
  - e.g., Landau energy

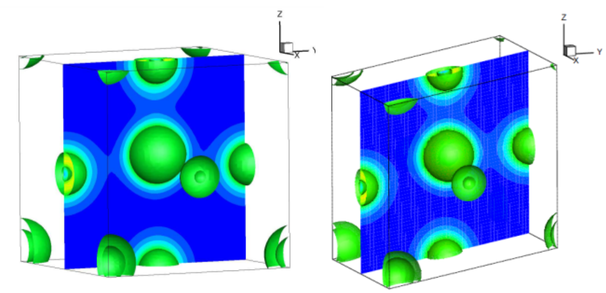
$$\psi(P) = \alpha_1 P^2 + \alpha_{11} P^4 + \alpha_{111} P^6$$



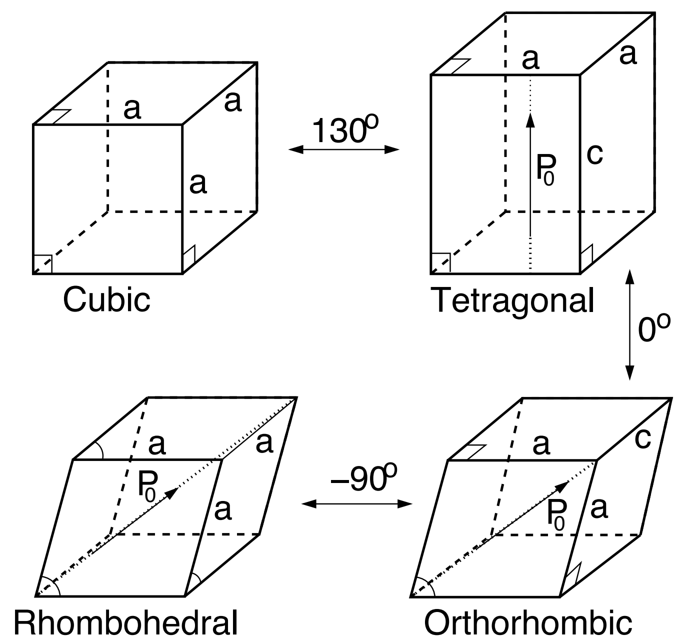
Landau energy



Lead Titanate Zirconate (PZT)



DFT Electronic Structure Simulation



UQ and SA Issues:

- Is 6th order term required to accurately characterize material behavior?

- **Note:** Determines molecular structure

Global Sensitivity Analysis: Analysis of Variance

Sobol' Representation: $Y = f(q)$

$$f(q) = f_0 + \sum_{i=1}^{p} f_i(q_i) + \sum_{i \leqslant i < j \leqslant p} f_{ij}(q_i, q_j) + \cdots + f_{12\cdots p}(q_1, \ldots, q_p)$$

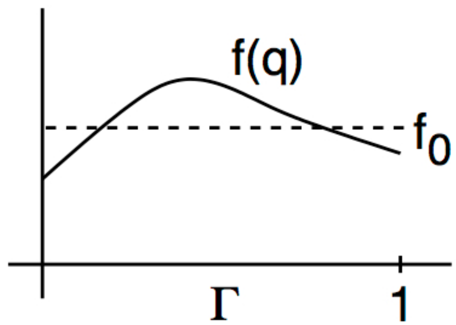
$$= f_0 + \sum_{i=1}^{p} \sum_{|u|=i} f_u(q_u)$$

where

$$f_0 = \int_\Gamma f(q)\rho(q)dq = \mathbb{E}[f(q)]$$

$$f_i(q_i) = \mathbb{E}[f(q)|q_i] - f_0$$

$$f_{ij}(q_i, q_j) = \mathbb{E}[f(q)|q_i, q_j] - f_i(q_i) - f_j(q_j) - f_0$$



Typical Assumption: $q_1, q_2, \ldots, q_p$ independent. Then

$$\int_\Gamma f_u(q_u) f_v(q_v)\rho(q)dq = 0 \quad \text{for } u \neq v$$

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

Sobol' Indices:

$$S_u = \frac{\text{var}[f_u(q_u)]}{\text{var}[f(q)]} \quad , \quad T_u = \sum_{v \subseteq u} S_v$$

Note: Magnitude of S_i, T_i quantify contributions of q_i to $\text{var}[f(q)]$

Global Sensitivity Analysis

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:

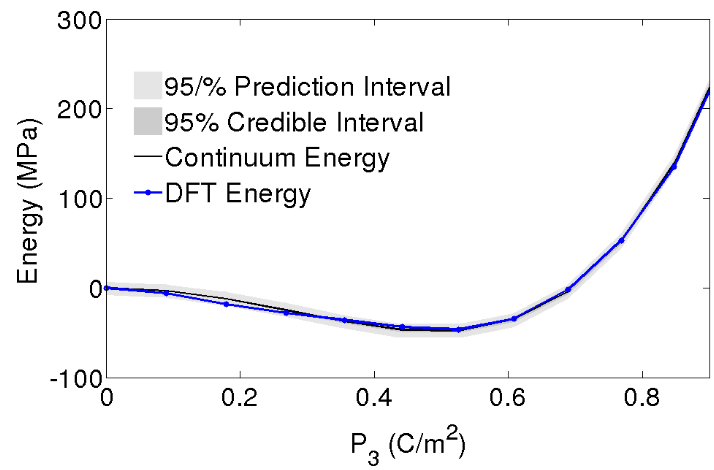
$$q = [\alpha_1, \alpha_{11}, \alpha_{111}]$$

Global Sensitivity Analysis:

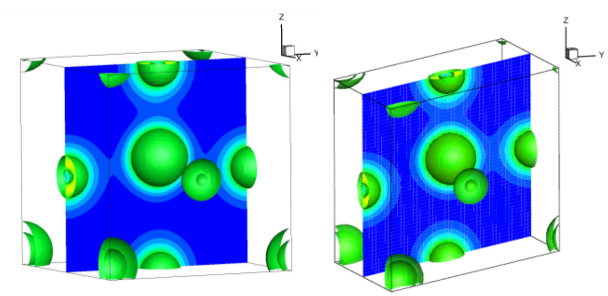
	α_1	α_{11}	α_{111}
S_k	0.62	0.39	0.01
T_k	0.66	0.38	0.06
μ_k^*	0.17	0.07	0.03

Conclusion:

α_{111} insignificant and can be fixed



Landau energy



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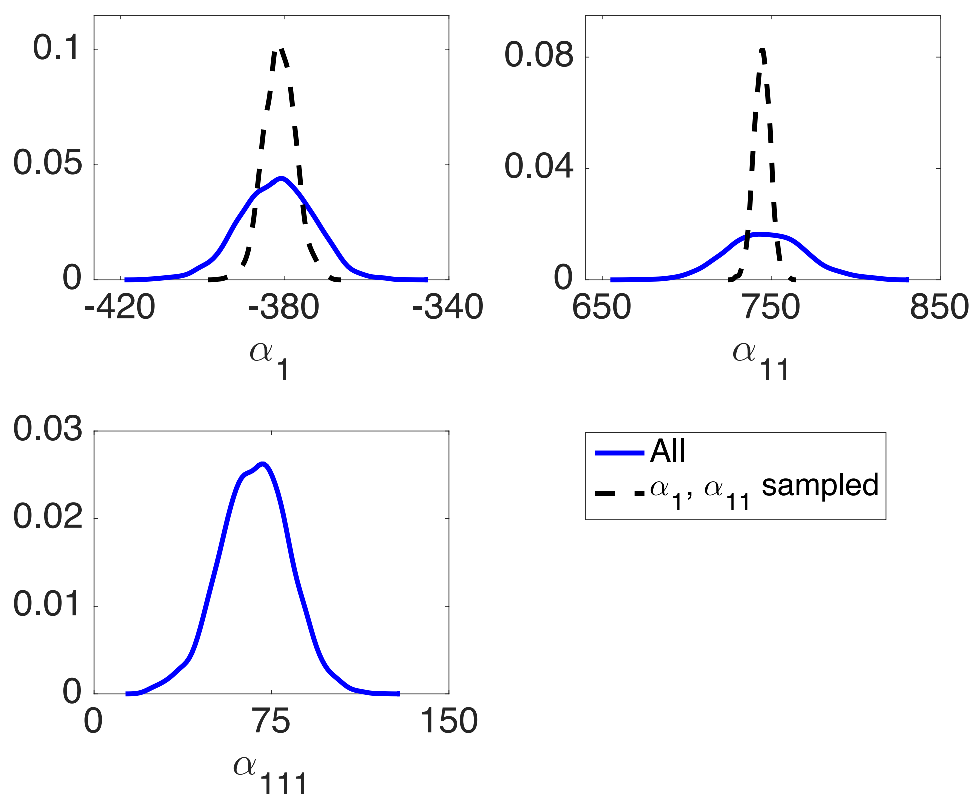
Problem: We obtain different distributions when we perform Bayesian inference with fixed non-influential parameters



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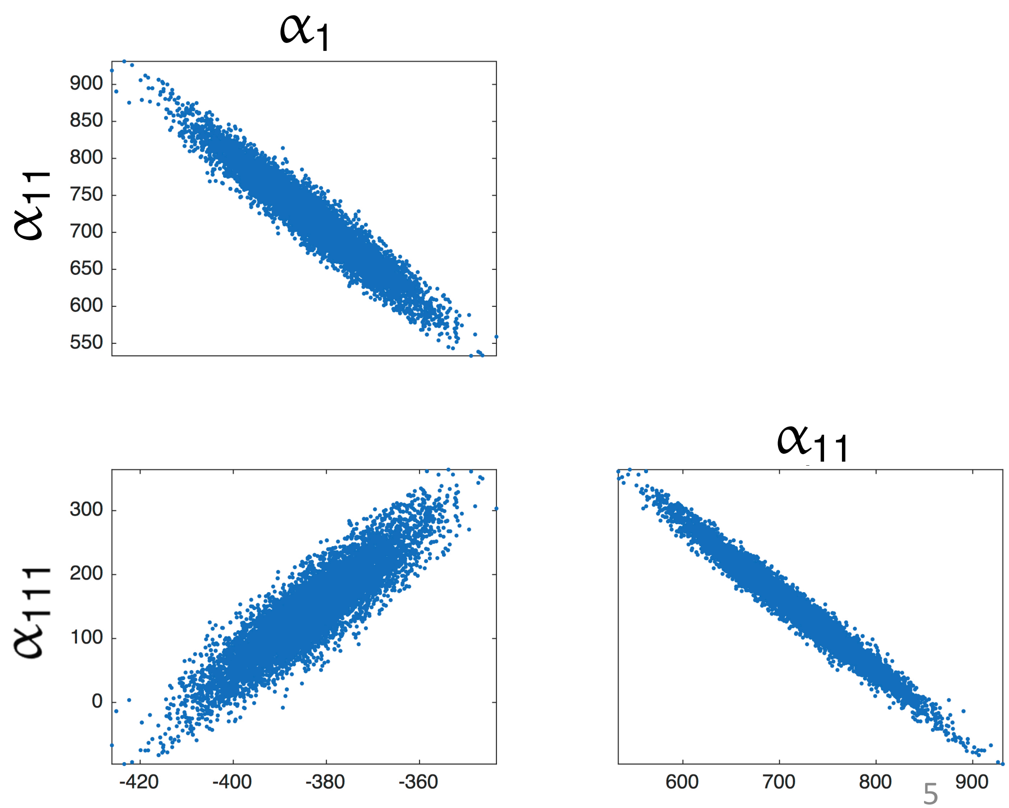
Note: Must accommodate correlation

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.

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.

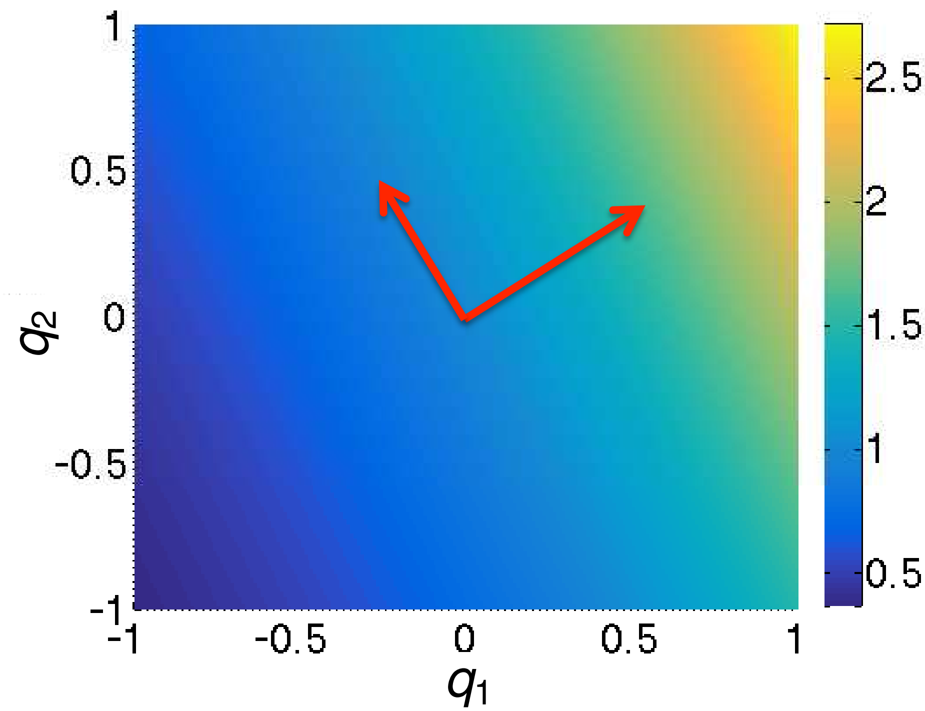
Active Subspaces

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



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.

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

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

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

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

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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

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

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

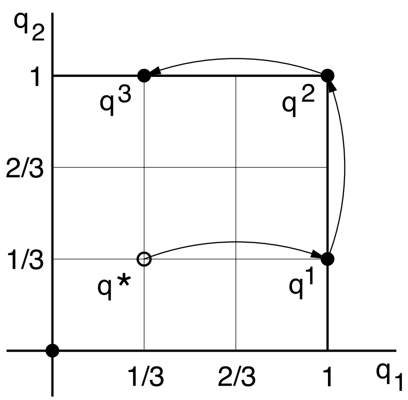
One Goal: Develop efficient algorithm for codes that do not have adjoint capabilities

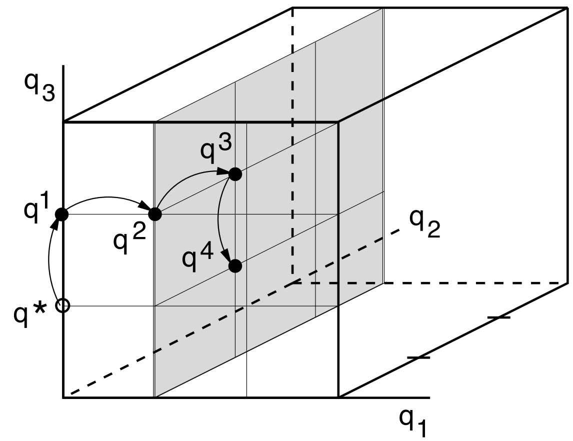
Note: Finite-difference approximations tempting but not effective for high-D

Strategy: Algorithm based on initialized adaptive Morris indices

Morris Screening: Random Sampling of Approximated Derivatives

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





Elementary Effect:

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

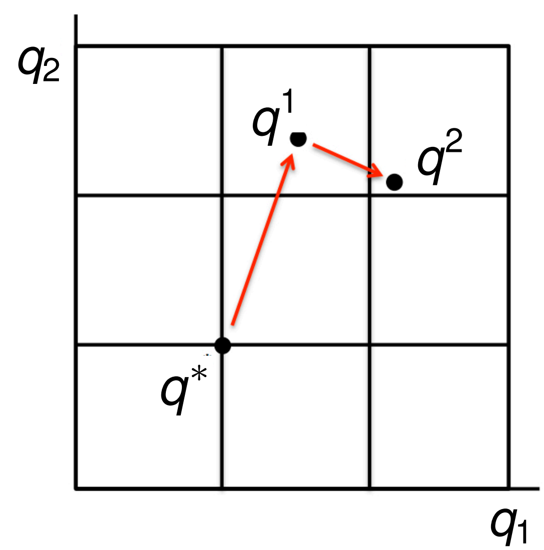
Global Sensitivity Measures: r samples

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

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

Adaptive Algorithm:

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



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