

Notes on minimax approaches in nonparametric regression

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1. Introduction

Consider the nonparametric regression model

$$Y_i = g(t_i) + \varepsilon_i, \quad i = 1, \dots, n,$$

where observations are taken at design points t_i for $i = 1, \dots, n$, and the errors ε_i are independent identically distributed as normal distribution with mean zero and variance σ^2 . The normality assumption is unnecessary in Section 2. The response function g is assumed to belong to a space $W = \{g: g \text{ and } g' \text{ are absolutely continuous, and } \int_0^1 |g''(t)|^2 dt < \infty\}$.

We deal with minimax estimators of g and σ^2 in some sense, based on a restricted class of the response function $W_C = \{g \in W: \int_0^1 |g''(t)|^2 dt < C\}$. To simplify the minimax problem, we shall use a natural coordinate system. Demmler and Reinsch [3] showed that there is a basis for the natural cubic splines, $\phi_1(\cdot), \dots, \phi_n(\cdot)$, determined essentially uniquely by

$$\sum_{i=1}^n \phi_j(t_i) \phi_k(t_i) = \delta_{jk}, \quad \int_0^1 \phi_j''(t) \phi_k''(t) dt = \delta_{jk} \omega_k$$

with $0 = \omega_1 = \omega_2 < \dots < \omega_n$. Here $\delta_{jk} = 1$ if $j = k$ and 0 otherwise. Let $\tilde{y} = (Y_1, \dots, Y_n)^T$ and $\tilde{g} = (g(t_1), \dots, g(t_n))^T$ be the vectors expressed with respect to a natural basis of \mathbf{R}^n , $\{\phi_j(t_i)\}$. To estimate g , Speckman [4] proposed the linear estimator of g which minimizes the expected summed squared criterion

$$J(\hat{g}) = n^{-1} \max_{g \in W_C} E \left[\sum_{i=1}^n \{\hat{g}(t_i) - g(t_i)\}^2 \right]$$

defined for any given estimator \hat{g} of g . Furthermore, he introduced a family of linear estimators \hat{g}_γ , $\gamma > 0$ which is optimal in the sense $\min J(\hat{g}) = \min_{\gamma > 0} J(\hat{g}_\gamma)$. In this paper, Section 2 gives an explicit expression of the minimax solution γ_0 for fixed value of C/σ^2 .

To estimate σ^2 , Buckley, Eagleson and Silverman [1] proposed the quadratic estimator of σ^2 which minimizes the expected squared criterion

$$M(\hat{\sigma}^2) = \max_{g \in W_C} E(\hat{\sigma}^2 - \sigma^2)^2$$

defined for given any estimator $\hat{\sigma}^2$ of σ^2 . Furthermore, they gave a family $\hat{\sigma}_\alpha^2$, $\alpha > 0$, which is optimal in the sense $\min M(\hat{\sigma}^2) = \min_{\alpha > 0} J(\hat{\sigma}_\alpha^2)$. In Section 3, we also give an explicit expression of the minimax solution α_0 for fixed value of C/σ^2 .

For an asymptotic approximation for large n , we use a particular series $\omega_j = \rho n^{-1} j^4$ ($3 \leq j \leq n$) for some constant ρ . Asymptotic expansions of the minimax solutions are given in Section 4.

2. Minimax solution for estimating g

Let \hat{g} be a linear estimator of \tilde{y} . Then we can write $(\hat{g}(t_1), \dots, \hat{g}(t_n))^T = A\tilde{y}$. For simplicity, write $(\hat{g}(t_1), \dots, \hat{g}(t_n))^T = (g_1, \dots, g_n)^T$, and $J(\hat{g}) = J(A)$. Let \mathcal{M} be the set of all $n \times n$ matrices. Then

$$J(A) = n^{-1} \max_{\sum \omega_i g_i^2 \leq C} \{ \tilde{g}^T (I - A)^T (I - A) \tilde{g} + \sigma^2 \text{tr} A^T A \}.$$

Speckman [4] proposed interpolating $A_0 \tilde{y}$ for A_0 which minimizes $J(A)$ over $A \in \mathcal{M}$. The following theorem gives an explicit expression for A_0 .

THEOREM 1. *For any fixed value of C/σ^2 , say r , the minimum over $A \in \mathcal{M}$ of $J(A)$ is attained when A is diagonal with diagonal elements a_{ii} given by*

$$\begin{aligned} a_{ii} &= 1 - (\gamma_0 \omega_i)^{1/2} & (i \leq v_J) \\ &= 0 & (i > v_J), \end{aligned}$$

where γ_0 and v_J are determined as follows: if for some $3 \leq j \leq n-1$

$$\sum_{i=3}^j \omega_i^{1/2} (\omega_j^{1/2} - \omega_i^{1/2}) \leq r \leq \sum_{i=3}^{j+1} \omega_i^{1/2} (\omega_{j+1}^{1/2} - \omega_i^{1/2})$$

then

$$v_J = j \quad \text{and} \quad \gamma_0 = \left(\frac{\sum_{i=3}^j \omega_i^{1/2}}{r + \sum_{i=3}^j \omega_i} \right)^2,$$

and if

$$\sum_{i=3}^n \omega_i^{1/2} (\omega_n^{1/2} - \omega_i^{1/2}) \leq r$$

then

$$v_J = n \quad \text{and} \quad \gamma_0 = \left(\frac{\sum_{i=3}^n \omega_i^{1/2}}{r + \sum_{i=3}^n \omega_i} \right)^2.$$

PROOF. Let $\mathcal{M}_D = \{A \in \mathcal{M} : A = \text{diag}(1, 1, a_3, \dots, a_n)\}$. Speckman [4] showed that $\min_{A \in \mathcal{M}} J(A) = \min_{A \in \mathcal{M}_D} J(A)$ and for $A = \text{diag}(1, 1, a_3, \dots, a_n)$

$$J(A) = n^{-1} \sigma^2 \left\{ r \max_{3 \leq i \leq n} (1 - a_i)^2 / \omega_i + \sum_{i=1}^n a_i^2 \right\}.$$

Now let $\mathcal{M}_\gamma = \{A \in \mathcal{M}_D : \max_{3 \leq i \leq n} (1 - a_i)^2 / \omega_i = \gamma\}$, $\gamma \geq 0$. We get

$$\begin{aligned} \min_{A \in \mathcal{M}_\gamma} nJ(A)/\sigma^2 &= r\gamma + 2 + \sum_{i=3}^n \max\{0, 1 - (\gamma\omega_i)^{1/2}\}^2, & \gamma \leq \omega_3^{-1} \\ &= r\gamma + 2 + (1 - (\gamma\omega_3)^{1/2})^2, & \gamma \geq \omega_3^{-1}. \end{aligned}$$

Define H by $H(\gamma^{1/2}) = \min_{A \in \mathcal{M}_\gamma} nJ(A)/\sigma^2$. Then for $\xi \geq 0$

$$\begin{aligned} H(\xi) &= r\xi^2 + 2 + \sum_{i=3}^n (1 - \xi\omega_i^{1/2})^2, & \xi \leq \omega_n^{1/2} \\ &= r\xi^2 + 2 + \sum_{i=3}^j (1 - \xi\omega_i^{1/2})^2, & \omega_{j+1}^{-1/2} \leq \xi \leq \omega_j^{-1/2} \\ &= r\xi^2 + 2 + (1 - \xi\omega_3^{1/2})^2, & \omega_3^{1/2} \leq \xi. \end{aligned}$$

The $H(\xi)$ has a continuous derivative and twice differentiable on $\{\xi > 0\}$ except for points $\omega_i^{-1/2}$ ($4 \leq i \leq n$). $H''(\xi) > 0$, $\lim_{\xi \rightarrow +0} H'(\xi) < 0$, and $H'(\omega_3^{-1/2}) \geq 0$. Therefore there uniquely exists $\xi_0 \in (0, \omega_3^{-1/2})$ which minimizes $H(\xi)$ over $\{\xi \geq 0\}$. Note that $H(\xi)$ is piecewise polynomial of degree 2. If $\xi_0 \leq \omega_n^{-1/2}$ then $(\sum_{i=3}^n \omega_i^{1/2}) / (r + \sum_{i=3}^n \omega_i) \leq \omega_n^{-1/2}$ and $\xi_0 = (\sum_{i=3}^n \omega_i^{1/2}) / (r + \sum_{i=3}^n \omega_i)$. If for some $3 \leq j \leq n$, $\omega_{j+1}^{-1/2} \leq \xi_0 \leq \omega_j^{-1/2}$ then $\omega_{j+1}^{-1/2} \leq (\sum_{i=3}^j \omega_i^{1/2}) / (r + \sum_{i=3}^j \omega_i) \leq \omega_j^{-1/2}$ and $\xi_0 = (\sum_{i=3}^j \omega_i^{1/2}) / (r + \sum_{i=3}^j \omega_i)$. Replacing ξ_0 by $\gamma_0^{1/2}$ we complete the proof of Theorem 1.

REMARK. We can write $\min_{A \in \mathcal{M}} J(A)/\sigma^2$ as $n^{-1} \{r\gamma_0 + \sum_{i=3}^{v_J} (1 - \gamma_0^{1/2} \omega_i^{1/2})^2\}$ in the proof of Theorem 1. By substituting our expression for γ_0 to this expression, we also have

$$\min_{A \in \mathcal{M}} J(A)/\sigma^2 = n^{-1} \left\{ v_J - \gamma_0^{1/2} \sum_{i=3}^{v_J} \omega_i^{1/2} \right\} = n^{-1} \text{tr } A_0.$$

3. Minimax solution for estimating σ^2

We restrict our attention to estimators of σ^2 whose form is $\hat{\sigma}^2(D) = \tilde{y}^T D \tilde{y} / \text{tr } D$, $D \in \mathcal{A}$. Here \mathcal{A} is the class of $n \times n$ symmetric non-negative definite matrices D for which $\hat{\sigma}^2(D)$ is unbiased when g is a straight line. For simplicity, write $M(\hat{\sigma}^2(D)) = M(D)$. Then

$$M(D) = \max_{\Sigma \omega_i \tilde{g}_i^2 \leq C} \{(\tilde{g}^T D \tilde{g})^2 + 4\sigma^2 \tilde{g}^T D^2 \tilde{g} + 2\sigma^4 \text{tr} D^2\} / (\text{tr} D)^2.$$

Buckley et al. [1] proposed minimizing $M(D)$ over $D \in \mathcal{A}$ of $M(D)$. The following theorem gives an explicit expression for D which minimizes $M(D)$.

THEOREM 2. For any fixed value of C/σ^2 , say r , the minimum over $D \in \mathcal{A}$ of $M(D)$ is attained when D is diagonal with diagonal elements d_{ii} given by

$$\begin{aligned} d_{ii} &= \alpha_0 \omega_i^+ & (i \leq v_M) \\ &= 1 & (i > v_M), \end{aligned}$$

with $\omega_i^+ = \omega_i(1 + 4\omega_i/r)^{-1/2}$, where α_0 and v_M are determined as follows: if for some $3 \leq j \leq n-1$

$$2 \sum_{i=3}^j \omega_i^+ (\omega_j^+ - \omega_i^+) \leq r^2 \leq 2 \sum_{i=3}^{j+1} \omega_i^+ (\omega_{j+1}^+ - \omega_i^+)$$

then

$$v_M = j \quad \text{and} \quad \alpha_0 = \frac{2 \sum_{i=3}^j \omega_i^+}{r^2 + 2 \sum_{i=3}^j (\omega_i^+)^2},$$

and if

$$2 \sum_{i=3}^n \omega_i^+ (\omega_n^+ - \omega_i^+) \leq r^2$$

then

$$v_M = n \quad \text{and} \quad \alpha_0 = \frac{2 \sum_{i=3}^n \omega_i^+}{r^2 + 2 \sum_{i=3}^n (\omega_i^+)^2}.$$

PROOF. Let $\mathcal{A}_D = \{D \in \mathcal{A} : D = \text{diag}(0, 0, d_3, \dots, d_n)\}$. Buckley et al. [1] reduced the problem of minimizing $M(D)$ to finding $D \in \mathcal{A}$ which minimizes

$$L(D) = \max_{\Sigma \omega_i \tilde{g}_i^2 \leq C} \{(\tilde{g}^T D \tilde{g})^2 + 4\sigma^2 \tilde{g}^T D^2 \tilde{g} + 2\sigma^4 \text{tr} D^2 - \lambda \text{tr} D\}$$

for any fixed Lagrangian multiplier λ . Furthermore they showed that $\min_{D \in \mathcal{A}} L(D) = \min_{D \in \mathcal{A}_D} L(D)$ and for $D = \text{diag}(0, 0, d_3, \dots, d_n)$

$$L(D) = \sigma^4 \{r^2 \max_{3 \leq i \leq n} (d_i/\omega_i^+)^2 + 2 \sum_{i=1}^n d_i (d_i - \lambda/2\sigma^4)\}.$$

If $\lambda \leq 0$, then $L(D)$ is minimized when D is zero matrix. Assume that $\lambda > 0$. Multiplying D by a positive constant does not change $M(D)$, so that we replace d_i by $\lambda d_i/4\sigma^4$ ($3 \leq i \leq n$). Then

$$L(D) = (\lambda^2/16\sigma^4) \left\{ r^2 \max_{3 \leq i \leq n} (d_i/\omega_i^+)^2 + 2 \sum_{i=1}^n d_i(d_i - 2) \right\}.$$

Now let $\Delta_\alpha = \{D \in \Delta_D : \max_{3 \leq i \leq n} d_i/\omega_i^+ = \alpha\}$, $\alpha \geq 0$. If $\alpha \leq (\omega_3^+)^{-1}$ then the minimum of $L(D)$ over $D \in \Delta_\alpha$ is attained when $d_i = \min\{1, \alpha\omega_i^+\}$ and if $\alpha \geq (\omega_3^+)^{-1}$ then the minimum of $L(D)$ over $D \in \Delta_\alpha$ is attained when $d_3 = \alpha\omega_3^+$ and $d_i = 1$ ($4 \leq i \leq n$). Define H by $H(\alpha) = \min_{D \in \Delta_\alpha} 16\sigma^4 L(D)/\lambda^2$. Then for $\alpha \geq 0$

$$\begin{aligned} H(\xi) &= \alpha^2 \left\{ r^2 + 2 \sum_{i=3}^n (\omega_i^+)^2 \right\} - 4\alpha \sum_{i=3}^n \omega_i^+, & \alpha &\leq (\omega_n^+)^{-1} \\ &= \alpha^2 \left\{ r^2 + 2 \sum_{i=3}^j (\omega_i^+)^2 \right\} - 4\alpha \sum_{i=3}^j \omega_i^+ - 2(n-j), & (\omega_{j+1}^+)^{-1} &\leq \alpha \leq (\omega_j^+)^{-1} \\ &= \alpha^2 \left\{ r^2 + 2(\omega_3^+)^2 \right\} - 4\alpha\omega_3^+ - 2(n-3), & (\omega_3^+)^{-1} &\leq \alpha. \end{aligned}$$

The $H(\alpha)$ has a continuous derivative and twice differentiable on $\{\alpha > 0\}$ except for points $(\omega_i^+)^{-1}$ ($4 \leq i \leq n$). $H''(\alpha) > 0$, $\lim_{\alpha \rightarrow +0} H'(\alpha) < 0$, and $H'((\omega_3^+)^{-1}) \geq 0$. Therefore there uniquely exists $\alpha_0 \in (0, (\omega_3^+)^{-1})$ which minimizes $H(\alpha)$ over $\{\alpha \geq 0\}$. Note that $H(\alpha)$ is piecewise polynomial of degree 2. If $\alpha_0 \leq (\omega_n^+)^{-1}$ then $(2 \sum_{i=3}^n \omega_i^+)/ (r^2 + 2 \sum_{i=3}^n \omega_i^+) \leq (\omega_n^+)^{-1}$ and $\alpha_0 = (2 \sum_{i=3}^n \omega_i^+) / (r^2 + 2 \sum_{i=3}^n (\omega_i^+)^2)$. If for some $3 \leq j \leq n-1$, $(\omega_{j+1}^+)^{-1} \leq \xi_0 \leq (\omega_j^+)^{-1}$ then $(\omega_{j+1}^+)^{-1} \leq (2 \sum_{i=3}^j \omega_i^+) / (r^2 + 2 \sum_{i=3}^j (\omega_i^+)^2) \leq (\omega_j^+)^{-1}$ and $\alpha_0 = (2 \sum_{i=3}^j \omega_i^+) / (r^2 + 2 \sum_{i=3}^j (\omega_i^+)^2)$. This completes the proof.

REMARK. We can write $\min_{D \in \Delta} M(D)/\sigma^4$ as $\{r^2\alpha_0^2 + \sum_{i=3}^{v_M} (\alpha_0\omega_i^+)^2 + n - v_M\} / \{\sum_{i=3}^{v_M} \alpha_0\omega_i^+ + n - v_M\}^2$ in the proof of Theorem 2. By substituting our expression for α_0 to this expression, we also have

$$\min_{D \in \Delta} M(D)/\sigma^4 = 2 \left\{ \alpha_0 \sum_{i=3}^{v_M} \omega_i^+ + n - v_M \right\}^{-1}.$$

Buckley et al. [1] defined a new criterion

$$K(D) = \max_{\sum \omega_i \tilde{g}_i^2 \leq C} \{(\tilde{g}^T D \tilde{g})^2 + 2\sigma^4 \text{tr } D^2\} / (\text{tr } D)^2$$

for estimating σ^2 , and discussed the relations between minimax estimators based on these two criteria. The following theorem gives an explicit expression for D which minimizes $K(D)$.

THEOREM 3. For any fixed value of C/σ^2 , say r , the minimum over $D \in \Delta$ of $K(D)$ is attained when D is diagonal with diagonal elements d_{ii} given by

$$\begin{aligned} d_{ii} &= \beta_0 \omega_i & (i \leq v_K) \\ &= 1 & (i > v_K), \end{aligned}$$

where β_0 and v_K are determined as follows: if for some $3 \leq j \leq n-1$

$$2 \sum_{i=3}^j \omega_i(\omega_j - \omega_i) \leq r^2 \leq 2 \sum_{i=3}^{j+1} \omega_i(\omega_{j+1} - \omega_i)$$

then

$$v_K = j \quad \text{and} \quad \beta_0 = \frac{2 \sum_{i=3}^j \omega_i}{r^2 + 2 \sum_{i=3}^j \omega_i^2},$$

and if

$$2 \sum_{i=3}^n \omega_i(\omega_n - \omega_i) \leq r^2$$

then

$$v_K = n \quad \text{and} \quad \beta_0 = \frac{2 \sum_{i=3}^n \omega_i}{r^2 + 2 \sum_{i=3}^n \omega_i^2}.$$

PROOF. Replacing ω_i^+ by ω_i in the proof of the Theorem 2 suffices the proof.

REMARK. We can write $\min_{D \in \Delta} K(D)/\sigma^4$ as $\{r^2 \beta_0^2 + \sum_{i=3}^{v_K} (\beta_0 \omega_i)^2 + n - v_K\} / \{\sum_{i=3}^{v_K} \beta_0 \omega_i + n - v_K\}^2$ in the proof of Theorem 3. By substituting our expression for β_0 to this expression, we also have

$$\min_{D \in \Delta} K(D)/\sigma^4 = 2 \left\{ \beta_0 \sum_{i=3}^{v_K} \omega_i + n - v_K \right\}^{-1}.$$

4. Asymptotic results

In this section we discuss the asymptotic behavior for large sample size of minimax solutions obtained in Sections 2 and 3. Speckman [4] showed that for large n the ω_j is approximately $n^{-1} \rho j^4$, where ρ is a constant.

Let \bar{v}_J be the solution of the equation $\sum_{i=3}^{\bar{v}_J} \omega_i^{1/2} (\omega_{\bar{v}_J}^{1/2} - \omega_i^{1/2}) = r$. Then the v_J is the largest integer that is smaller than n and \bar{v}_J by Theorem 1. By expanding \bar{v}_J in decreasing powers of n , we have the following theorem.

THEOREM 4. Under the assumption $\omega_j = \rho n^{-1} j^4$ ($3 \leq j \leq n$), $\bar{v}_J - 1 \leq v_J \leq \bar{v}_J$ and the \bar{v}_J is expanded as

$$(4.1) \quad \bar{v}_J = z + \frac{1}{4} z^{-1} + O(z^{-2})$$

with $z = (15rn/2\rho)^{1/5}$, as $n \rightarrow \infty$. Write $v_J = \bar{v}_J - a_J$ ($0 \leq a_J \leq 1$), then the γ_0 is expanded as

$$(4.2) \quad \gamma_0 = \frac{1}{15r} z [1 + (-6a_J^2 + 6a_J - 1)z^{-2} + O(z^{-3})].$$

The minimum of $J(A)/\sigma^2$ is

$$(4.3) \quad \frac{1}{n} \left[\frac{2}{3} z + \frac{1}{2} + O(z^{-2}) \right].$$

Speckman [4] obtained the leading terms of (4.1) and (4.2). Carter, Eagleson and Silverman [2] obtained the leading tem of (4.3).

Similarly the next theorem gives the asymptotic results on minimax solutions for estimating σ^2 based on two criterions $M(D)$ and $K(D)$.

THEOREM 5. *Under the assumption $\omega_j = \rho n^{-1} j^4$ ($3 \leq j \leq n$), $\bar{v}_M - 1 \leq v_M \leq \bar{v}_M$, $\bar{v}_K - 1 \leq v_K \leq \bar{v}_K$, and the \bar{v}_M and \bar{v}_K are expanded as*

$$(4.4) \quad \bar{v}_M = w + \frac{46}{117} \left(\frac{45}{8} \right)^{1/2} w^{1/2} - \frac{2095}{5746} - \frac{73016675}{63530649} \left(\frac{45}{8} \right)^{1/2} w^{-1/2} \\ + \frac{16413426245}{2160042066} w^{-1} + O(w^{-2})$$

$$(4.5) \quad \bar{v}_K = w + \frac{5}{12} w^{-1} + O(w^{-2})$$

with $w = (45r^2 n^2 / 8\rho^2)^{1/9}$, as $n \rightarrow \infty$. Write $v_M = \bar{v}_M - a_M$ ($0 \leq a_M < 1$), and $v_K = \bar{v}_K - a_K$ ($0 \leq a_K < 1$), respectively, then the α_0 and β_0 are expanded as

$$(4.6) \quad \alpha_0 = \left(\frac{8}{45} \right)^{1/2} \frac{w^{1/2}}{r} \left[1 + \frac{50}{117} \left(\frac{45}{8} \right)^{1/2} w^{-1/2} - \frac{8725}{7956} w^{-1} \right. \\ \left. - \frac{2922875}{9773946} \left(\frac{45}{8} \right)^{1/2} w^{-3/2} + \left(-10a_M^2 + 10a_M + \frac{908518055}{182860704} \right) w^{-2} \right. \\ \left. + O(w^{-3}) \right],$$

$$(4.7) \quad \beta_0 = \left(\frac{8}{45} \right)^{1/2} \frac{w^{1/2}}{r} \left[1 + \left(-10a_K^2 + 10a_K - \frac{5}{3} \right) w^{-2} + O(w^{-3}) \right].$$

The minimum of $M(D)/\sigma^4$ is

$$(4.8) \quad \frac{1}{n} \left[1 - \frac{9r}{2\rho} \left(\frac{8}{45} \right)^{1/2} w^{-7/2} - \frac{10r}{13\rho} w^{-4} \right. \\ \left. - \frac{10r(51714a_M + 31217)}{45986\rho} \left(\frac{8}{45} \right)^{1/2} w^{-9/2} + O(w^{-5}) \right].$$

The minimum of $K(D)/\sigma^4$ is

$$(4.9) \quad \frac{1}{n} \left[1 - \frac{9r}{2\rho} \left(\frac{8}{45} \right)^{1/2} w^{-7/2} - \frac{45r(2a_M + 1)}{16\rho} \left(\frac{8}{45} \right)^{1/2} w^{-9/2} + O(w^{-5}) \right].$$

Buckley et al. [1] obtained the leading term in (4.5), (4.7) and (4.9). Carter et al. [2] obtained the second order term in (4.9). They made use of approximations of sums by integrals.

References

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