#2 Let $f(x)=\sum_{0}^{3}\beta_j x^j+\sum_{1}^{K}\theta_k\cdot(X-\xi_k)_+^3$

Let's prove: $\beta_2=0,\ \beta_3=0,\ \sum_{k=1}^{K}\theta_k=0,\ \sum_{k=1}^{K}\xi_k\theta_k=0.$

Then: $\begin{cases} N_1(x)=1,\ N_2(x)=X,\ N_{k+2}(x)=d_k(x)-d_{K-1}(X) \\ d_k(x)=\dfrac{(X-\xi_k)_+^3-(X-\xi_K)_+^3}{\xi_K-\xi_k} \end{cases}$

对于$(-\infty,\xi_1)$: $f'(x)=\beta_1+2\beta_2X+3\beta_3X^2$

$f''(x)=2\beta_2+6\beta_3X=0 \Rightarrow \beta_2=\beta_3=0.$ ($\forall X\in(-\infty,\xi_1)$成立)

对于$(\xi_K,+\infty)$: $f(x)=\sum_{j=0}^{3}\beta_j x^j+\sum_{k=1}^{K}\theta_k(X-\xi_k)^3$

$f'(x)=\beta_1+3\sum_{k=1}^{K}\theta_k(X-\xi_k)^2$

$\left.\begin{aligned} f''(x)=6\sum_{k=1}^{K}\theta_k(X-\xi_K)=0 \\ f(\xi_K)=0 \end{aligned}\right\} \Rightarrow \sum_{k=1}^{K}\theta_k=0,\ \sum_{k=1}^{K}\xi_k\theta_k=0.$

即 $\begin{cases} \theta_{K-1}+\theta_K=-\sum_{k=1}^{K-2}\theta_k \\ \xi_{K-1}\theta_{K-1}+\xi_K\theta_K=-\sum_{k=1}^{K-2}\theta_k\xi_k. \end{cases}$

$\Rightarrow \theta_{K-1}=\dfrac{\sum_{k=1}^{K-2}\theta_k(\xi_k-\xi_K)}{\xi_K-\xi_{K-1}};\quad \theta_K=\dfrac{\sum_{k=1}^{K-2}\theta_k(\xi_{K-1}-\xi_k)}{\xi_K-\xi_{K-1}}$

$\therefore F(x)=\beta_0+\beta_1X+\sum_{k=1}^{K-2}\theta_k(X-\xi_k)_+^3+\theta_{K-1}\cdot(X-\xi_{K-1})_+^3+\theta_K(X-\xi_K)_+^3$

$=\beta_0+\beta_1X+\sum_{k=1}^{K-2}\theta_k\cdot\left[(\xi_K-\xi_k)\cdot\dfrac{(X-\xi_k)_+^3-(X-\xi_K)_+^3}{\xi_K-\xi_k}-(\xi_K-\xi_k)\cdot\dfrac{(X-\xi_{K-1})^3-(X-\xi_K)_+^3}{\xi_K-\xi_{K-1}}\right]$

$=\beta_0+\beta_1X+\sum_{k=1}^{K-2}\theta_k(\xi_K-\xi_k)[d_k(x)-d_{K-1}(x)]$

$=\beta_0N_1(x)+\beta_1N_2(x)+\sum_{k=1}^{K-2}\theta_k(\xi_K-\xi_k)\cdot N_{k+2}(x).$

即得自然三次样条的基函数.

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#3. $\hat{f} = N\cdot(N^TN+\lambda\Omega_N)^{-1}\cdot N^Ty$

$= S_\lambda y.$ S_λ 仅依赖 x_i 和 λ.

S_λ 为对称.半正定矩阵.

$S_\lambda \cdot S_\lambda \preceq S_\lambda$. (RHS = LHS + 半正定矩阵)

$\mathrm{rank}(S_\lambda) = N$.

定义 $df_\lambda = \mathrm{trace}(S_\lambda)$ 原因:

S_λ 满秩: $S_\lambda = (N^{-T}\cdot(N^TN+\lambda\Omega_N)N^{-1})^{-1}$

$= (I+\lambda N^{-T}\Omega_N\cdot N^{-1})^{-1}$

令 $K = N^{-T}\Omega_N N^{T}$, 则 $S_\lambda = \underbrace{(I+\lambda K)^{-1}}_{\text{(分解)}}$. 其中 K 不依赖 λ.

$\because \hat{f} = S_\lambda y$ 为令 $(y-f)^T(y-f)+\lambda f^TKf$ 最小的解.

$\Rightarrow S_\lambda = \sum_{k=1}^{N}\rho_k(\lambda)u_ku_k^T$, $\rho_k(\lambda) = \frac{1}{1+\lambda d_k}$. d_k 为 K 的特征值.

此时 $df_\lambda = \mathrm{trace}(S_\lambda) = \sum_{k=1}^{N}\rho_k(\lambda)$ u_k 为基.

此变体能展示拟合参数、基函数,并更好地对光滑样条参量化.

$df(\lambda) = \sum_{k=1}^{N}\frac{1}{1+\lambda d_k}$, $K = N^{-T}\Omega_N N^{T}$

$= \sum_{i=1}^{n}\frac{\partial\hat{y}_i}{\partial y_i}$. (即有效独立参数的数量).