

## Parameter Subset Selection

- Given  $\tilde{S}_j = \frac{\partial f}{\partial \theta_j}$ , we know that given  $J(\hat{\theta})$  to be minimized

$$\Rightarrow J(\hat{\theta}) = \frac{1}{n} \sum (y - f)^2 \Rightarrow J(\hat{\theta} + \Delta \hat{\theta}) \approx \frac{1}{n} [\sum \Delta \hat{\theta}]^T [\sum \Delta \hat{\theta}]$$

So  $J(\hat{\theta} + \Delta \hat{\theta}) = \frac{1}{n} \Delta \hat{\theta}^T (\sum \tilde{S}_j^T \tilde{S}_j) \Delta \hat{\theta}$ ,  $\hat{\theta} \in \mathbb{R}^p$

- If  $\Delta \hat{\theta}$  is an eigenvector of  $\sum \tilde{S}_j^T \tilde{S}_j \Rightarrow \sum \tilde{S}_j^T \tilde{S}_j \Delta \hat{\theta} = \tilde{\lambda} \Delta \hat{\theta}$ ,  $\tilde{\lambda} > 0$ ,  $\tilde{\lambda}$  are eig. values of  $\sum \tilde{S}_j^T \tilde{S}_j$

$$\Rightarrow J(\hat{\theta} + \Delta \hat{\theta}) \approx \frac{1}{n} \tilde{\lambda} \|\Delta \hat{\theta}\|_2^2$$

- If any  $\lambda_i \approx 0$ , then  $\theta_i$  has relatively little impact  $J(\hat{\theta})$

## Global Sensitivity Analysis (GSA) (Chapter 4)

- GSA quantifies the uncertainty in  $y$  that is apportioned to  $\hat{\theta}$ .

### Variance-Based Methods

- Consider a scalar, nonlinear model

$$y = F(\hat{\theta}), \quad \hat{\theta} \in \Gamma + \theta_i \overset{\text{independent}}{\sim} \mathcal{U}(0, 1) \quad (\text{so } \Gamma = [0, 1]^p)$$

- We can decompose  $f(\hat{\theta})$  into a hierarchical form

$$F(\hat{\theta}) = f_0 + \sum_{i=1}^p f_i(\theta_i) + \sum_{1 \leq i < j \leq p} f_{ij}(\theta_i, \theta_j) + \dots$$

where

$f_0 \equiv$  mean over  $\Gamma$   
 $f_i$  ... response from  $\theta_i$

where

$f_0 \equiv \text{mean over } \Gamma$

$f_i \equiv \text{first order response from } \theta_i$

$f_{ij} \equiv \text{Second order interactions from } \theta_i + \theta_j$

- We assume that the functions satisfy

$$\int_0^1 f_i(\theta_i) d\theta_i = 0$$

$$\int_0^1 f_{ij}(\theta_i, \theta_j) d\theta_i = \int_0^1 f_{ij}(\theta_i, \theta_j) d\theta_j = 0$$

i.e. each  $f$  is orthogonal.

- Each  $f$  can be expressed as:

$$f_0 = \int_{\Gamma} F(\vec{\theta}) d\vec{\theta} = E[F(\vec{\theta})]$$

$$f_i(\theta_i) = \int_{\Gamma^{p-1}} F(\vec{\theta}) d\vec{\theta}_{\sim i} - f_0 = E[F(\vec{\theta}) | \theta_i] - f_0$$

$$f_{ij}(\theta_i, \theta_j) = \int_{\Gamma^{p-2}} F(\vec{\theta}) d\vec{\theta}_{\sim ij} - f_i - f_j - f_0 = E[F(\vec{\theta}) | \theta_i, \theta_j] - f_i - f_j - f_0$$

where  $\vec{\theta}_{\sim i} = \vec{\theta} \setminus \theta_i$ ,  $\vec{\theta}_{\sim ij} = \vec{\theta} \setminus \{\theta_i, \theta_j\}$

- This is a (functional) analysis of variance (ANOVA) decomposition of  $F(\vec{\theta})$ .

• Hoeffding-Sobol decomposition.

- If  $\theta_i$  are independent

$$\Rightarrow \int_{\Gamma} f_i(\theta_i) f_j(\theta_j) d\vec{\theta} = 0$$

$$\Rightarrow \int_{\Gamma} f_i(\theta_i) f_j(\theta_j) d\vec{\theta} = 0$$

- Let the Variance of  $F(\vec{\theta}) = Y$

$$D = \text{Var}[Y] = \int_{\Gamma} (F(\vec{\theta}))^2 d\vec{\theta} - f_0^2$$

- Since each  $f$  term is orthogonal, then

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

where

$$D_i = \int_0^1 f_i^2(\theta_i) d\theta_i = \text{Var}[f_i(\theta_i)]$$

$$D_{ij} = \int_0^1 \int_0^1 f_{ij}^2(\theta_i, \theta_j) d\theta_i d\theta_j = \text{Var}[f_{ij}(\theta_i, \theta_j)]$$

Because

$$\text{Var}[f_i] = E[f_i^2] - (E[f_i])^2$$

$$+ E[f_i] = \int_0^1 f_i(\theta_i) d\theta_i = 0$$

Sobol Indices