Surrogates + Reduced Order Models

- Consider $\vec{y}_{HF} = f_{HF}(\vec{x}; \vec{\theta})$, $\vec{\theta} \in \mathbb{R}^P$ HF: High Fidelity

- We are interested in generating
$$f_{HF}(\vec{x}; \vec{\theta}) \approx f_{LF}(\vec{x}; \vec{\theta}), \quad \text{LF: Low fidelity}$$

  - Let's assume $\vec{x}$ is fixed $\Rightarrow f_{HF}(\vec{\theta}) \approx f_{LF}(\vec{\theta})$.

Polynomials as Surrogate

- An intuitive approach is letting f_{LF} be a polynomial, i.e.
$$f_{LF}^{K}(\vec{\theta}) = \sum_{q=0}^{K} a_q \psi_q(\vec{\theta})$$

where K is the "order" of the polynomial, + a_q are weights or coefficients. ψ_q represents polynomials.

Interpolation

- Consider $\theta \in \mathbb{R}$. A simple 1D polynomial is
$$f_{LF}^{K} = \sum_{q=0}^{K} a_q \theta^q = a_0 + a_1\theta + a_2\theta^2 + \dots + a_K\theta^K$$

- Given training data, $y^n = f_{HF}(\theta^n)$, $n = 1, \dots, M$, we enforce matching of f_{LF} at each θ^n.

- Given ... matching of f_{LF} at each Θ^n.

. This gives

$$\vec{y} = \underset{\sim}{X}\vec{a}, \quad \underset{\sim}{X} = \begin{bmatrix} 1 & \Theta^0 & (\Theta^0)^2 & \cdots & (\Theta^0)^K \\ \vdots & \vdots & \vdots & & \\ 1 & \Theta^M & (\Theta^M)^2 & \cdots & (\Theta^M)^K \end{bmatrix}$$

. Then solve

$$\vec{a} = (\underset{\sim}{X}^T \underset{\sim}{X})^{-1} \underset{\sim}{X}^T \vec{y} = \underset{\sim}{X}^+ \vec{y}$$

where $\underset{\sim}{X}^+ = (\underset{\sim}{X}^T \underset{\sim}{X})^{-1} \underset{\sim}{X}^T$ is penrose pseudo inverse.

Lagrange Polynomials

- The interpolating polynomial given by Lagrange polynomials is given by

$$f_{LF}^M = \sum_{m=0}^{M} y_m L_m(\Theta)$$

$$L_m(\theta) = \prod_{\substack{j=0 \\ j\neq m}}^{M} \frac{\Theta - \Theta^j}{\Theta^m - \Theta^j} = \frac{(\Theta-\theta^0)(\theta-\theta^1)\cdots(\Theta-\Theta^M)}{(\theta^m-\theta^0)\cdot(\theta^m-\theta^1)\cdots(\Theta^m-\Theta^M)}$$

which satisfies $L_m(\theta^j) = \delta_{mj}, \quad 0 \le m, j \le M$

. Note: Choice of Θ^j can have effects on f_{LF} accuracy.

Ex) $f(\Theta) = (6\theta - 2)^2 \sin(12\theta - 4), \quad \theta \in [0,1]$

. Note that boundaries have sharp changes.

- Once we have f_{LF}, we can use it for uncertainty propagation

- Assume $\theta \sim \rho(\theta)$ with support Γ. Then

$$E\left[f_{HF}\right] \approx E\left[f_{LF}\right] = \int_{\Gamma} f_{LF}(\theta)\, \rho(\theta)\, d\theta$$

· Use Lagrange polynomials

$$\Rightarrow E\left[f_{LF}\right] = E\left[\sum_{m=0}^{M} f_{HF}(\theta^m)\, L_m(\theta)\right]$$

$$= \sum_{m=0}^{M} f_{HF}(\theta^m) \int_{\Gamma} L_m(\theta)\, \rho(\theta)\, d\theta$$

· To evaluate integral, we approximate using quadrature

$$\Rightarrow E\left[f_{LF}\right] \approx \sum_{m=0}^{M} f_{HF}(\theta^m) \sum_{r=0}^{R} L_m(\theta^r)\, \rho(\theta^r)\, \omega^r$$

where θ^r + ω^r come from quadrature.

- If we choose $\theta^r = \theta^m$, $R = M$, then

$$E\left[f_{LF}\right] \approx \sum_{m=0}^{M} f_{HF}(\theta^m)\, \underbrace{L_m(\theta^m)}_{\text{goes away}}\, \rho(\theta^m)\, \omega^m$$

· Note that L_m are orthogonal w.r.t. any density, $\rho(\theta)$

$$\Rightarrow E\left[f_{LF}\right] \approx \sum_{m=0}^{M} f_{HF}(\theta^m)\, \rho(\theta^m)\, \omega^m = \bar{f}_{LF}$$

- Similarly

$$\left[\;\cdot\;\right] \int \left[f(\theta) - \bar{f}_{LF} \right]^2 \rho(\theta)\, d\theta$$

- Similarly

$$Var[f_{LF}] = \int_{\Gamma} [f_{LF}(\theta) - \bar{f}_{LF}]^2 \rho(\theta)\, d\theta$$

$$\approx \sum_{m=0}^{M} [f_{LF}(\theta^m) - \bar{f}_{Lf}]^2 \rho(\theta^m)\, \omega^m$$

* See more on Sparse grids *

Spectral Surrogates

- Polynomials as surrogates provide some analytical advantages over purely data-driven approaches.
- Here, we employ polynomials that exhibit orthogonality w.r.t. a specific pdf, $\rho(\theta)$.
  - Spectral expansions are often called "polynomial chaos expansion" (PCEs)
- Throughout, assume $\vec{\theta} \sim N(0, \underset{\sim}{I}_p)$ or $\vec{\theta} \sim U([-1,1]^p)$, $\vec{\theta} \in \mathbb{R}^p$
  - we assume each θ_i is independent.
- The general spectral expansion is

$$f_{LF}(\vec{\theta}) = \sum_{l=0}^{K} a_l \Psi_l(\vec{\theta})$$

Gaussian θ

- Assume $\theta \in \mathbb{R}$ is Gaussian, $\theta \sim N(0,1)$.
  - The pdf, $\rho(\theta)$, is

$$\frac{1}{} \exp\left(-\frac{1}{2}\theta^2\right)$$

· The pdf, $\rho(\theta)$, is

$$\rho(\theta) = \frac{1}{\sqrt{2\pi}} \exp\left(-\frac{1}{2}\theta^2\right)$$

since $E[\theta] = 0$.

- Consider the Hermitian Polynomials, $H_n(x)$, given

$$H_n(x) = (-1)^n \exp(x^2/2) \cdot \frac{d^n}{dx^n} \exp(-x^2/2)$$

$H_0(x) = 1$, $H_1(x) = x$, $H_2(x) = x^2 - 1$, $H_3(x) = x^3 - 3x$

- Note, for any $m, n \in \mathbb{N}_0$

$$\int_{\mathbb{R}} H_n(\theta) H_m(\theta) \rho(\theta) d\theta$$

$$= \int_{\mathbb{R}} (-1)^{n+m} e^{\theta^2} \frac{d^n}{d\theta^n}\left(e^{-\theta^2/2}\right) \frac{d^m}{d\theta^m}\left(e^{-\theta^2/2}\right) \cdot \frac{1}{\sqrt{2\pi}} e^{-\frac{1}{2}\theta^2} d\theta$$

$$= \begin{cases} 0, & \text{if } n \neq m \\ n!, & \text{if } n = m \end{cases}$$