Nested kriging / model aggregation

$\xi \sim \mathcal{N}(0, k)$

data $X_1, \dots, X_N$

$f(X_1), \dots, f(X_N)$

$$\xi \mid \xi(X) = f(X) \sim \mathcal{N}(m, C)$$

$$m(x) = \mathbb{E}[\xi(x) \mid \xi(X) = f(X)]$$

$$= k(x, X)\, K(X, X)^{-1} f(X)$$

$$C(x, x') = k(x, x') - k(x, X)\, K(X, X)^{-1} K(X, x')$$

Partition the data $X^1, \dots, X^q$

$\rightarrow$ q predictions $m^i = \mathbb{E}[\xi(x) \mid \xi(X^i) = f(X^i)]$

How to combine them to get a better prediction?

$\rightarrow$ q submodel predictions

$$M(x) = (\mathbb{E}[\xi(x) \mid \xi(X^1)], \dots, \underbrace{\mathbb{E}[\xi(x) \mid \xi(X^q)]}_{M^q})$$

$\searrow$ Gaussian vector

$(M(x), \xi(x))$: Gaussian vector

$$K_M(x) = \mathrm{Cov}(M(x))$$

$$k_M(x) = \mathrm{Cov}(\xi(x), M(x))$$

$\hookrightarrow 1 \times q$ vector

sub-model aggregation

$$M_A(x) = k_M(x) K_M(x)^{-1} M(x)$$

given $M(x) = m(x) = (m^1(x), \dots, m^q(x))$

best prediction is

$$m_A(x) = k_M(x) K_M(x)^{-1} m(x)$$

<u>Prop</u> M_A is the best linear unbiased predictor of $\xi(x)$ that writes

and nonlinear

$$\sum_i \alpha_i(x) M^i(x)$$

$$\alpha = k_M(x) K_M(x)^{-1}$$

$$v_A(x) = \mathbb{E}[|\xi(x) - M_A(x)|^2]$$

$$= K(x,x) - k_M(x) K_M(x)^{-1} k_M^T(x)$$

Prop

(i) M linear in $\xi(X) \Leftrightarrow M(x) = \Lambda(x)\,\xi(X)$

$q \times N$ mat

$$\Downarrow$$

$$M_A(x) = \lambda_A(x)^T \xi(X)$$

$$v_A(x) = K(x,x) - \lambda_A^T(x) K(X,x)$$

$$\lambda_A(x)^T = K(x,X)\,\Lambda(x)^T \left(\Lambda(x) K(X,X) \Lambda(x)^T\right)^{-1} \Lambda(x)$$

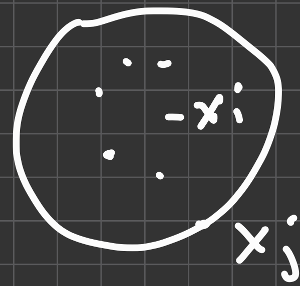
(ii) $M_A(X) = \xi(X)$

$v_A(X) = 0$

(iii) $\mathbb{E}[\xi(x) \mid M(x)] = M_A(x)$

$\mathrm{Var}[\xi(x) \mid M(x)] = v_A(x)$

$$\begin{cases} -\Delta u = f & \Omega \\ u = g & \partial\Omega \end{cases}$$



$$\bar{u} = \arg \begin{cases} \min \|v\|_K \\ \text{s.t.} \quad -\Delta v(x_i) = f(x_i) & \Omega \\ \qquad\quad v(x_i) = g(x_i) & \partial\Omega \end{cases}$$

Assume q sets of points

$j = 1, \dots, q \qquad X^j \longrightarrow \bar{u}^j$

f or g at those points

How to combine $\overbrace{\bar{u}^1, \dots, \bar{u}^q}^{M(x)}$ to get a better model?

$$k_M(x) = \mathrm{Cor}\big(\xi(x), \mathbb{E}[\xi(x) \mid \xi(\phi^j)]\big)$$

ϕ^j: $\delta_{x_i^j}$ or $\delta_{x_i^j} \circ (-\Delta)$

$$K_M(x) = \mathrm{Cor}\big(\mathbb{E}[\xi(x) \mid \xi(\phi^j)]\big)$$

$$\bar{U}_A(x) = k_M(x)\, K_M^{-1}(x)\, M(x)$$

What about nonlinear PDEs?

$$\begin{cases} -\Delta u + \tau(u) = f & \Omega \\ u = g & \partial\Omega \end{cases}$$

$$\bar{U} = \arg \left| \begin{array}{l} \min \|v\|_K^2 \\ \text{s.t. } \left.\begin{array}{l} -\Delta v + \tau(v) = f \\ v = g \end{array}\right\} \text{ at collocation points} \end{array} \right.$$

$$\Longleftrightarrow \quad \left| \begin{array}{lll} \min \|v\|_K^2 & & \\ \text{s.t. } -\Delta v(x_i) = z_i^2 & v(x_i) = z_i^1 & \\ \quad z_i^2 + \tau(z_i^1) = f(x_i) & & x_i \in \Omega \\ \quad z_i^1 = g(x_i) & & x_i \in \partial\Omega \end{array} \right.$$

$$M^j(x) = \mathbb{E}\left[\xi(x) \,\middle|\, \begin{array}{l} -\Delta \xi(x_i^j) \\ \xi(x_i^j) \end{array}\right]$$

→ won't work

Alternative approach

$$\bar{u}^{n+1} = \bar{u}^{n} + \delta \bar{u}^{n}$$

$$-\Delta\left(\bar{u}^{n} + \delta \bar{u}^{n}\right) + \tau(u^{n}) + \tau'(u^{n})\,\delta u^{n} = f$$

$$\bar{u}^{n} + \delta \bar{u}^{n} = g$$

$$\Updownarrow$$

Linear PDE $\rightsquigarrow$

$$-\Delta \delta \bar{u}^{n} + \tau'(u^{n})\,\delta u^{n} = f + \Delta u^{n} - \tau(u^{n})$$

$$\delta \bar{u}^{n} = g - \bar{u}^{n}$$

$$\begin{tikzcd}
 & X \arrow[dl] \arrow[dr] & & \\
X^{1} \arrow[d] & \cdots & X^{q} \arrow[d] & \bar{u}^{n} \arrow[l] \arrow[dd, Rightarrow] \\
\delta \bar{u}^{1,n} \arrow[dr] & & \delta \bar{u}^{q,n} \arrow[dl] & \\
 & \delta \bar{u}^{n}_{A} \arrow[rr] & & \bar{u}^{n+1}
\end{tikzcd}$$

$$M^{j,n} = \mathbb{E}[\xi \mid \mathcal{G}^{n} \xi]$$

linearized PDE

$$\min \|v\|^{2}$$

$$-\Delta v + \tau'(u_n)\, v = f + \Delta u_n - \tau(u_n) \quad \Omega$$

$$v = g - u_n \quad \partial\Omega$$

$$\bar{U}^n_A \qquad X^j$$

$$\bar{U}^n_A \downarrow \mathcal{L}^n \downarrow M^{j,n} \downarrow \delta\bar{U}^n_A \downarrow \bar{U}^{n+1}$$

$$\mathbb{E}\left[\xi(x) \,\middle|\, \begin{matrix}\Delta\xi(x^j) \\ \xi(x^j)\end{matrix}\right]$$

$$\mathbb{E}[X \mid Y, Z] = \alpha Y + \beta Z$$

$$\mathbb{E}[X \mid aY + bZ] = \gamma\,(aY + bZ)$$