Global Sensitivity Analysis

- Let $\hat{\underset{\sim}{C}} = \frac{1}{M} \sum_{i=1}^{M} (\nabla_\theta f^i)(\nabla_\theta f^i)^T$ be defined by

$$\hat{\underset{\sim}{C}} = \hat{\underset{\sim}{W}} \hat{\underset{\sim}{\Lambda}} \hat{\underset{\sim}{W}}^T, \quad \hat{\underset{\sim}{\Lambda}} = \begin{bmatrix} \lambda_1 \dots & \\ & \lambda_p \end{bmatrix}, \in \mathbb{R}^{p \times p}$$

- Let $\hat{\underset{\sim}{\Lambda}} = \begin{bmatrix} \hat{\underset{\sim}{\Lambda}}_1 & \\ & \hat{\underset{\sim}{\Lambda}}_2 \end{bmatrix}$, $\hat{\underset{\sim}{W}} = \left[\hat{\underset{\sim}{W}}_1 \quad \hat{\underset{\sim}{W}}_2 \right]$
- Let $\hat{\underset{\sim}{W}}_1$ be the active subspace, $\hat{\underset{\sim}{W}}_1 \in \mathbb{R}^{p \times m}$

- The activity score, a_i, is given by

$$a_i = \sum_{j=1}^{m} \lambda_j w_{ij}^2, \quad i = 1, \dots, p$$

where w_{ij} is the ith component of the jth eigenvector, $\vec{\omega}_j$

- So the most significant average change in f occurs in direction $\vec{\omega}_1$, then $\vec{\omega}_2$, etc.
- The sum of λ_j tell us how each θ_i contributes in direction $\vec{\omega}_j$.

Surrogate Modeling

- Suppose $\hat{\underset{\sim}{W}}_1$ effectively describe how $\vec{\theta}$ affects $f(\vec{\theta})$, where $\lambda_m >> \lambda_{m+1}$, $m < p$.

- Suppose $\underset{\sim}{W}_1$ effectively describe how ... $m < P$.

. Let $\vec{z} = \underset{\sim}{\hat{W}}_1^T \vec{\theta}$, $\underset{\sim}{\hat{W}}_1 \in \mathbb{R}^{P \times m}$, $\vec{\theta} \in \mathbb{R}^P \Rightarrow \vec{z} \in \mathbb{R}^m$

- Could we derive a surrogate, $\tilde{f}(\vec{z})$, that is sufficiently accurate, i.e.

$$f(\vec{\theta}) \approx \tilde{f}(\vec{z}) = \tilde{f}(\hat{W}_1^T \vec{\theta}) \ ?$$

- <u>Idea</u>: Given new data, $\vec{z}^j = \underset{\sim}{\hat{W}}_1^T \vec{\theta}^j$, build surrogate, e.g., regression

$$\tilde{f}(\vec{z}^j) = \underset{\sim}{B} \vec{z}, \quad \underset{\sim}{B} = \left[\vec{1} \ \vec{z} \ \vec{z}^2 \ \ldots \right]$$

Ex) $f(x; \vec{q}) = q_1 + q_2 x + q_3 x^2 + q_4 x^3$

- when $x \approx 0$

$$\Rightarrow \lambda_1 >> \lambda_2 > \lambda_3 > \lambda_4 \Rightarrow \vec{z} = \underset{\sim}{\hat{W}}_1 \vec{q} \in \mathbb{R}$$

. For a 1^{st} degree polynomial

$$\tilde{f} = b_0 + b_1 \vec{z} = \left[1 \ \vec{z} \right] \vec{b}$$

. To build $\tilde{f}$

$$\text{Let } \underset{\sim}{Z} = \left[\vec{1} \ \vec{z} \right] \Rightarrow \tilde{f} = \underset{\sim}{Z} \vec{b}$$

. Generate $y_i = f(x, \vec{q})$, $i = 1, \ldots, N_y$

$$\Rightarrow \vec{y} = Z \vec{b} + \vec{\varepsilon}$$

$$\Rightarrow \quad \vec{y} = \underset{\sim}{Z}\vec{b} + \vec{\varepsilon}$$

- Solve $\quad \vec{b} = (\underset{\sim}{Z}^T \underset{\sim}{Z})^{-1} \underset{\sim}{Z}^T \vec{y}$

- $\hat{f} = \underset{\sim}{Z}\vec{b}$

Ex) PDE's with random fields

- Consider the PDE in 1D

$$\frac{\partial u}{\partial t} = \frac{\partial}{\partial x}\left(\alpha(x)\frac{\partial u}{\partial x}\right) + f(x,t), \quad x \in (-1,1), \; t > 0$$

$$u(-1,t) = u_L, \quad u(1,t) = u_R, \quad \forall\, t > 0$$

$$u(x,0) = \bar{u}_0(x), \quad x \in [-1,1]$$

where $\alpha(x)$ is spatial conductivity.

- $\alpha(x) = \alpha(x, \vec{\theta})$ is a random field.

- Recall the KL expansion

$$\alpha(\vec{x}, \vec{\omega}) = \bar{\alpha}(x) + \sum_{n=1}^{\infty} \sqrt{\lambda_n}\, \varphi_n(x)\, \Theta_n(\omega)$$

$$\approx \bar{\alpha}(x) + \sum_{n=1}^{A} \sqrt{\lambda_n}\, \varphi_n(x)\, \Theta_n(\omega)$$

where λ_n & φ_n are eigenpairs of covariance, & $\Theta_n \sim N(0,1)$

- We can try to identify

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$$\vec{z} \in \mathbb{R}^m, \quad \vec{z} = \underset{\sim}{\hat{W}}^{+} \vec{\Theta}, \quad \Theta \in \mathbb{R}^A, \quad m \ll A.$$

· For an inverse problem

$$\min_{\vec{\Theta}} \| \vec{y}_u - u(\vec{x}, \vec{t}; \vec{\theta}) \|_2^2 \approx \min_{\vec{z}} \| \vec{y}_u - \hat{f}(\vec{z}) \|_2^2$$

p-dimension PDE constrained opt. problem

m dimensional linear problem