Parameter Selection Techniques

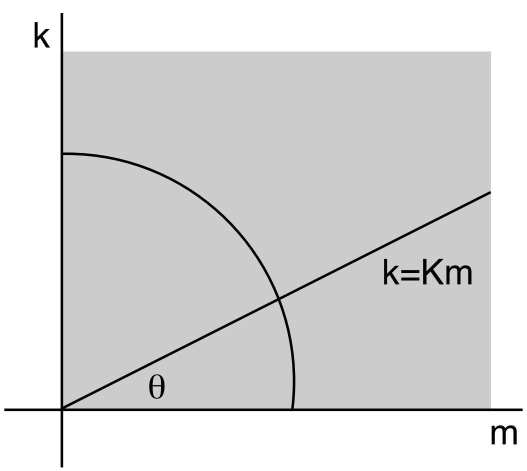
Motivation: Consider spring model

$$m\frac{d^2z}{dt^2} + kz = 0$$
$$z(0) = z_0 \ , \ \frac{dz}{dt}(0) = 0$$

with solution $z(t) = z_0 \cos(\sqrt{k/m} \cdot t)$.

Observation: Parameters q = [k,m] not uniquely determined by displacement data.

Admissible Parameter Space: $\mathbb{Q} = (0,\infty) \times (0,\infty)$



Note: Determination of slope equivalent to specifying θ

$$I(q) = \{\theta = \arctan(k/m) \,|\, 0 < \theta < \pi/2\}$$
$$NI(q) = \left\{r = \sqrt{k^2+m^2} \,|\, r > 0\right\}$$

Note: $\mathbb{Q} = I(q) \oplus NI(q)$

Parameter Selection Techniques

HIV Model:

$$\dot{T}_1 = \lambda_1 - d_1 T_1 - (1-\varepsilon) k_1 V T_1$$

$$\dot{T}_2 = \lambda_2 - d_2 T_2 - (1-f\varepsilon) k_2 V T_2$$

$$\dot{T}_1^* = (1-\varepsilon) k_1 V T_1 - \delta T_1^* - m_1 E T_1^*$$

$$\dot{T}_2^* = (1-f\varepsilon) k_2 V T_2 - \delta T_2^* - m_2 E T_2^*$$

$$\dot{V} = N_T \delta (T_1^* + T_2^*) - cV - [(1-\varepsilon)\rho_1 k_1 T_1 + (1-f\varepsilon)\rho_2 k_2 T_2] V$$

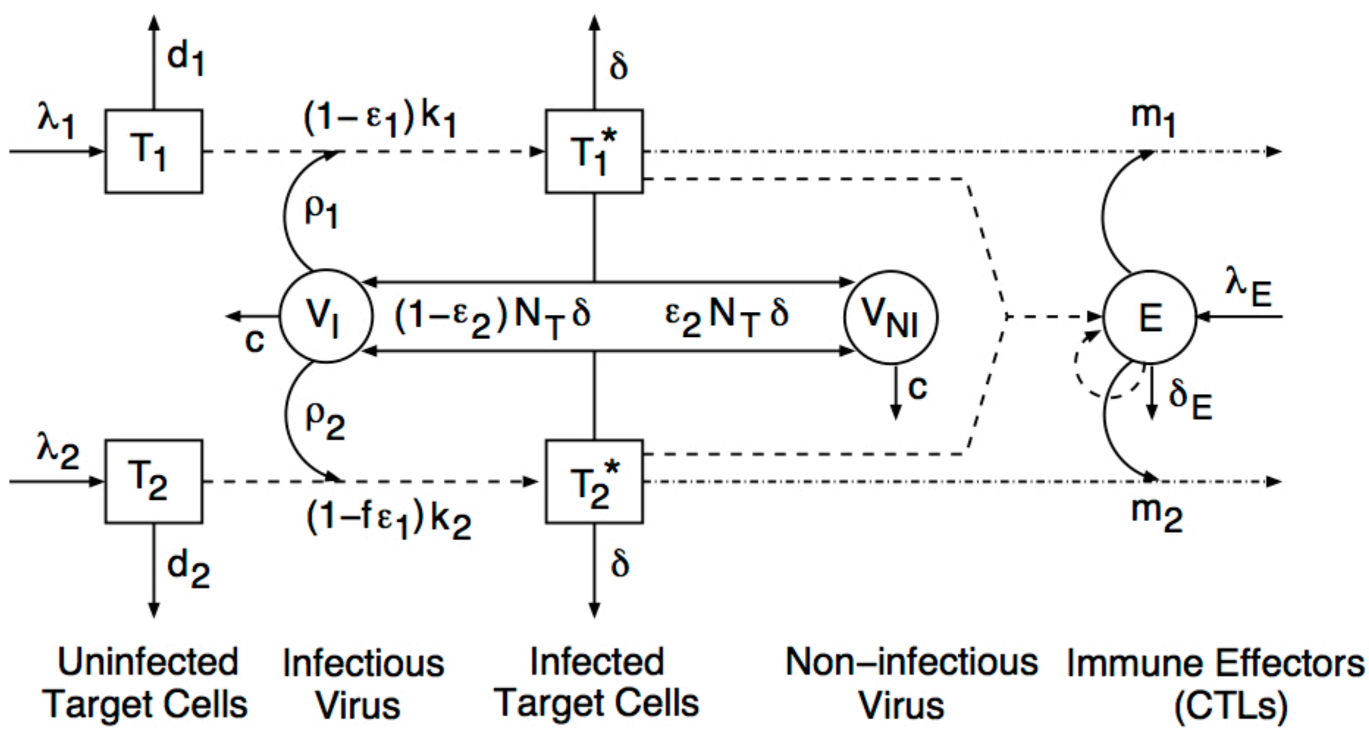
$$\dot{E} = \lambda_E + \frac{b_E (T_1^* + T_2^*)}{T_1^* + T_2^* + K_b} E - \frac{d_E (T_1^* + T_2^*)}{T_1^* + T_2^* + K_d} E - \delta_E E$$

Notes: 21 parameters

[Adams, Banks et al., 2005]

Notation: $\dot{E} \equiv \frac{dE}{dt}$

Compartments:



Parameter Selection Techniques

HIV Model: Used for characterization and control treatment regimes.

$$\dot{T}_1 = \lambda_1 - d_1 T_1 - (1-\varepsilon) k_1 V T_1$$

$$\dot{T}_2 = \lambda_2 - d_2 T_2 - (1-f\varepsilon) k_2 V T_2$$

$$\dot{T}_1^* = (1-\varepsilon) k_1 V T_1 - \delta T_1^* - m_1 E T_1^*$$

$$\dot{T}_2^* = (1-f\varepsilon) k_2 V T_2 - \delta T_2^* - m_2 E T_2^*$$

$$\dot{V} = N_T \delta (T_1^* + T_2^*) - cV - [(1-\varepsilon)\rho_1 k_1 T_1 + (1-f\varepsilon)\rho_2 k_2 T_2] V$$

$$\dot{E} = \lambda_E + \frac{b_E (T_1^* + T_2^*)}{T_1^* + T_2^* + K_b} E - \frac{d_E (T_1^* + T_2^*)}{T_1^* + T_2^* + K_d} E - \delta_E E$$

Parameters: Most are unknown and must be estimated from data

λ_1	Target cell 1 production rate	ρ_1	Ave. virions infecting type 1 cell
λ_2	Target cell 2 production rate	ρ_2	Ave. virions infecting type 2 cell
d_1	Target cell 1 death rate	b_E	Max. birth rate immune effectors
d_2	Target cell 2 death rate	d_E	Max. death rate immune effectors
k_1	Population 1 infection rate	K_b	Birth constant, immune effectors
k_2	Population 2 infection rate	K_d	Death constant, immune effectors
c	Virus natural death rate	λ_E	Immune effector production rate
δ	Infected cell death rate	δ_E	Natural death rate, immune effectors
ε	Population 1 treatment efficacy	N_T	Virions produced per infected cell
m_1	Population 1 clearance rate	f	Treatment efficacy reduction
m_2	Population 2 clearance rate		

Pressurized Water Reactors (PWR)

3-D Neutron Transport Equations:

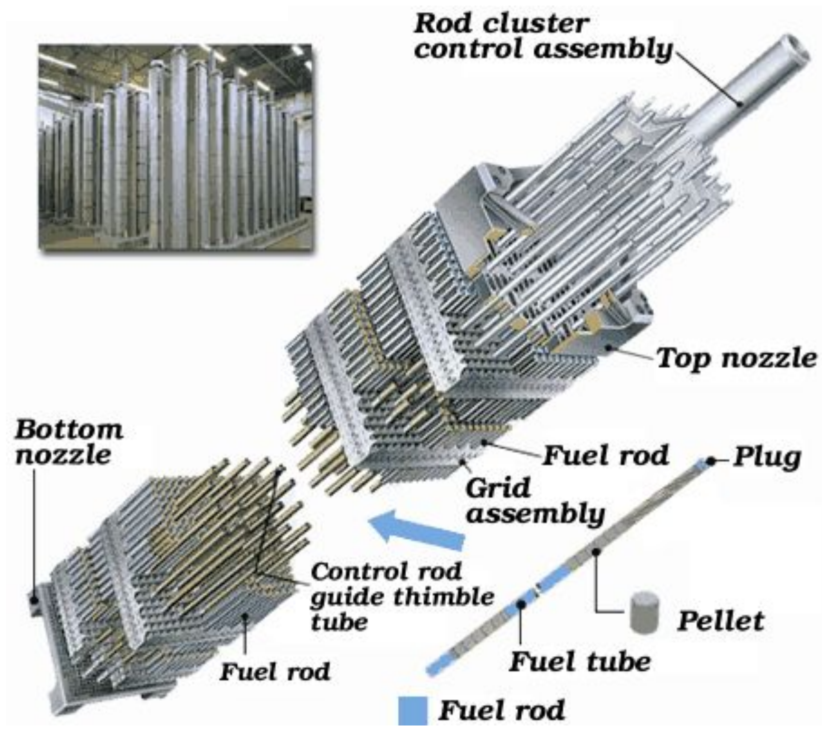
$$\frac{1}{|v|}\frac{\partial\varphi}{\partial t} + \Omega\cdot\nabla\varphi + \Sigma_t(r,E)\varphi(r,E,\Omega,t)$$
$$= \int_{4\pi} d\Omega' \int_0^\infty dE' \Sigma_s(E'\to E, \Omega'\to\Omega)\varphi(r,E',\Omega',t)$$
$$+ \frac{\chi(E)}{4\pi}\int_{4\pi} d\Omega' \int_0^\infty dE' \nu(E')\Sigma_f(E')\varphi(r,E',\Omega',t)$$

Challenges:

- Linear in the state but function of 7 independent variables:

$$r = x,y,z; E; \Omega = \theta,\phi; t$$

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



- SCALE TRITON has adjoint capabilities via TSUNAMI-2D and NEWT.

Parameter Subspaces

Definition: Consider

$$y = f(q) \quad , \; q = [q_1, ..., q_p]$$

The parameters are identifiable at q^* if $f(q) = f(q^*)$ implies that $q = q^*$ for all admissible $q \in \mathbb{Q}$. The parameters are identifiable with respect to a space $I(q)$, termed the identifiable subspace, if this holds for all $q^* \in I(q)$. The nonidentifiable subspace $NI(q)$ is the orthogonal complement of $I(q)$ with respect to $\mathbb{Q}$.

Example: Consider $q = [q_1, q_2]$ in $\mathbb{Q} = \mathbb{R}^2$ and $y = q_1$. Then

$$NI(q) = \{q_2 \in \mathbb{R}\} \, , \; I(q) = \{q_1 \in \mathbb{R}\}$$

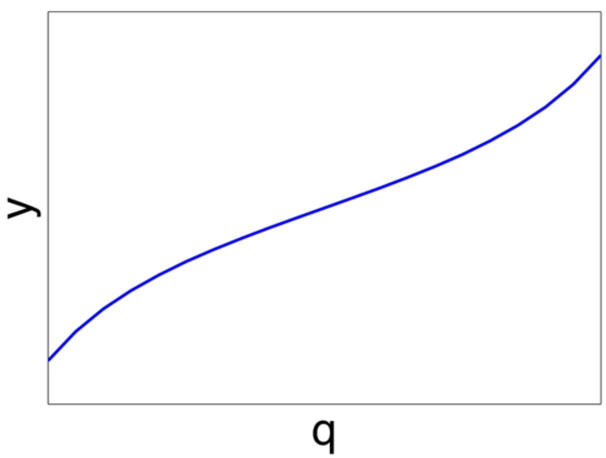
Example: Take $y = q_1 - q_2$. Then

$$NI(q) = \{(q_1, q_2) \in \mathbb{R}^2 \,|\, q_1 = q_2\}$$

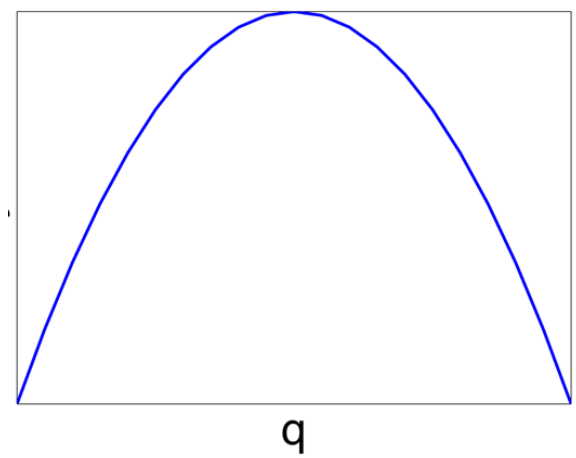
$$I(q) = \{(q_1, q_2) \in \mathbb{R}^2 \,|\, q_1 = -q_2\}$$

Parameter Subspaces

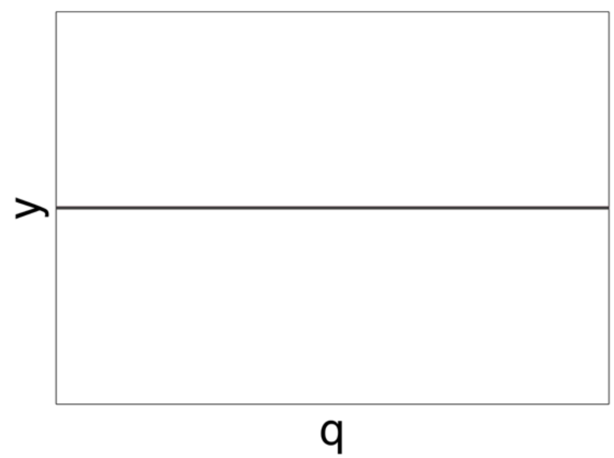
Definition: The parameters $q = [q_1, \ldots, q_p]$ are noninfluential on the space $\mathcal{NI}(q)$ if $|f(q) - f(q^*)| < \varepsilon$ for all $q, q^* \in \mathcal{NI}(q)$. The space $\mathcal{I}(q)$ of influential parameters is the orthogonal complement of $\mathcal{NI}(q)$ with respect to $\mathbb{Q}$ using the Euclidean inner product.



Identifiable



Unidentifiable
(Non-identifiable)

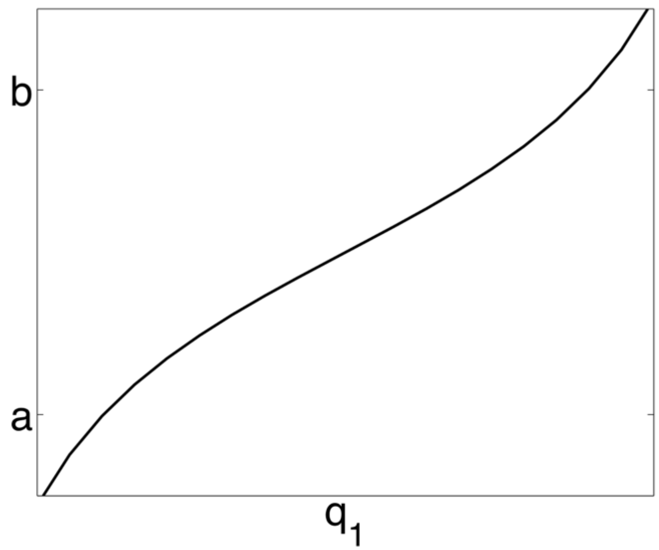


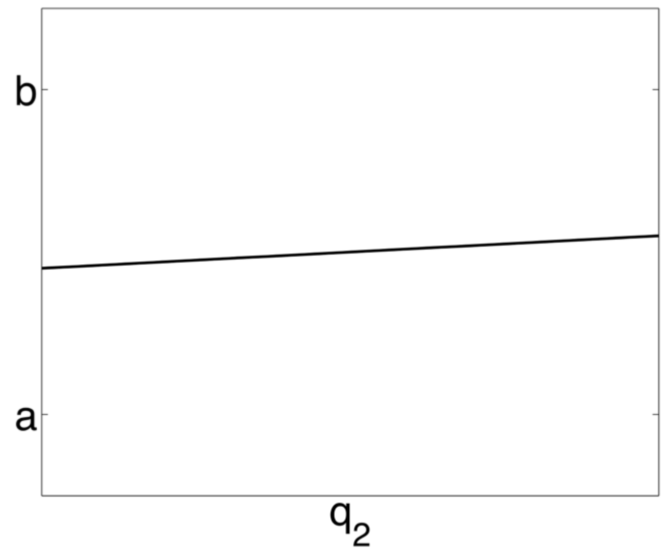
Noninfluential

Parameter Subspaces

Definition: The parameters $q = [q_1, ..., q_p]$ are noninfluential on the space $\mathcal{NI}(q)$ if $|f(q) - f(q^*)| < \varepsilon$ for all $q, q^* \in \mathcal{NI}(q)$. The space $\mathcal{I}(q)$ of influential parameters is the orthogonal complement of $\mathcal{NI}(q)$ with respect to $\mathbb{Q}$ using the Euclidean inner product.

Note: q_1 is more influential than q_2





Parameter Selection Techniques

Techniques: $y = f(q)$

1. Local sensitivity analysis: Based on derivatives $\dfrac{\partial y}{\partial q_i}$

2. Global sensitivity analysis: Quantifies how uncertainties in model outputs are apportioned to uncertainties in model inputs; e.g., ANOVA

3. Active subspace techniques based on QR or SVD

Note: 1 and 2 determine subsets of parameters whereas 3 determines subspace

Local Sensitivity Analysis

Strategy: Approximate derivatives

$$s_i = \frac{\partial f}{\partial q_i}(q^*)$$

Issues:

- Does not quantify uncertainties
- Local at q^*

Example: Spring model

$$\frac{d^2z}{dt^2} + C\frac{dz}{dt} + Kz = 0$$

$$z(0) = 2 \, , \; \frac{dz}{dt}(0) = -C$$

Displacement Observations:

$$y = [1 \;\; 0]\begin{bmatrix} z \\ \dot{z} \end{bmatrix} = z$$

Then $y(t) = 2e^{-Ct/2}\cos\left(\sqrt{K - C^2/4} \cdot t\right)$

Techniques to Compute Local Sensitivities:

1. Analytic
2. Sensitivity equations
3. Finite-difference or complex step
4. Automatic differentiation

Techniques for Local Sensitivity Analysis

1. Analytic: Use symbolic package; e.g., Maple, Mathematica

$$\frac{\partial y}{\partial K} = \frac{-2t}{\sqrt{4K - C^2}} e^{-Ct/2} \sin\left(\sqrt{K - C^2/4} \cdot t\right)$$

$$\frac{\partial y}{\partial C} = e^{-Ct/2}\left[\frac{Ct}{\sqrt{4K - C^2}} \sin\left(\sqrt{K - C^2/4} \cdot t\right) - t\cos\left(\sqrt{K - C^2/4} \cdot t\right)\right]$$

Sensitivity Matrix: $q = (C, K)$

$$\chi(q) = \begin{bmatrix} \frac{\partial y}{\partial C}(t_1, q^*) & \frac{\partial y}{\partial K}(t_1, q^*) \\ \vdots & \vdots \\ \frac{\partial y}{\partial C}(t_n, q^*) & \frac{\partial y}{\partial K}(t_n, q^*) \end{bmatrix}$$

Fisher Information Matrix: $\mathcal{F} = \chi^T \chi$

Techniques for Local Sensitivity Analysis

2. Sensitivity Equations:

$$\frac{d}{dK}\left[\frac{d^2 z}{dt^2} + C\frac{dz}{dt} + Kz\right] = 0$$

$$\Rightarrow \frac{d^2 z_K}{dt^2} + C\frac{dz_K}{dt} + Kz_K = -z \quad , \; z_K \equiv \frac{\partial z}{\partial K}$$

System:

$$\frac{d^2 z_K}{dt^2} + C\frac{dz_K}{dt} + Kz_K = -z \quad , \; z_K(0) = \frac{dz_K}{dt}(0) = 0$$

$$\frac{d^2 z}{dt^2} + C\frac{dz}{dt} + Kz = 0 \quad z(0) = 2, \frac{dz}{dt}(0) = 0$$

Similarly:

$$\frac{d^2 z_C}{dt^2} + C\frac{dz_C}{dt} + Kz_C = -\frac{dz}{dC} \quad , \; z_C \equiv \frac{\partial z}{\partial C}$$

$$z_C(0) = 0 \; , \; \frac{dz_C}{dt}(0) = -1$$

Techniques for Local Sensitivity Analysis

3. Finite-Difference or Complex Step:

$$\frac{\partial y}{\partial K}(t) \approx \frac{z(t, K + h_K, C) - z(t, K, C)}{h_K}$$

$$\frac{\partial y}{\partial C}(t) \approx \frac{z(t, K, C + h_C) - z(t, K, C)}{h_C}$$

Issues:

1) Stepsizes h_K, h_C must reflect magnitudes of coefficients; e.g., $h_K = 10^{-6}|K|$

2) $\frac{\text{small}}{\text{small}}$ can be inaccurate

Solution: Complex steps

4. Automatic Differentiation:

• Perform differentiation of basic operations – e.g., addition, subtraction, multiplication, division, composition – at the compiler level;

• Good software for ODE and some for PDE

Fisher Information Matrix

Relate Sensitivities to Taylor Expansion: Note that

$$f(t_i, q) \approx f(t_i, q^*) + \nabla_q(t_i, q^*) \cdot \Delta q$$

where

$$\nabla_q f(t_i, q^*) = \left[\frac{\partial f}{\partial q_1}(t_i, q^*), \ldots, \frac{\partial f}{\partial q_p}(t_i, q^*)\right]$$
$$\Delta q = q - q^*$$

Functional: Since $y_i \approx f(t_i, q^*)$,

$$\begin{aligned} J(q) &= \frac{1}{n}\sum_{i=1}^{n}[y_i - \psi(P_i, q)]]^2 \\ &\approx \frac{1}{n}\sum_{i=1}^{n}[\nabla_q \psi(P_i, q^*) \cdot \Delta q]^2 \\ &= \frac{1}{n}(\chi \Delta q)^T(\chi \Delta q) \end{aligned}$$

Sensitivity Matrix:

$$\chi(q^*) = \begin{bmatrix} \frac{\partial f}{\partial q_1}(t_1, q^*) & \cdots & \frac{\partial f}{\partial q_p}(t_1, q^*) \\ \vdots & & \vdots \\ \frac{\partial f}{\partial q_1}(t_n, q^*) & \cdots & \frac{\partial f}{\partial q_p}(t_n, q^*) \end{bmatrix}_{n \times p}$$

Note:

$$J(q^* + \Delta q) \approx \frac{1}{n}\Delta q^T \chi^T \chi \Delta q$$

Fisher Information Matrix

Note:

$$J(q^* + \Delta q) \approx \frac{1}{n} \Delta q^T \chi^T \chi \Delta q$$

Strategy: Take Δq to be eigenvector of $\boxed{\chi^T \chi}$ Fisher Information

$$\Rightarrow \chi^T \chi \Delta q = \lambda \Delta q$$

$$\Rightarrow J(q^* + \Delta q) \approx \frac{\lambda}{n} \|\Delta q\|_2^2$$

Note: $\lambda \approx 0 \Rightarrow$ Perturbations $J(q^* + \Delta q) \approx 0$

$\Rightarrow$ Nonidentifiable

Note: Estimator for covariance matrix

$$V = s^2 \left[\chi^T \chi\right]^{-1} = \begin{bmatrix} \mathrm{var}(q_1) & \mathrm{cov}(q_1, q_2) & \cdots & \mathrm{cov}(q_1, q_n) \\ \mathrm{cov}(q_2, q_1) & \mathrm{var}(q_2) & \mathrm{cov}(q_2, q_3) & \\ \vdots & & & \vdots \\ \mathrm{cov}(q_n, q_1) & \cdots & \cdots & \mathrm{var}(q_n) \end{bmatrix}$$

Parameter Subset Selection

Note:

$$J(q^* + \Delta q) \approx \frac{1}{n} \Delta q^T \chi^T \chi \Delta q$$

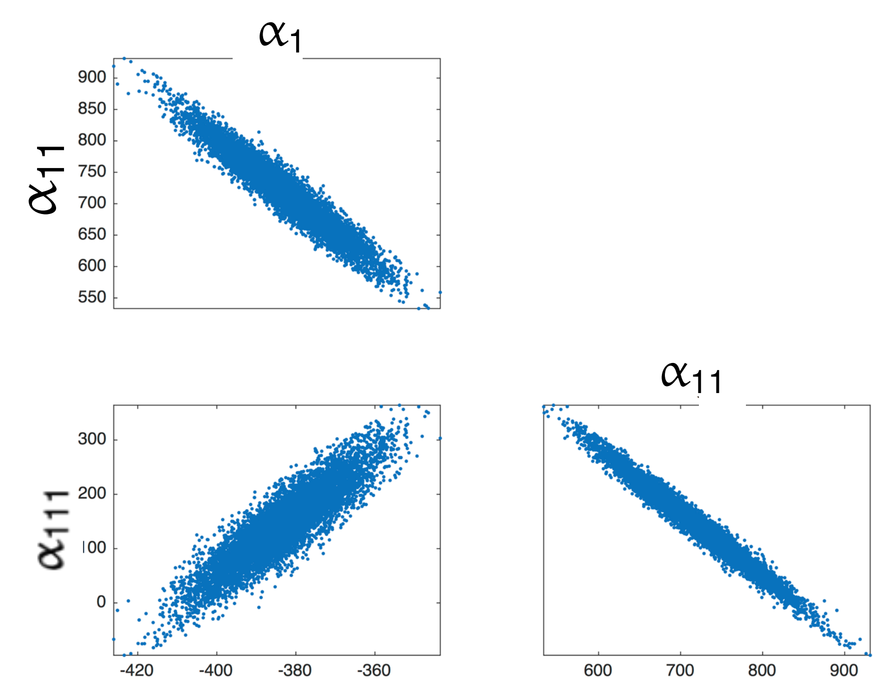
Strategy: Take Δq to be eigenvector of $\chi^T \chi$ Fisher Information

$$\Rightarrow \chi^T \chi \Delta q = \lambda \Delta q$$

$$\Rightarrow J(q^* + \Delta q) \approx \frac{\lambda}{n} \|\Delta q\|_2^2$$

$\lambda \approx 0 \Rightarrow$ Perturbations $J(q^* + \Delta q) \approx 0$

$\Rightarrow$ Nonidentifiable



Example:

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

Parameters:

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

Result: rank($\chi^T \chi$) = 3 so all parameters identifiable

Fisher Information Matrix

Parameter Subset Selection (PSS) Algorithm:

1. Set $n = p$ and threshhold ε

2. Compute eigenvalues $\lambda_1, \ldots, \lambda_n$ and eigenvectors $v_1, \ldots, v_n$ of $\chi^T\chi$ and order the eigenvalues by magnitude:

$$|\lambda_1| \leqslant |\lambda_2| \leqslant \ldots \leqslant |\lambda_n|$$

3. If $|\lambda_1| > \varepsilon$, stop

4. If $|\lambda_1| < \varepsilon$, one or more parameters is not identifiable

   - Identify component of v_1 with largest magnitude. This corresponds to least identifiable parameter

   - Remove column of $\chi^T\chi$ that corresponds to this component and set $n = n-1$

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.
- Does not accommodate potential correlation between parameters.
- Sensitive to units and magnitudes of parameters.

Global Sensitivity Analysis

Example: Portfolio model

$$Y = c_1 Q_1 + c_2 Q_2$$

Note:

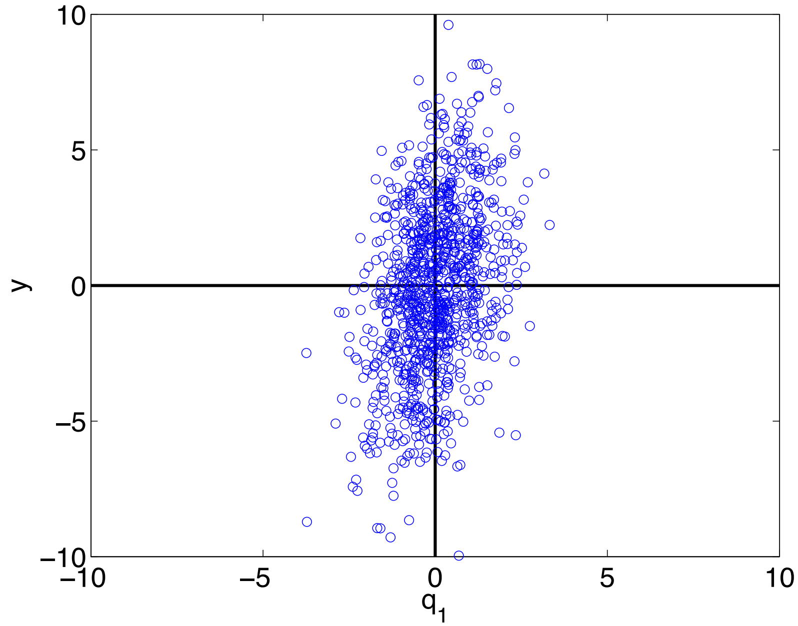
- Q_1 and Q_2 represent hedged portfolios
- c_1 and c_2 amounts invested in each portfolio

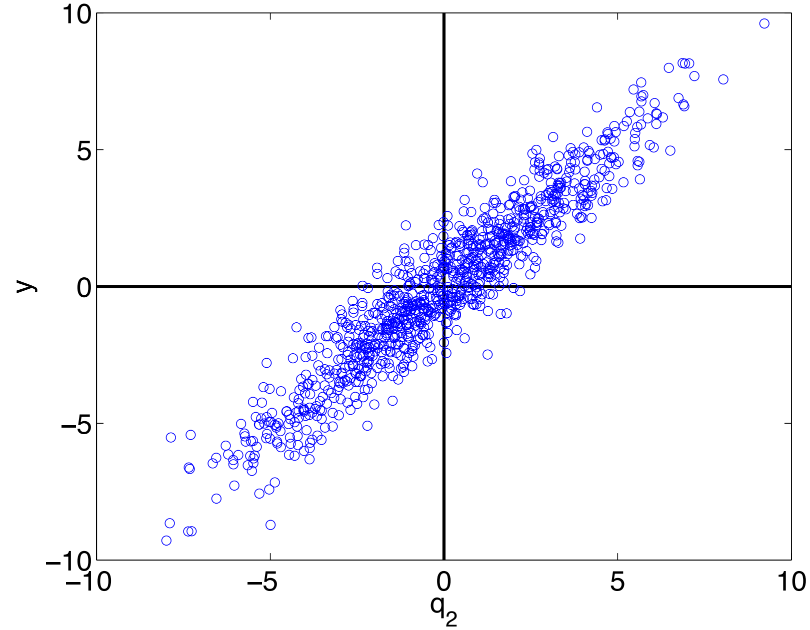
Take

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

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

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





Local Sensitivities:

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

Solutions:

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

Global Sensitivity Analysis: Variance-Based Methods

Example: Portfolio model

$$Y = c_1 Q_1 + c_2 Q_2$$

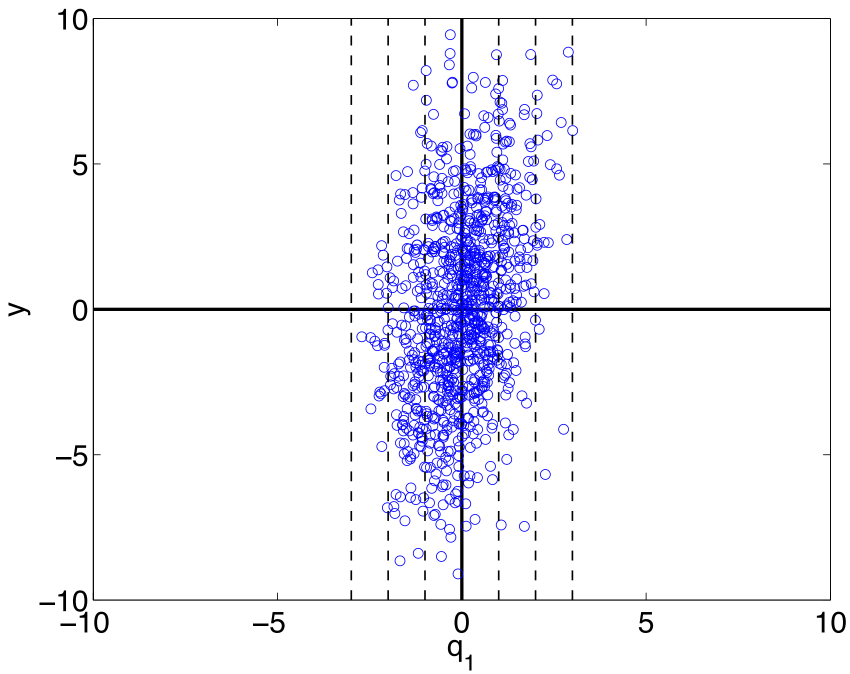
Take $c_1 = 2\,,\; c_2 = 1$

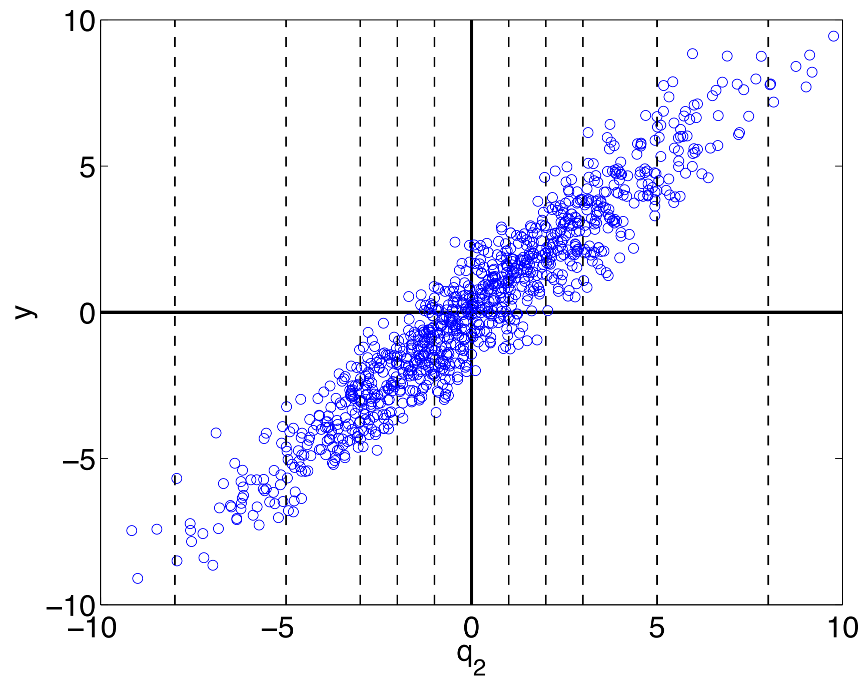
$$Q_1 \sim N(0,1)$$

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

Statistical Motivation: Consider variability of expected values

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





Note: Here $D_2 > D_1$

Analysis of Variance (ANOVA): Sobol Analysis

Initial Assumption: Independent uniformly distributed parameters

$$Q = [Q_1, \ldots, Q_p] \sim \mathcal{U}([0,1]^p)$$

Sobol Representation: Truncate at 2nd order – exact if pth order

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

Notes:

- Analogies: Taylor or Fourier series
- Need constraints to construct unique representation
    - Derivatives: Taylor
    - Orthogonality: Fourier

Example: $f(q) = \sin(\pi q)$

Taylor: $f(q) = \pi q - \frac{(\pi q)^3}{3!} + \frac{(\pi q)^5}{5!} + \ldots \approx \pi q$

Fourier: $f(q) = \sum_{m=1}^{\infty} B_m \sin(m\pi q) = \sin(\pi q)$

Analysis of Variance (ANOVA): Sobol Analysis

Sobol Representation: Truncate at 2nd order – exact if pth order

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

Sobol Constraints:

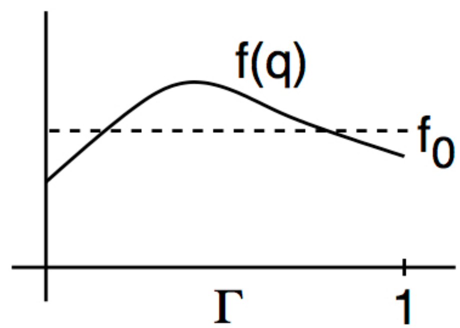
$$\int_0^1 f_i(q_i) dq_i = \int_0^1 f_{ij}(q_i, q_j) dq_i = \int_0^1 f_{ij}(q_i, q_j) dq_j = 0$$

Coefficients:

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

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

$$f_{ij}(q_i, q_j) = \int_{\Gamma^{p-2}} f(q) dq_{\sim\{ij\}} - f_i(q_i) - f_j(q_j) - f_0$$



Note: $q_{\sim i} = [q_1, \cdots, q_{i-1}, q_{i+1}, \cdots, q_p]$

Analysis of Variance (ANOVA)

Example: $y = aq_1 + bq_2$

Then

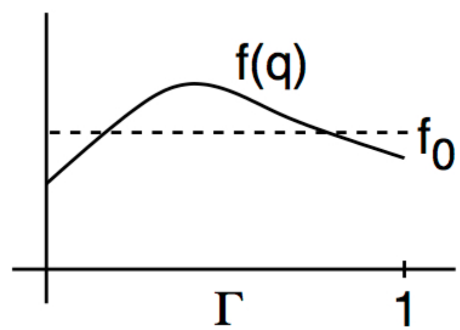
$$f_0 = \int_0^1 \int_0^1 [aq_1 + bq_2] dq_1 dq_2 = \frac{a+b}{2}$$

$$f_1(q_1) = \int_0^1 [aq_1 + bq_2] dq_2 - f_0 = aq_1 - \frac{a}{2}$$

$$f_2(q_2) = \int_0^1 [aq_1 + bq_2] dq_1 - f_0 = aq_2 - \frac{b}{2}$$

Coefficients:

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



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

$$f_{ij}(q_i, q_j) = \int_{\Gamma^{p-2}} f(q) dq_{\sim\{ij\}} - f_i(q_i) - f_j(q_j) - f_0$$

Analysis of Variance (ANOVA)

Statistical Interpretations:

$$\mathbb{E}(Y|q_i) = \int_{\Gamma^{p-1}} f(q) dq_{\sim i}$$

$$\mathbb{E}(Y|q_i, q_j) = \int_{\Gamma^{p-2}} f(q) dq_{\sim \{ij\}}$$

Recall: $f_{X_1}(x_1) = \int_{\mathbb{R}} f_X(x_1, x_2) dx2$

Note:

$$f_0 = \mathbb{E}(Y)$$

$$f_i(q_i) = \mathbb{E}(Y|q_i) - f_0$$

$$f_{ij}(q_i, q_j) = \mathbb{E}(Y|q_i, q_j) - f_i(q_i) - f_j(q_j) - f_0.$$

Total Variance:

$$D = \mathrm{var}(Y) = \int_{\Gamma} f^2(q) dq - f_0^2$$

$$= \sum_{i=1}^{p} D_i + \sum_{1 \leqslant i < j \leqslant p} D_{ij}$$

Partial Variances:

$$D_i = \int_0^1 f_i^2(q_i) dq_i \quad \text{since} \int_0^1 f_i(q_i) dq_i = 0$$

$$D_{ij} = \int_0^1 \int_0^1 f_{ij}^2(q_i, q_j) dq_i dq_j.$$

Analysis of Variance (ANOVA)

Sobol Indices:

$$S_i = \frac{D_i}{D} \quad , \; S_{ij} = \frac{D_{ij}}{D} \quad , \; i, j = 1, \cdots, p$$

$$S_{T_i} = S_i + \sum_{j=1}^{p} S_{ij}$$

Variance Interpretations: Verified shortly

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

and

$$S_{T_i} = \frac{\mathbb{E}[\mathrm{var}(Y|q_{\sim i})]}{\mathrm{var}(Y)}$$

Note:

$$S_{T_i} \approx 0 \Rightarrow \mathbb{E}[\mathrm{var}(Y|q_{\sim i})] \approx 0$$

$$\Rightarrow \mathrm{var}(Y|q_{\sim i}) \approx 0 \;\text{ since }\; \mathrm{var}(Y|q_{\sim i}) \geqslant 0$$

$\Rightarrow$ Parameter is noninfluential

Analysis of Variance (ANOVA)

Sobol Indices:

$$S_i = \frac{D_i}{D} \quad , \; S_{ij} = \frac{D_{ij}}{D} \quad , \; i,j = 1, \cdots, p$$

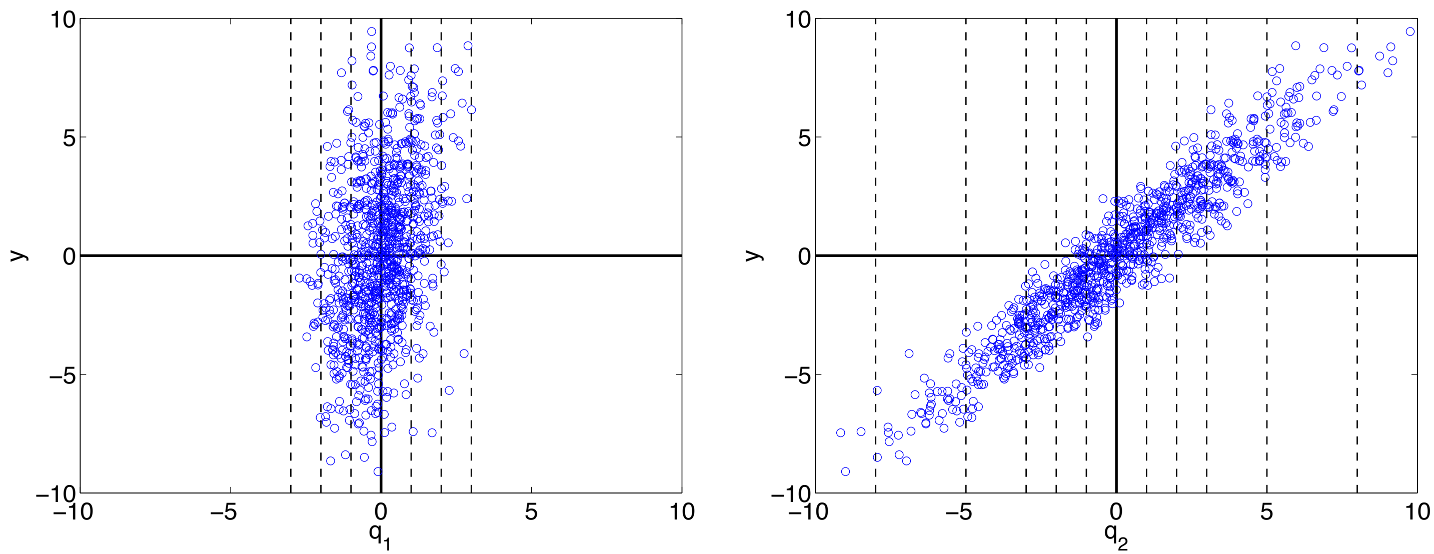
$$S_{T_i} = S_i + \sum_{j=1}^{p} S_{ij}$$

Variance Interpretations: Verified shortly

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

Example: Portfolio model

$$Y = c_1 Q_1 + c_2 Q_2$$



Analysis of Variance (ANOVA)

Example: Portfolio model

$$Y = c_1 Q_1 + c_2 Q_2$$

Take

$$Q_1 \sim \mathcal{N}(0, \sigma_1^2) \qquad \Rightarrow \qquad \rho(q_1) = \frac{1}{\sigma_1 \sqrt{2\pi}} e^{-q_1^2/2\sigma_1^2}$$

$$Q_2 \sim \mathcal{N}(0, \sigma_2^2) \qquad\qquad \rho(q_2) = \frac{1}{\sigma_2 \sqrt{2\pi}} e^{-q_2^2/2\sigma_2^2}$$

and

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

$$\sigma_1 = 1 \, , \; \sigma_2 = 3$$

Then

$$f_0 = \iint_{\mathbb{R}^2} [c_1 q_1 + c_2 q_2] \rho(q_1) \rho(q_2) dq_1 dq_2 = 0$$

$$f_1(q_1) = \int_{\mathbb{R}} [c_1 q_1 + c_2 q_2] \rho(q_2) dq_2 = c_1 q_1$$

$$f_2(q_2) = \int_{\mathbb{R}} [c_1 q_1 + c_2 q_2] \rho(q_1) dq_1 = c_2 q_2$$

$$f_{12}(q_1, q_2) = 0$$

Analysis of Variance (ANOVA)

Example: Portfolio model

$$Y = c_1 Q_1 + c_2 Q_2 \qquad c_1 = 2\,,\; c_2 = 1 \qquad \sigma_1 = 1\,,\; \sigma_2 = 3$$

Variances:

$$D_i = \int_{\mathbb{R}} f_i^2(q_i)\rho(q_i)dq_i = \int_{\mathbb{R}} c_i^2 q_i^2 \rho(q_i)dq_i = c_i^2\sigma_i^2$$

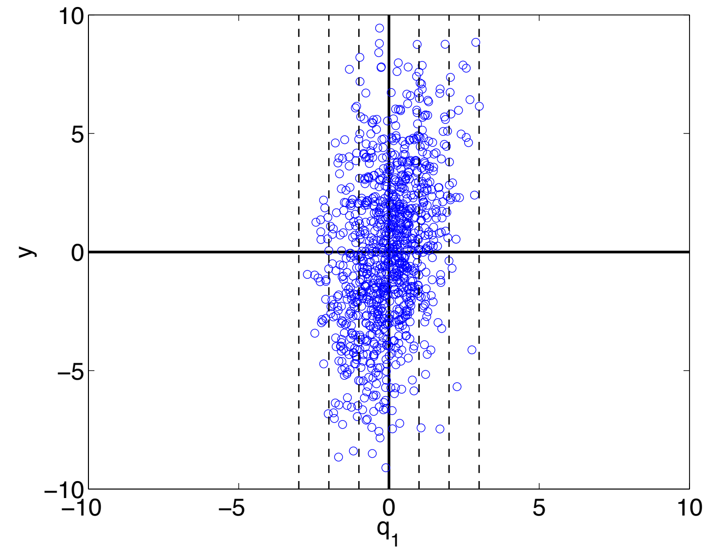
$$D_{12} = \iint_{\mathbb{R}^2} f_{12}^2 \rho(q_1)\rho(q_2)dq_1 dq_2 = 0$$

so

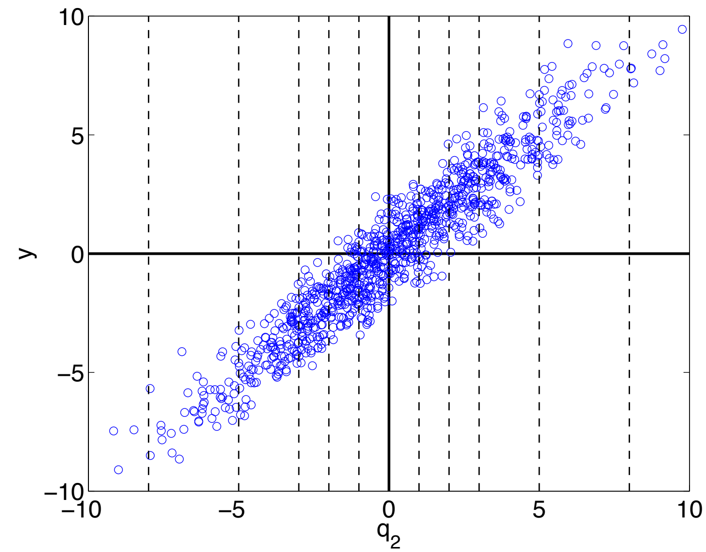
$$D = D_1 + D_2 + D_{12} = c_1^2\sigma_1^2 + c_2^2\sigma_2^2$$

Sobol Indices:

$$S_i = \frac{c_i^2\sigma_i^2}{c_1^2\sigma_1^2 + c_2^2\sigma_2^2} \Rightarrow \boxed{S_1 = \frac{4}{13}\,,\; S_2 = \frac{9}{13}}$$



$D_1 = 4$



$D_2 = 9$

Analysis of Variance (ANOVA)

Verification: Recall that $\text{var}(f) = \mathbb{E}(f^2) - [\mathbb{E}(f)]^2$

Then

$$
\begin{aligned}
D_i &= \int_0^1 f_i^2(q_i)dq_i \\
&= \int_0^1 \left[\int_{\Gamma^{p-1}} f(q)dq_{\sim i} - f_0\right]^2 dq_i \\
&= \int_0^1 \left[\int_{\Gamma^{p-1}} f(q)dq_{\sim i}\right]^2 dq_i - f_0^2 \quad \star \\
&= \mathbb{E}\left[\mathbb{E}(Y|q_i)\right]^2 - \left[\mathbb{E}[\mathbb{E}(Y|q_i)]^2\right] \\
&= \mathrm{var}[\mathbb{E}(Y|q_i)]
\end{aligned}
$$

since

$$
\mathbb{E}[\mathbb{E}(Y|q_i)] = \int_0^1 \left[\int_{\Gamma^{p-1}} f(q)dq_{\sim i}\right] dq_i = f_0
$$

$\star$

Morris Screening

Model: $y = f(Q)$

Initial Assumption: Independent uniformly distributed parameters

$$Q = [Q_1, \ldots, Q_p] \sim \mathcal{U}([0,1]^p)$$

Elementary Effects: Coarse derivative approximations

$$d_i - \frac{f(q_1, \ldots, q_{i-1}, q_i + \Delta, q_{i+1}, \ldots, q_p) - f(q)}{\Delta}$$

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

$$\Delta \in \left\{ \frac{1}{\ell - 1}, \ldots, 1 - \frac{1}{\ell - 1} \right\} \; , \; \ell \text{ is level; e.g., } \Delta = \frac{1}{100}$$

$$e_i = [0, \ldots, 0, 1, 0 \ldots, 0]$$

Global Sensitivity Measures: i=1, …, p

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

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

Morris Screening

Issues:

- Provides relative than absolute rankings
- Parameters often correlated and hence not independent. One can make incorrect conclusions based on incorrect assumption of independence.
- How does one construct indices for time or space-dependent responses or, more generally infinite-dimensional responses? Same question for vector-valued responses.

SIR Disease Example

SIR Model:

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

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

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

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

Assumed Parameter Distribution:

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

Infection Coefficient	Interaction Coefficient	Recovery Rate	Birth/death Rate

Response:

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

SIR Disease Example

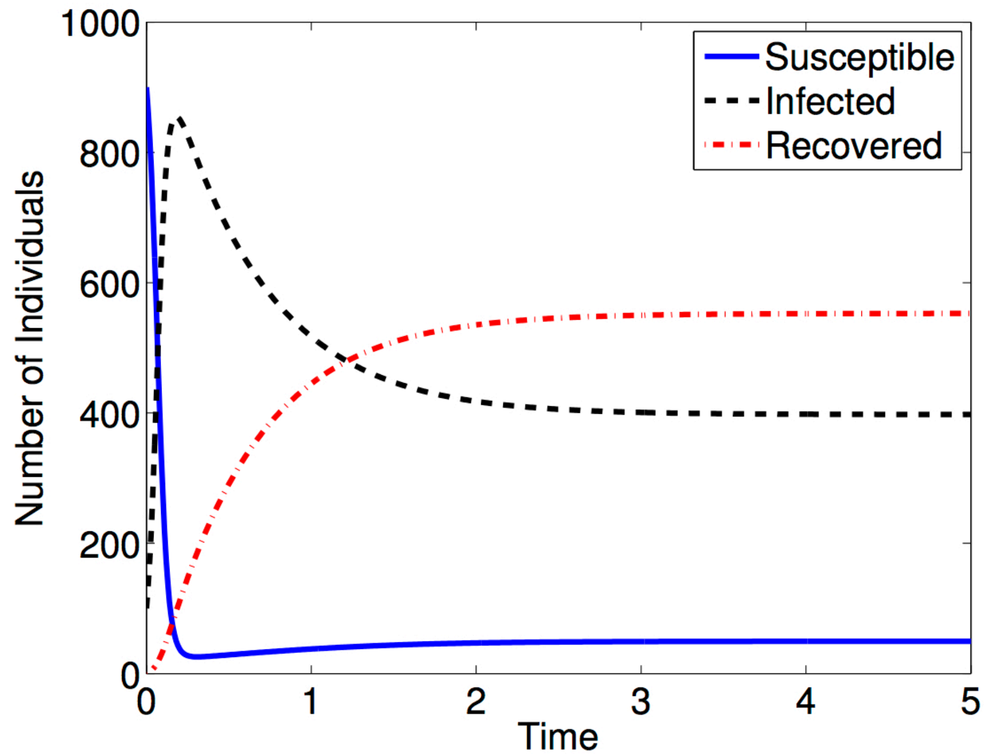
SIR Model:

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

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

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

Typical Realization:

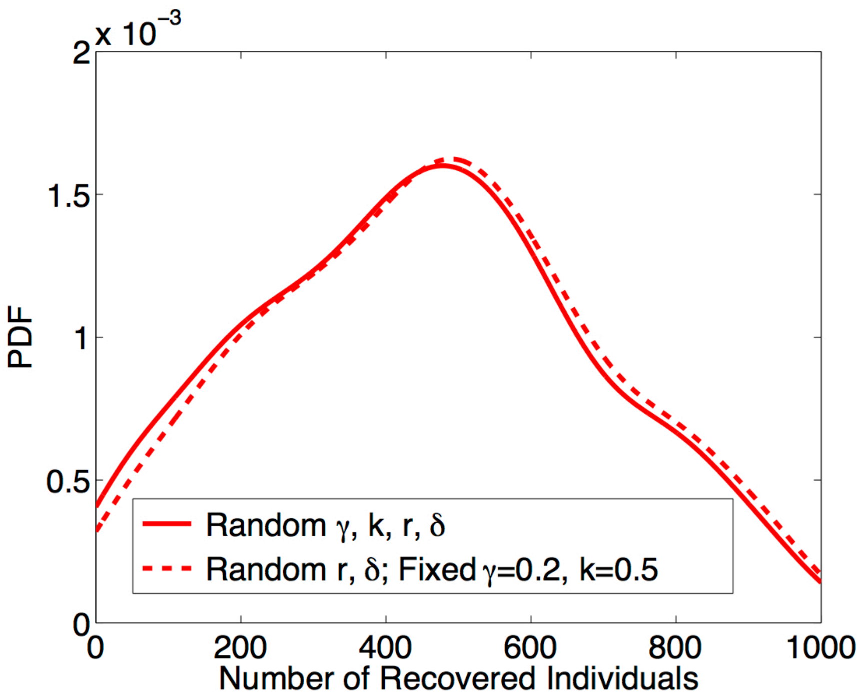


SIR Disease Example

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

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



Note: Can fix non-influential parameters

Global Sensitivity Analysis

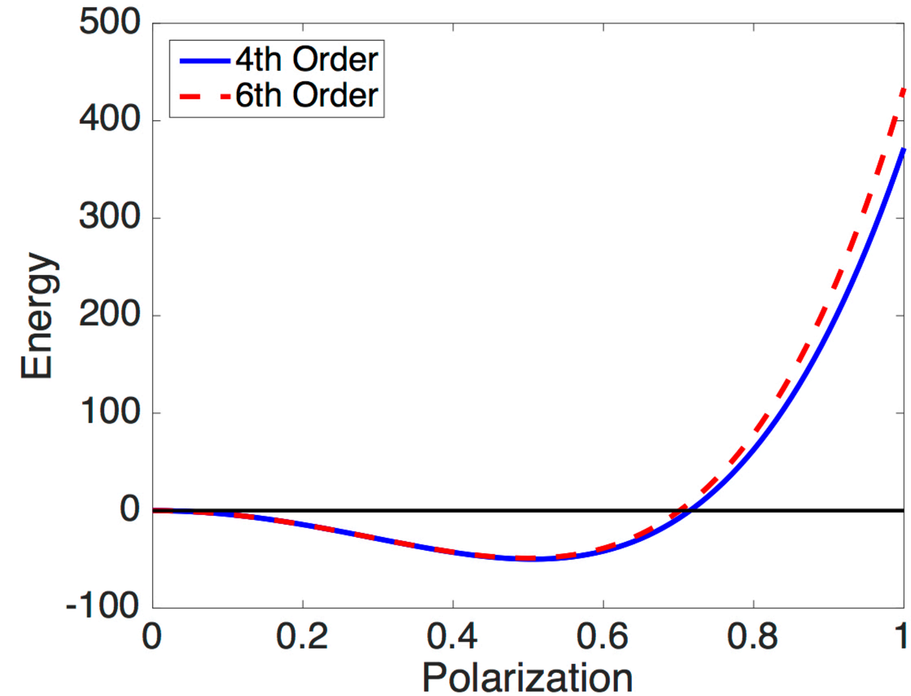
Example: Quantum-informed continuum model

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

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

Parameters:

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



Global Sensitivity Analysis:

	α_1	α_{11}	α_{111}
S_i	0.62	0.39	0.01
S_{T_i}	0.66	0.38	0.06
μ_i^*	0.17	0.07	0.03

Conclusion: α_{111} insignificant and can be fixed

Global Sensitivity Analysis

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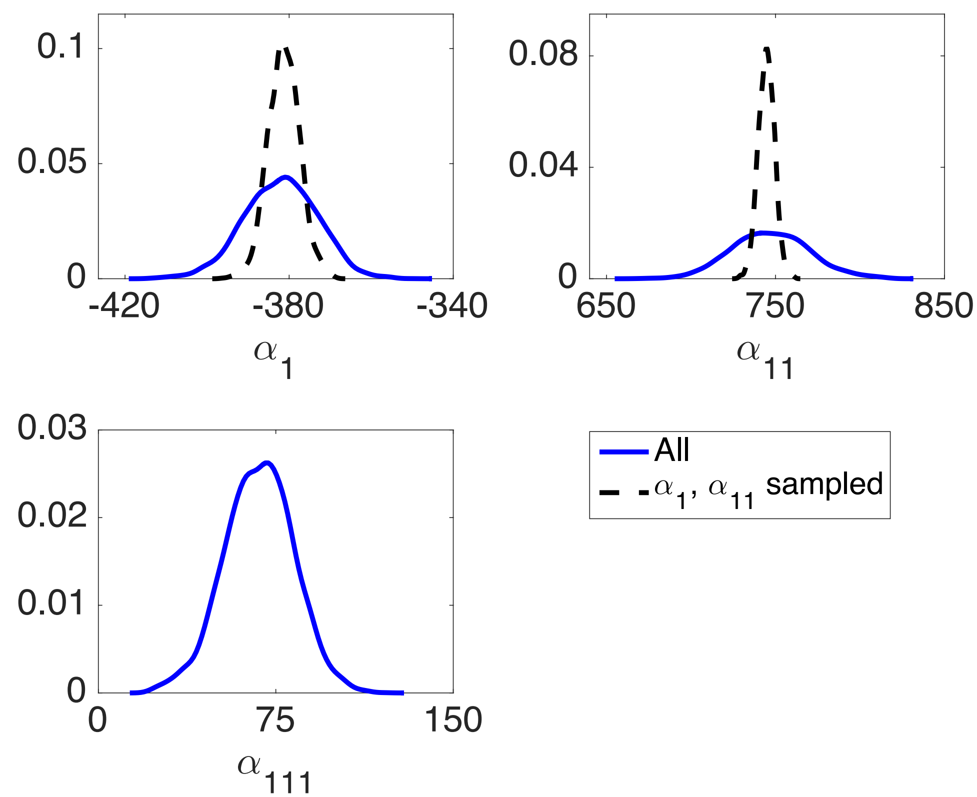
μ_i^*	0.17	0.07	0.03

Conclusion:

α_{111} insignificant and can be fixed

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



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:

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

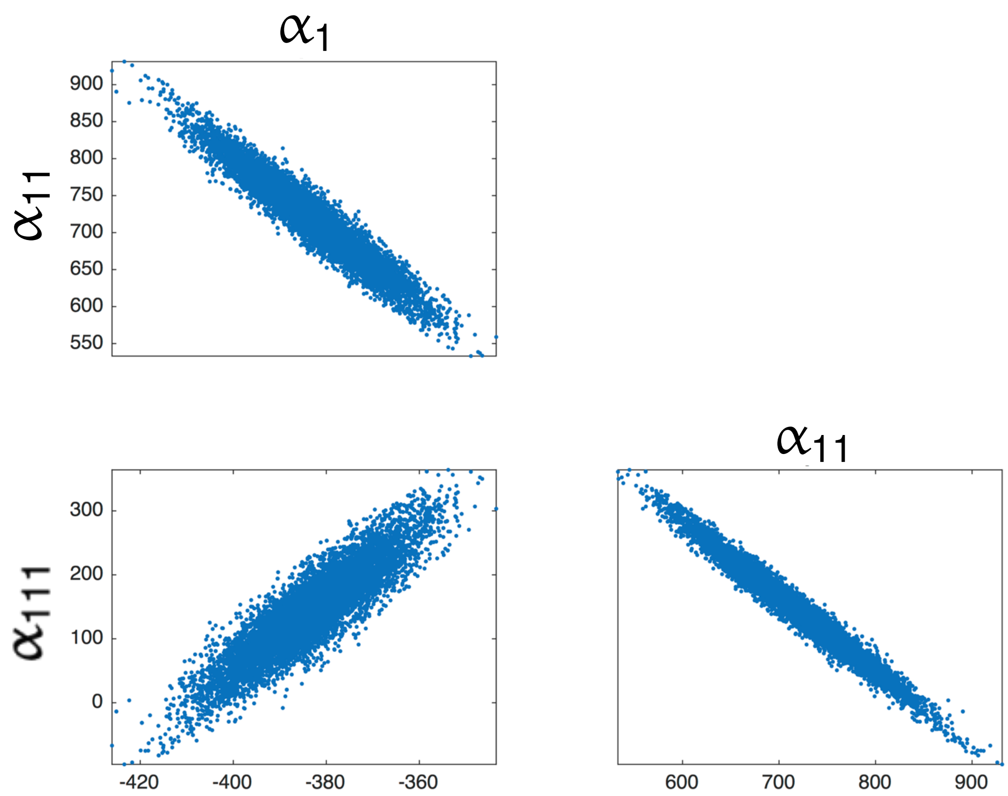
Global Sensitivity Analysis:

	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

Note: Must accommodate correlation

Problem:

- Parameters correlated
- Cannot fix α_{111}

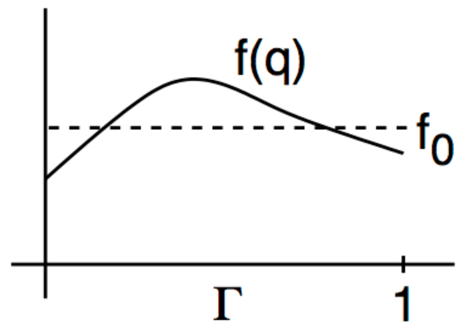


Global Sensitivity Analysis: Analysis of Variance

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

$$\begin{aligned} f(q) &= f_0 + \sum_{i=1}^{p} f_i(q_i) + \sum_{i \leqslant i < j \leqslant p} f_{ij}(q_i, q_j) + \cdots + f_{12 \cdots p}(q_1, \ldots, q_p) \\ &= f_0 + \sum_{i=1}^{p} \sum_{|u|=i} f_u(q_u) \end{aligned}$$

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: 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:

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

Alternative: Construct active subspaces

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

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.

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

One Solution: Parameter Subset Selection

Note:

$$J(q^* + \Delta q) \approx \frac{1}{n} \Delta q^T \chi^T \chi \Delta q$$

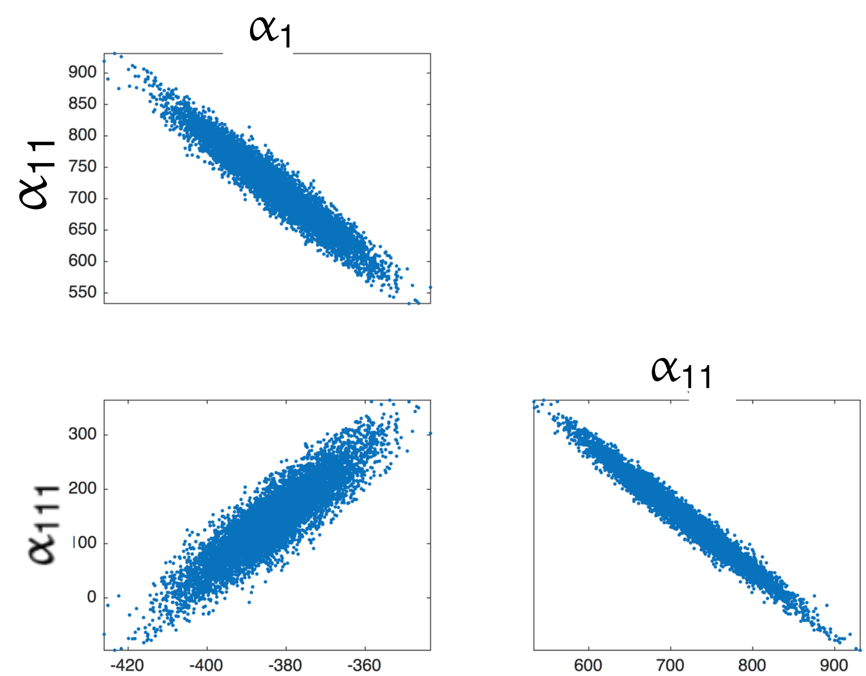
Strategy: Take Δq to be eigenvector of $\chi^T \chi$ Fisher Information

$$\Rightarrow \chi^T \chi \Delta q = \lambda \Delta q$$

$$\Rightarrow J(q^* + \Delta q) \approx \frac{\lambda}{n} \|\Delta q\|_2^2$$

$\lambda \approx 0 \Rightarrow$ Perturbations $J(q^* + \Delta q) \approx 0$

$\Rightarrow$ Nonidentifiable



Example:

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

Parameters:

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

Result: rank($\chi^T \chi$) = 3 so all parameters identifiable