The max-MSE's of minimax estimators of variance in nonparametric regression

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1. Introduction and notations

Consider the nonparametric regression model

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

where observations are taken at design points t_i for $1 \le i \le n$, and the errors ε_i are independent and identically distributed as normal distribution with mean zero and variance σ^2 . The response function g is assumed to belong to the 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 σ^2 defined in Buckley, Eagleson and Silverman [1]. They are based on a restricted class of the response functions $W_C = \{g \in W : \int_0^1 |g''(t)|^2 dt \le C\}$. Define the max-MSE criterion as

$$M(\hat{\sigma}^2; \sigma^2, C) = \max_{\alpha \in W_C} \frac{1}{\sigma^4} E(\hat{\sigma}^2 - \sigma^2)^2$$

for any given estimator $\hat{\sigma}^2$ of σ^2 . To simplify the minimax problem, we shall use a natural coordinate system. Demmler and Reinsch [2] showed that there is a basis for the natural cubic splines, $\phi_1(\cdot)$, ..., $\phi_n(\cdot)$, determined essentially uniquely by

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

with $0 = \omega_1 = \omega_2 < \cdots < \omega_n$. Here $\delta_{jk} = 1$ if j = k and 0 otherwise. Let $\tilde{y} = (Y_1, \ldots, Y_n)^T$ and $\tilde{g} = (g(t_1), \ldots, g(t_n))^T$ be the vectors expressed with respect to a natural basis of R^n , $\{(\phi_j(t_i))\}$. Our attention is restricted to a class of estimators of σ^2 whose form is $\hat{\sigma}^2(D) = \tilde{y}^T D \tilde{y} / \text{tr } D$, $D \in \Delta$. Here Δ 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. Buckley, Eagleson and Silverman [1] proposed minimax estimators defined as the estimator which minimizes $M(\hat{\sigma}^2(D); \sigma^2, C)$ over $D \in \Delta$. Their minimax estimators depend on σ^2 and C through C/σ^2 . The explicit expressions of them were obtained in Fujioka [3] as follows. Putting $\omega_i^+(r) = \omega_i (1 + 4\omega_i/r)^{-1/2}$ for $3 \le i \le n$, we set for $3 \le k \le n - 1$

$$R_k = \left\{ r > 0 : 2 \sum_{i=3}^k \omega_i^+(r) (\omega_k^+(r) - \omega_i^+(r)) < r^2 \le 2 \sum_{i=3}^{k+1} \omega_i^+(r) (\omega_{k+1}^+(r) - \omega_i^+(r)) \right\},$$

and

$$R_n = \left\{ r > 0 : 2 \sum_{i=3}^k \omega_i^+(r)(\omega_k^+(r) - \omega_i^+(r)) < r^2 \right\}.$$

We also set for $3 \le k \le n$

$$d_i^+(r) = \min \left\{ \alpha_k^+(r)\omega_i^+(r), 1 \right\}, \qquad 3 \le i \le n, \qquad r \in R_k,$$

where

$$\alpha_k^+(r) = \frac{2\sum_{i=3}^k \omega_i^+(r)}{r^2 + 2\sum_{i=3}^k \omega_i^+(r)^2}.$$

Then, the minimax estimators of σ^2 are expressed as $\hat{\sigma}^2(D^+)$ with

$$D^+ = \text{diag}(0, 0, d_3^+(r), \ldots, d_n^+(r)).$$

Rewrite $\hat{\sigma}^2(D^+) = \hat{\sigma}^2(r)$ as a function of r > 0. In this paper, we investigate the behavior of $M(\hat{\sigma}^2(r); \sigma^2, C)$ for any fixed value of C/σ^2 .

2. Theorems

Each component of \tilde{y} corresponds to the basis function ϕ_j and $\hat{\sigma}^2(r)$ is a weighted sum of squared components of \tilde{y} . Now, for r > 0 we define

$$x_j(r) = \frac{d_j^+(r)}{d_{j-1}^+(r)}, \quad 4 \le i \le n.$$

We have the following property of the ratios of the weights.

THEOREM 1. $\lim_{r\to +0} x_4(r) = 1$ and for $5 \le j \le n$, $x_4(r) = 1$ on $\bigcup_{i< j-1} R_i$. Furthermore, for $4 \le j \le n$, $x_j(r)$ is strictly monotone increasing function of r on $\bigcup_{i\ge j-1} R_i$.

If $C/\sigma^2 = s$, then $\hat{\sigma}^2(s)$ minimizes $M(\hat{\sigma}^2(D); \sigma^2, C)$ over $D \in \Delta$. Hence, $\hat{\sigma}^2(s)$ minimizes $M(\hat{\sigma}^2(r); \sigma^2, C)$ over r > 0. We have prominent properties of the class of minimax estimators $\hat{\sigma}^2(r): r > 0$.

THEOREM 2. For any fixed value of C/σ^2 , say s, $M(\hat{\sigma}^2(r); \sigma^2, C)$ is strictly monotone decreasing function of r on (0, s) and strictly monotone increasing function of r on (s, ∞) .

THEOREM 3. For any fixed value of C/σ^2 , say s,

$$M(\hat{\sigma}^2(+0); \sigma^2, C) = \frac{s^2 + 4\omega_3 s + 2(n-2)\omega_3^2}{(n-2)^2 \omega_3^2},$$
(2.1)

and

$$M(\hat{\sigma}^{2}(+\infty); \sigma^{2}, C) = \frac{s^{2} + 4\omega_{n}s + 2\sum_{i=3}^{n}\omega_{i}^{2}}{(\sum_{i=3}^{n}\omega_{i})^{2}}.$$
 (2.2)

Furthermore, there exists an $s_0 > 0$ such that

$$M(\hat{\sigma}^2(+0); \sigma^2, C) \leq M(\hat{\sigma}^2(+\infty); \sigma^2, C) \Leftrightarrow s \leq s_0$$
. (2.3)

COROLLARY. If $s \le s_0$, then we have the inequality:

$$M(\hat{\sigma}^2(s); \sigma^2, C) < \frac{s^2 + 4\omega_3 s + 2(n-2)\omega_3^2}{(n-2)^2\omega_3^2}.$$

If $s \ge s_0$, then we have the inequality:

$$M(\hat{\sigma}^2(s); \sigma^2, C) < \frac{s^2 + 4\omega_n s + 2\sum_{i=3}^n \omega_i^2}{(\sum_{i=3}^n \omega_i)^2}.$$

Note that $\hat{\sigma}^2(+0)$ is the ordinary least squared estimator in linear regression:

$$\hat{\sigma}^2(+0) = \sum_{i=3}^n \tilde{y}_i^2/(n-2)$$
.

Also note that $\hat{\sigma}^2(+\infty)$ is the estimator which minimizes $\max_{g \in W} \frac{1}{\sigma^4} E(\hat{\sigma}^2(D) - \sigma^2)^2$ over $D \in \Delta$:

$$\hat{\sigma}^2(+\infty) = \sum_{i=3}^n \omega_i \tilde{y}_i^2 \left/ \left(\sum_{i=3}^n \omega_i \right) \right.$$

A comparison of three estimators, $\hat{\sigma}^2(+0)$, $\hat{\sigma}^2(+\infty)$, $\hat{\sigma}^3(s)$, is given in Theorem 3 and Corollary.

3. Proofs of Theorems

Proof of Theorem 1: If $r \in R_k$ $(3 \le k \le n-1)$, then

$$x_j(r) = \frac{\omega_j^+(r)}{\omega_{j-1}^+(r)}\,, \qquad 4 \le j \le k\,,$$

$$x_{k+1}(r) = \frac{r^2 + 2\sum_{i=3}^{k} \omega_i^+(r)^2}{2\omega_k^+(r)\sum_{i=3}^{k} \omega_i^+(r)}$$

$$x_i = 1 , \qquad k+1 < j \le n .$$

If $r \in R_n$, then

$$x_j(r) = \frac{\omega_j^+(r)}{\omega_{j-1}^+(r)}, \qquad 4 \le j \le n.$$

We have $\lim_{r\to +0} x_4(r) = \lim_{r\to +0} (r^2 + 2\omega_3^+(r)^2)/2\omega_3^+(r)^2 = 1$. If r > s > 0, then for $4 \le j \le n$

$$\frac{\omega_{j}^{+}(r)}{\omega_{j-1}^{+}(r)} \frac{\omega_{j-1}^{+}(s)}{\omega_{j}^{+}(s)} = \left\{ 1 + \frac{4(r-s)(\omega_{j}-\omega_{j-1})}{(r+4\omega_{j})(s+4\omega_{j-1})} \right\}^{1/2} > 1.$$
 (3.1)

Thus, for $4 \le j \le n$, $\omega_j^+(r)/\omega_{j-1}^+(r)$ is strictly monotone increasing function of r. Now, it suffices to prove that if $2\sum_{i=3}^k \omega_i^+(r)(\omega_k^+(r)-\omega_i^+(r)) < r^2$,

$$F_k(r) = \frac{r^2 + 2\sum_{i=3}^k \omega_i^+(r)^2}{2\omega_k^+(r)\sum_{i=3}^k \omega_i^+(r)}$$

is strictly monotone increasing function of r for $3 \le k \le n$. Putting $z_i = \omega_i^+(r)/r$ $(3 \le k \le n)$, we have

$$F_k(r) = \frac{1 + 2\sum_{i=3}^k z_i^2}{2z_k \sum_{i=3}^k z_i},$$

and

$$1 - 2z_k \sum_{i=3}^k z_i + 2 \sum_{i=3}^k z_i^2 > 0.$$

We can get

$$\frac{\partial F_k}{\partial z_i} = \frac{4z_i \sum_{i=3}^k z_i - (1 + 2\sum_{i=3}^k z_i^2)}{2z_k (\sum_{i=3}^k z_i)^2}, \quad 3 \le i \le k-1,$$

$$\frac{\partial F_k}{\partial z_k} = \frac{4z_k^2 \sum_{i=3}^k z_i - (1 + 2 \sum_{i=3}^k z_i^2)(z_k + \sum_{i=3}^k z_i)}{2z_k^2 (\sum_{i=3}^k z_i)^2},$$

and

$$\frac{dz_i}{dr} = -\frac{z_i(r+2\omega_i)}{r(r+4\omega_i)}, \quad 3 \le i \le k.$$

By substituting these equations to the relation

$$\frac{dF_k}{dr} = \sum_{i=3}^k \frac{\partial F_k}{\partial z_i} \frac{dz_i}{dr},$$

we can obtain

$$\begin{split} 2rz_k \bigg(\sum_{i=3}^k z_i \bigg)^2 \frac{dF_k}{dr} &= \bigg(1 - 2z_k \sum_{i=3}^k z_i + 2 \sum_{i=3}^k z_i^2 \bigg) \sum_{i=3}^k \bigg(\frac{r + 2\omega_i}{r + 4\omega_i} + \frac{r + 2\omega_k}{r + 4\omega_k} \bigg) z_i \\ &+ 2 \bigg(\sum_{i=3}^k z_i \bigg) \sum_{i=3}^k \left\{ \frac{r + 2\omega_i}{r + 4\omega_i} (z_k - z_i) z_i + \bigg(\frac{r + 2\omega_k}{r + 4\omega_k} z_k - \frac{r + 2\omega_i}{r + 4\omega_i} z_i \bigg) z_i \right\}. \end{split}$$

By using the fact that both $\{z_i\}$ and $\left\{\frac{r+2\omega_i}{r+4\omega_i}z_i\right\}$ are increasing sequences, we can show $dF_k/dr > 0$.

Proof of Theorem 2: For any fixed value of C/σ^2 , say s, we have

$$M(\hat{\sigma}^{2}(r); \sigma^{2}, C) = \left\{ s^{2} \max_{3 \leq i \leq n} \left(\frac{d_{i}^{+}(r)}{\omega_{i}^{+}(s)} \right)^{2} + 2 \sum_{i=3}^{n} d_{i}^{+}(r)^{2} \right\} / \left(\sum_{i=3}^{n} d_{i}^{+}(r) \right)^{2},$$

as is shown in Buckley, Eagleson and Silverman [1]. Let l(r, s) denote

$$\min \left\{ l : \max_{3 \le i \le n} \frac{d_i^+(r)}{\omega_i^+(s)} = \frac{d_i^+(r)}{\omega_i^+(s)} \right\}.$$

The inequality (3.1) ensures that $\{\omega_i^+(r)/\omega_i^+(s)\}$ is a monotone sequence. We evaluate the value of l(r, s). Assume that $r \in R_k$ ($3 \le k \le n - 1$). If $r \le s$, then

$$\frac{\alpha_{k}^{+}(r)\omega_{3}^{+}(r)}{\omega_{3}^{+}(s)} \ge \cdots \ge \frac{\alpha_{k}^{+}(r)\omega_{k}^{+}(r)}{\omega_{k}^{+}(s)} \ge \frac{1}{\omega_{k+1}^{+}(s)} > \cdots > \frac{1}{\omega_{n}^{+}(s)}.$$

Thus, l(r, s) = 3. If r > s and $r^2 \le 2 \sum_{i=3}^k \omega_i^+(r) \left(\frac{\omega_{k+1}^+(s)}{\omega_k^+(s)} \omega_k^+(r) - \omega_i^+(r) \right)$, then

$$\frac{\alpha_k^+(r)\omega_3^+(r)}{\omega_3^+(s)} < \dots < \frac{\alpha_k^+(r)\omega_k^+(r)}{\omega_k^+(s)} \ge \frac{1}{\omega_{k+1}^+(s)} > \dots > \frac{1}{\omega_n^+(s)}.$$

Thus, l(r, s) = k. If r > s and $r^2 > 2 \sum_{i=3}^k \omega_i^+(r) \left(\frac{\omega_{k+1}^+(s)}{\omega_k^+(s)} \omega_k^+(r) - \omega_i^+(r) \right)$, then

$$\frac{\alpha_k^+(r)\omega_3^+(r)}{\omega_3^+(s)} < \dots < \frac{\alpha_k^+(r)\omega_k^+(r)}{\omega_k^+(s)} < \frac{1}{\omega_{k+1}^+(s)} > \dots > \frac{1}{\omega_n^+(s)}.$$

Thus, l(r, s) = k + 1. Assume that $r \in R_n$. If $r \le s$, then

$$\frac{\alpha_n^+(r)\omega_3^+(r)}{\omega_3^+(s)} \ge \cdots \ge \frac{\alpha_n^+(r)\omega_n^+(r)}{\omega_n^+(s)}.$$

Thus, l(r, s) = 3. If r > s, then

$$\frac{\alpha_k^+(r)\omega_3^+(r)}{\omega_3^+(s)} < \dots < \frac{\alpha_n^+(r)\omega_n^+(r)}{\omega_n^+(s)}.$$

Thus, l(r, s) = n.

We express $M(\hat{\sigma}^2(r); \sigma^2, C)$ as a function of $x_4(r), \ldots, x_n(r)$ and proceed to prove Theorem 2. For notational convenience, put $x_3 = 1$. For $3 \le k \le n$, define

$$H_k(x_4, \ldots, x_n) = \frac{A_k x_3^2 \cdots x_k^2 + \sum_{i=3}^n x_3^2 \cdots x_i^2}{(\sum_{i=3}^n x_3 \cdots x_i)^2}$$

with $A_k = \frac{s^2}{2\omega_k^+(s)^2}$. Then, we have $M(\hat{\sigma}^2(r); \sigma^2, C) = 2H_k(x_4, \dots, x_n)$ if l(r, s) = k.

Assume that l(r, s) = 3. We have

$$\frac{\partial H_3}{\partial x_j} = \frac{2}{x_j \left(\sum_{i=3}^n x_3 \cdots x_i\right)^3} \left\{ \left(\sum_{i=3}^{j-1} x_3 \cdots x_i\right) \left(\sum_{i=j}^n x_3^2 \cdots x_i^2\right) - \left(A_3 + \sum_{i=3}^{j-1} x_3^2 \cdots x_i^2\right) \left(\sum_{i=j}^n x_3 \cdots x_i\right) \right\}.$$

Let U_j , V_j be functions defined by

$$U_j(x_4,\ldots,x_n)=\frac{x_j(\sum_{i=3}^n x_3\cdots x_i)^3}{2}\frac{\partial H_3}{\partial x_i}, \qquad 4\leq j\leq n,$$

and

$$V_j(x_4, \ldots, x_j) = x_3 \cdots x_j \sum_{i=3}^{j-1} x_3 \cdots x_i - \sum_{i=3}^{j-1} x_3^2 \cdots x_i^2, \quad 4 \le j \le n.$$

We get

$$U_{j}-U_{j+1}=x_{3}\cdots x_{j}\left\{V_{j}-A_{3}+x_{3}\cdots x_{j}\sum_{i=j+1}^{n}x_{3}\cdots x_{i}(1-x_{j+1}\cdots x_{i})\right\},\,4\leq j\leq n\,,$$

and

$$U_n(x_4, \ldots, x_n) = x_3 \cdots x_n(V_n(x_4, \ldots, x_n) - A_3).$$

Three cases: (i) $r \in R_3$ (ii) s > r, $r \in R_k$ $(4 \le k \le n - 1)$ (iii) s > r, $r \in R_n$ are considered. (i) Substituting $x_4 = \frac{1}{\alpha_4^+(r)\omega_4^+(r)}$, $x_i = 1$ $(5 \le i \le n)$ to U_4 yields

$$\begin{split} U_4(x_4, \dots, x_n) &= (n-3)x_3x_4(V_4(x_4) - A_3) \\ &= (n-3)x_3x_4\left(\frac{r^2}{2\omega_3^+(r)^2} - \frac{s^2}{2\omega_3^+(s)^2}\right) \lessapprox 0 \Leftrightarrow r \lessapprox s \; . \end{split}$$

From Theorem 1, it follows that $\frac{dx_4}{dr} > 0$, $\frac{dx_i}{dr} = 0$ ($5 \le i \le n$). Therefore, $\frac{dH_3}{dr} = \frac{\partial H_3}{\partial x_4} \frac{dx_4}{dr} \lessapprox 0 \Leftrightarrow r \lessapprox s$. (ii) Substituting $x_i = \frac{\omega_i^+(r)}{\omega_{i-1}^+(r)}$ ($4 \le i \le k$), $x_{k+1} = \frac{1}{\alpha_k^+(r)\omega_k^+(r)}$, $x_i = 1$ ($k + 2 \le i \le n$) to V_j ($4 \le j \le k$) yields

$$V_j(x_4,\ldots,x_j) = \frac{1}{\omega_3^+(r)^2} \sum_{i=3}^j \omega_i^+(r)(\omega_j^+(r) - \omega_i^+(r)).$$

Thus, we have $V_4 < \cdots < V_k$. Furthermore, $V_k - A_3$ is a monotone decreasing function of s and if s = r

$$V_k - A_3 = \frac{-1}{\omega_3^+(r)^2} \left\{ r^2 - \sum_{i=3}^k \omega_i^+(r) (\omega_j^+(r) - \omega_i^+(r)) \right\} < 0 \; .$$

Hence, $V_k - A_3 < 0$. Consequently, for $3 \le j \le k$, $V_j - A_3 < 0$. In addition, from Theorem 1, $x_i \ge 1$ $(3 \le i \le n)$. Thus, we have $U_j - U_{j+1} < 0$ $(4 \le j \le k)$, that is, $U_4 < \cdots < U_{k+1}$. On the other hand, substituting $x_i = \frac{\omega_i^+(r)}{\omega_{i-1}^+(r)}$ $(4 \le i \le k)$, $x_{k+1} = \frac{1}{\alpha_k^+(r)\omega_i^+(r)}$, $x_i = 1$ $(k+2 \le i \le n)$ to U_{k+1} yields

$$\begin{aligned} U_{k+1}(x_4, \dots, x_n) &= (n-k)x_3 \cdots x_{k+1}(V_{k+1}(x_4, \dots, x_n) - A_3) \\ &= (n-k)x_3 \cdots x_{k+1} \left(\frac{r^2}{2\omega_3^+(r)^2} - \frac{s^2}{2\omega_3^+(s)^2} \right) < 0 \; . \end{aligned}$$

Hence, for $4 \le j \le k+1$, $U_j < 0$. From Theorem 1, it follows that $\frac{dx_j}{dr} > 0$ $(4 \le j \le k+1)$, $\frac{dx_j}{dr} = 0$ $(k+2 \le j \le n)$. Therefore, $\frac{dH_3}{dr} = \sum_{j=4}^{k+1} \frac{\partial H_3}{\partial x_j} \frac{dx_j}{dr} < 0$. (iii) By arguments similar to the case (ii), we have $V_j - A_3 < 0$ $(3 \le j \le n)$, so that $U_4 < \cdots < U_n < 0$. From Theorem 1, it follows that $\frac{dx_j}{dr} > 0$ $(4 \le j \le n)$. Therefore, $\frac{dH_3}{dr} = \sum_{j=4}^n \frac{\partial H_3}{\partial x_i} \frac{dx_j}{dr} < 0$.

Assume that $l(r, s) = k \ (4 \le k \le n - 1)$. We have

$$\frac{\partial H_k}{\partial x_j} = \frac{2}{x_j (\sum_{i=3}^n x_3 \cdots x_i)^3} \left\{ A_k x_3^2 \cdots x_k^2 \sum_{i=3}^{j-1} x_3 \cdots x_i + \sum_{i=j}^n x_3 \cdots x_i \sum_{m=3}^{j-1} x_3^2 \cdots x_m^2 (x_{m+1} \cdots x_i - 1) \right\}, \quad 4 \le j \le k,$$

and

$$\begin{split} \frac{\partial H_k}{\partial x_{k+1}} &= \frac{2}{x_{k+1} \left(\sum_{i=3}^n x_3 \cdots x_i\right)^3} \left\{ \left(\sum_{i=3}^k x_3 \cdots x_i\right) \left(\sum_{i=k+1}^n x_3^2 \cdots x_i^2\right) \right. \\ &\left. - \left(A_k x_3^2 \cdots x_i^2 + \sum_{i=3}^k x_3^2 \cdots x_i^2\right) \left(\sum_{i=k+1}^n x_3 \cdots x_i\right) \right\}. \end{split}$$

From Theorem 1, $x_i \ge 1$ $(3 \le i \le n)$, so that $\frac{\partial H_k}{\partial x_j} > 0$ $(4 \le j \le k)$. Two cases: (i) s < r, $r \in R_{k-1}$ (ii) s < r, $r \in R_k$ are considered. (i) From Theorem 1, it follows that $\frac{dx_j}{dr} > 0$ $(4 \le j \le k)$, $\frac{dx_j}{dr} = 0$ $(k+1 \le j \le n)$. Therefore, $\frac{dH_k}{dr} = \sum_{j=4}^k \frac{\partial H_3}{\partial x_j} \frac{dx_j}{dr} > 0$. (ii) Substituting $x_i = \frac{\omega_i^+(r)}{\omega_{i-1}^+(r)}$ $(4 \le i \le k)$, $x_{k+1} = \frac{1}{\omega_k^+(r)\omega_k^+(r)}$, $x_i = 1$ $(k+2 \le i \le n)$ to $\frac{\partial H_k}{\partial x_{k+1}}$ yields

$$\begin{split} \frac{\partial H_k}{\partial x_{k+1}} &= \frac{2(n-k)x_3^3 \cdots x_k^3}{\left(\sum_{i=3}^n x_3 \cdots x_i\right)^3} \left\{ \frac{1}{x_3^2 \cdots x_k^2} V_{k+1}(x_4, \dots, x_{k+1}) - A_k \right\} \\ &= \frac{2(n-k)x_3^3 \cdots x_k^3}{\left(\sum_{i=3}^n x_3 \cdots x_i\right)^3} \left\{ \frac{r^2}{2\omega_k^+(r)^2} - \frac{s^2}{2\omega_k^+(s)^2} \right\} > 0 \; . \end{split}$$

From Theorem 1, it follows that $\frac{dx_j}{dr} > 0$ $(4 \le j \le k+1)$, $\frac{dx_j}{dr} = 0$ $(k+2 \le j \le n)$.

Therefore, $\frac{dH_k}{dr} = \sum_{j=4}^{k+1} \frac{\partial H_3}{\partial x_j} \frac{dx_j}{dr} > 0$.

Assume that l(r, s) = n. We have

$$\begin{split} \frac{\partial H_n}{\partial x_j} &= \frac{2}{x_j (\sum_{i=3}^n x_3 \cdots x_i)^3} \left\{ A_k x_3^2 \cdots x_n^2 \sum_{i=3}^{j-1} x_3 \cdots x_i \right. \\ &\left. + \sum_{i=j}^n x_3 \cdots x_i \sum_{m=3}^{j-1} x_3^2 \cdots x_m^2 (x_{m+1} \cdots x_i - 1) \right\}, \qquad 4 \le j \le n \,. \end{split}$$

From Theorem 1, $x_i \ge 1$ $(3 \le i \le n)$, so that $\frac{\partial H_n}{\partial x_j} > 0$ for $4 \le j \le n$. From Theorem 1, it follows that if $r \in R_{n-1}$ or $r \in R_n$, then $\frac{dx_j}{dr} > 0$ $(4 \le j \le n)$. Therefore, $\frac{dH_3}{dr} = \sum_{j=4}^n \frac{\partial H_3}{\partial x_j} \frac{dx_j}{dr} > 0$. In conclusion, we have

$$\frac{d}{dr}M(\hat{\sigma}^2(r); \sigma^2, C) \leq 0 \Leftrightarrow r \leq s.$$

Proof of Theorem 3: If r < s and $r \in R_3$, then l(r, s) = 3 and $M(\hat{\sigma}^2(r); \sigma^2, C) = 2H_3(x_4, 1, ..., 1)$. From Theorem 1, we have $\lim_{r \to +0} x_4(r) = 1$, so that

$$\lim_{r\to +0} M(\hat{\sigma}^2(r); \sigma^2, C) = 2H_3(1, \ldots, 1).$$

On the other hand, if r > s and $r \in R_n$, then l(r, s) = n and $M(\hat{\sigma}^2(r); \sigma^2, C) = 2H_n(x_4, \ldots, x_n)$. Since $\lim_{r \to \infty} x_j(r) = \lim_{r \to \infty} \omega_j^+(r)/\omega_{j-1}^+(r) = \omega_j/\omega_{j-1}$, we have

$$\lim_{r\to\infty} M(\hat{\sigma}^2(r); \sigma^2, C) = 2H_n\left(\frac{\omega_4}{\omega_3}, \dots, \frac{\omega_n}{\omega_{n-1}}\right).$$

Thus, we obtain (2.1) and (2.2). Furthermore, $M(\hat{\sigma}^2(+0); \sigma^2, C) - M(\hat{\sigma}^2(\infty); \sigma^2, C)$ is a quadratic function of s with the positive coefficient of s^2 and the negative constant term. Hence there exists an s_0 satisfying (2.3).

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