Multidimensional Splines

Single dimensional: $f(x) = \underset{f \in W_2^{(2)}}{\arg\inf} \sum_{i=1}^{n} (y_i - f(x_i))^2 + \lambda R(f)$

$$W_2^{(2)} = \left\{ f : f : [0,1] \to C,\ R(f) = \int f''(x)^2 < \infty \right\}$$

Goal: Extend to $x \in \mathbb{R}^p$, $f \in W_2^{(2)} [0,1]^p$

$$W_2^{(2)} [0,1]^p = \left\{ f : \int_{[0,1]^p} (\Delta f)^2 \, dx < \infty \right\}$$

$$\Delta f = \left(\frac{\partial}{\partial x_1} f + \frac{\partial}{\partial x_2} + \cdots + \frac{\partial}{\partial x_p} f \right)$$

$$f(x) = \underset{f \in W_2^{(2)}[0,1]}{\arg\inf} \sum_{i=1}^{n} (y_i - f(x_i))^2 + \lambda \int_0^1 (\Delta f(x))^2 \, dx$$

Even in the multidimensional case the solution is a natural cubic spline with knots at the data points (finite dimensional) with basis $\{N_i(x)\}_{i=1}^{m}$ on the set $[0,1]^p$

Suppose we have a dimensional dataset

Goal find $\hat{f}(x) = \sum_{j=1}^{m} N_j(x)\,\theta_j$

$$\hat{f} = \operatorname{arginf}_{f = \sum \theta_k N_k(x)} \sum_{i=1}^{n} (y_i - f(x_i))^2$$

Define $N = \begin{bmatrix} N_1(x_1) & \cdots & N_m(x) \\ \vdots & & \\ N_1(x_n) & \cdots & N_m(\vec{x}_n) \end{bmatrix}$

$$(\Delta f)^2 = \sum_i \sum_j \Delta N_j(x)\,\Delta N_i(x)\,\theta_i\,\theta_j$$

Then we estimate with the penalty

$$\hat{f} = \operatorname{argmin}_{\theta \in \mathbb{R}^m} (Y - N\theta)^T (Y - N\theta) + \lambda \int (\Delta f)^2\,dx$$

$$\hat{f} = \operatorname{argmin}_{\theta \in \mathbb{R}^m} (Y - N\theta)^T (Y - N\theta) + \lambda\,\theta^T \Omega\,\theta$$

$$\Omega = (\Omega)_{jk} = \int_{[0,1]^p} \Delta N_j(x)\,\Delta N_k(x)\,d\vec{x}$$

$$\boxed{\hat{\theta} = (N^T N + \lambda \Omega)^{-1} N^T Y}$$

$$\hat{f}(\vec{x}) = (\hat{f}(x_1) \ldots \hat{f}(x_n))^T = (\hat{y}_1, \ldots, \hat{y}_n)$$

$$= N\hat{\theta} = \underbrace{N(N^T N + \lambda\Omega)^{-1}N^T}_{S_\lambda} y$$

Smoothing Operator

Typically we define $df = tr(S_\lambda)$

Functional Analysis Overview