

An unbiased C_p type criterion for ANOVA model with a tree order restriction

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ABSTRACT. In this paper, we consider a C_p type criterion for ANOVA model with a tree ordering (TO) $\theta_1 \leq \theta_j$, ($j = 2, \dots, l$) where $\theta_1, \dots, \theta_l$ are population means. In general, under ANOVA model with the TO, the usual C_p criterion has a bias to a risk function, and the bias depends on unknown parameters. In order to solve this problem, we calculate a value of the bias, and we derive its unbiased estimator. By using this estimator, we provide an unbiased C_p type criterion for ANOVA model with the TO, called TOC_p . A penalty term of the TOC_p is simply defined as a function of an indicator function and maximum likelihood estimators. Furthermore, we show that the TOC_p is the uniformly minimum-variance unbiased estimator (UMVUE) of a risk function.

1. Introduction

In real data analysis, ANOVA model is often used for analyzing cluster data. Moreover, a model whose parameters μ_1, \dots, μ_l are restricted such as a Simple Ordering (SO) given by $\mu_1 \leq \dots \leq \mu_l$, is also important in the field of applied statistics (e.g., Robertson et al., [14]). In addition, Brunk [4], Lee [11], Kelly [9] and Hwang and Peddada [7] showed that maximum likelihood estimators (MLEs) for mean parameters of ANOVA model with the SO are more efficient than those of ANOVA model without any restriction when the assumption of the SO is true.

However, in general, the classical asymptotic theory does not hold for the model with parameter restrictions. For example, Anraku [2] showed that the ordinal Akaike information criterion (AIC, Akaike [1]) for ANOVA model with the SO, whose penalty term is $2 \times$ the number of parameters, is not an asymptotically unbiased estimator of a risk function. In order to solve this problem, Inatsu [8] derived an asymptotically unbiased AIC for ANOVA model with the SO, called AIC_{SO} . Furthermore, a penalty term of the AIC_{SO} can be simply defined as a function of MLEs of mean parameters. On the

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other hand, Anraku and Nomakuchi [3] investigated the k -variate normal distribution with mean $\boldsymbol{\theta} = (\theta_1, \dots, \theta_k)'$ and covariance $\boldsymbol{\Sigma}$ where $\boldsymbol{\theta}$ is an unknown parameter vector, and $\boldsymbol{\Sigma}$ is a known positive definite matrix. In this setting, they proposed an unbiased AIC when the parameter $\boldsymbol{\theta}$ is restricted on a closed convex polyhedral cone. Nevertheless, above previous studies only considered the AIC under order restrictions, and they do not consider other criteria such as C_p type criteria (see, Mallows [13], Fujikoshi and Satoh [6]). Furthermore, particularly in Inatsu [8], the considered restriction is the SO. In practice, the tree ordering (TO) given by $\mu_1 \leq \mu_j$ ($j = 2, \dots, l$), is also often used in applied statistics (see, e.g., Hwang and Peddada [7]).

In this paper, we consider ANOVA model with the TO. For this model, we derive an unbiased C_p type criterion. The remainder of the present paper is organized as follows: In Section 2, we define the true model and candidate model. Moreover, we derive MLEs of parameters in the candidate model. In Section 3, we provide the C_p type criterion for ANOVA model with the TO, called $\text{TO}C_p$. In addition, we show that the $\text{TO}C_p$ is the uniformly minimum-variance unbiased estimator (UMVUE). In Section 4, we show some properties of the $\text{TO}C_p$ through numerical experiments. In Section 5, we conclude our discussion. Technical details are provided in Appendix.

2. ANOVA model with a tree order restriction

In this section, we define the true model, and candidate models with order restrictions. The MLE for the considered candidate model is given in Subsection 2.3.

2.1. True and candidate models. Let Y_{ij} be an observation variable on the j th individual in the i th cluster, where $1 \leq i \leq k^*$, $j = 1, \dots, N_i$ for each i , and $k^* \geq 2$. Here, we put $N = N_1 + \dots + N_{k^*}$ and $\mathbf{Y}_i = (Y_{i1}, \dots, Y_{iN_i})'$ for each i . Also we put $\mathbf{Y} = (\mathbf{Y}'_1, \dots, \mathbf{Y}'_{k^*})'$ and $\mathbf{N} = (N_1, \dots, N_{k^*})'$.

Suppose that $Y_{11}, \dots, Y_{k^*N_{k^*}}$ are mutually independent, and Y_{ij} is distributed as

$$Y_{ij} \sim N(\mu_{i,*}, \sigma_*^2), \quad (1)$$

for any i and j . Here, $\mu_{i,*}$ and σ_*^2 are unknown true values satisfying $\mu_{i,*} \in \mathbb{R}$ and $\sigma_*^2 > 0$, respectively. In other words, the true model is given by (1).

Next, we define a candidate model. Let Q_1, \dots, Q_k be non-empty disjoint sets satisfying $Q_1 \cup \dots \cup Q_k = \{1, 2, \dots, k^*\}$, where $2 \leq k \leq k^*$. Then, we assume that $Y_{11}, \dots, Y_{k^*N_{k^*}}$ are mutually independent, and distributed as

$$Y_{ij} \sim N(\mu_i, \sigma^2), \quad (2)$$

where μ_1, \dots, μ_{k^*} and $\sigma^2 (> 0)$ are unknown parameters. In addition, for the parameters μ_1, \dots, μ_{k^*} , we assume that

$$\forall s \in \{1, \dots, k\}, \quad \forall u_1, u_2 \in Q_s, \quad \mu_{u_1} = \mu_{u_2}, \quad (3)$$

and

$$\forall t \in \{2, \dots, k\}, \quad \forall v \in Q_t, \quad \mu_q \leq \mu_v, \quad (4)$$

where $q \in Q_1$. Then, a candidate model \mathcal{M} is defined as the model (2) with (3) and (4). In particular, the order restriction (4) is called a Tree Ordering (TO). For example, when $k^* = 7$, $k = 4$, $Q_1 = \{1, 3, 7\}$, $Q_2 = \{2\}$, $Q_3 = \{4, 5\}$ and $Q_4 = \{6\}$, the unknown parameters μ_1, \dots, μ_7 for the candidate model \mathcal{M} are restricted as

$$\mu_1 = \mu_3 = \mu_7 \leq \mu_2, \quad \mu_1 = \mu_3 = \mu_7 \leq \mu_4 = \mu_5, \quad \mu_1 = \mu_3 = \mu_7 \leq \mu_6.$$

2.2. Notation and lemma. In this subsection, we define several notations. After that, we provide the related lemma. Let l be an integer with $l \geq 2$. Then, define

$$\mathbb{N}_l = \{x \in \mathbb{N} \mid x \leq l\} = \{1, \dots, l\}.$$

Moreover, let x_1, \dots, x_l be real numbers, and let N_1, \dots, N_l be positive numbers. We put $\mathbf{x} = (x_1, \dots, x_l)'$ and $\mathbf{N} = (N_1, \dots, N_l)'$. Furthermore, let $A = \{a_1, \dots, a_l\}$ be a non-empty subset of \mathbb{N}_l , where $a_1 < \dots < a_l$ when $l \geq 2$.

Next, define

$$\mathbf{x}_A = (x_{a_1}, \dots, x_{a_l})', \quad \tilde{\mathbf{x}}_A = \sum_{s \in A} x_s, \quad \bar{\mathbf{x}}_A^{(N)} = \frac{\sum_{s \in A} N_s x_s}{\sum_{s \in A} N_s} = \frac{\sum_{s \in A} N_s x_s}{\tilde{N}_A}.$$

For example, when $l = 10$ and $A = \{2, 3, 5, 10\}$, \mathbf{x}_A , $\tilde{\mathbf{x}}_A$ and $\bar{\mathbf{x}}_A^{(N)}$ are given by

$$\mathbf{x}_A = (x_2, x_3, x_5, x_{10})', \quad \tilde{\mathbf{x}}_A = x_2 + x_3 + x_5 + x_{10},$$

$$\bar{\mathbf{x}}_A^{(N)} = \frac{N_2 x_2 + N_3 x_3 + N_5 x_5 + N_{10} x_{10}}{N_2 + N_3 + N_5 + N_{10}}.$$

In particular, when A has only one element a , i.e., $A = \{a\}$, it holds that $\mathbf{x}_A = (x_a)'$, $\tilde{\mathbf{x}}_A = x_a$ and $\bar{\mathbf{x}}_A^{(N)} = x_a$. On the other hand, when $A = \mathbb{N}_l$, it holds that $\mathbf{x}_A = \mathbf{x}$. For simplicity, we often represent $\bar{\mathbf{x}}_A^{(N)}$ as $\bar{\mathbf{x}}_A$. In addition, let $A^{(l)}$ be a set defined as

$$A^{(l)} = \{(x_1, \dots, x_l)' \in \mathbb{R}^l \mid \forall j \in \mathbb{N}_l \setminus \{1\}, x_1 \leq x_j\}$$

$$= \{(x_1, \dots, x_l)' \in \mathbb{R}^l \mid x_1 \leq x_2, \dots, x_1 \leq x_l\}.$$

Furthermore, for any integer i with $1 \leq i \leq l$, we consider a family of sets $\mathcal{J}_i^{(l)}$ defined by

$$\mathcal{J}_i^{(l)} = \{J \subset \mathbb{N}_l \mid 1 \in J, \#J = i\},$$

where $\#J$ means the number of elements of the set J . For example, when $l = 3$, it holds that

$$\mathcal{J}_1^{(3)} = \{\{1\}\}, \quad \mathcal{J}_2^{(3)} = \{\{1, 2\}, \{1, 3\}\}, \quad \mathcal{J}_3^{(3)} = \{\{1, 2, 3\}\} = \{\mathbb{N}_3\}.$$

Here, note that $\mathcal{J}_1^{(l)} = \{\{1\}\}$ and $\mathcal{J}_l^{(l)} = \{\mathbb{N}_l\}$ for any $l \geq 2$. Similarly, for any integer i with $1 \leq i \leq l$ and for any set J in $\mathcal{J}_i^{(l)}$, we consider the following set $A^{(l)}(J)$:

$$A^{(l)}(J) = \{(x_1, \dots, x_l)' \in \mathbb{R}^l \mid \forall s \in J, x_1 = x_s, \forall t \in \mathbb{N}_l \setminus J, x_1 < x_t\}.$$

Note that when $J = \mathbb{N}_l$, it holds that $\mathbb{N}_l \setminus J = \emptyset$. In this case, the proposition

$$\forall t \in \emptyset, \quad x_1 < x_t$$

is always true. For example, when $l = 3$, it holds that

$$A^{(3)}(\{1\}) = \{\mathbf{x} = (x_1, \dots, x_3)' \in \mathbb{R}^3 \mid x_1 < x_2, x_1 < x_3\},$$

$$A^{(3)}(\{1, 2\}) = \{\mathbf{x} \in \mathbb{R}^3 \mid x_1 = x_2, x_1 < x_3\},$$

$$A^{(3)}(\{1, 3\}) = \{\mathbf{x} \in \mathbb{R}^3 \mid x_1 = x_3, x_1 < x_2\},$$

$$A^{(3)}(\{1, 2, 3\}) = \{\mathbf{x} \in \mathbb{R}^3 \mid x_1 = x_2 = x_3\}.$$

It is clear that these four sets are disjoint sets and

$$\bigcup_{i=1}^3 \bigcup_{J \in \mathcal{J}_i^{(3)}} A^{(3)}(J) = \{\mathbf{x} \in \mathbb{R}^3 \mid x_1 \leq x_2, x_1 \leq x_3\} = A^{(3)}.$$

Similarly, in the case of $l \geq 2$, it holds that

$$\bigcup_{i=1}^l \bigcup_{J \in \mathcal{J}_i^{(l)}} A^{(l)}(J) = \{\mathbf{x} \in \mathbb{R}^l \mid x_1 \leq x_2, \dots, x_1 \leq x_l\} = A^{(l)}, \quad (5)$$

and $A^{(l)}(J) \cap A^{(l)}(J^*) = \emptyset$ when $J \neq J^*$.

Next, for a vector $\mathbf{x} = (x_1, \dots, x_l)'$, an integer s with $1 \leq s \leq l$ and a real number a , $\mathbf{x}[s; a]$ stands for an l -dimensional vector whose s th element is a and t th element ($t \in \mathbb{N}_l \setminus \{s\}$) is x_t . For example, if $\mathbf{x} = (1, 4, 4, 3)'$, then $\mathbf{x}[2; -1] = (1, -1, 4, 3)'$ and $\mathbf{x}[4; 5] = (1, 4, 4, 5)'$. Moreover, for any integer s (≥ 2) with $1 \leq s \leq l$ and for any set $J = \{j_1, \dots, j_s\}$ of $\mathcal{J}_s^{(l)}$, where $j_1 < \dots < j_s$, we define

a matrix $\mathbf{D}_J^{(N)}$ as follows. First, in the case of $s = 1$, the family of sets $\mathcal{J}_1^{(l)}$ has only one set $J = \{1\}$, and we define $\mathbf{D}_J^{(N)} = \mathbf{0}$. On the other hand, in the case of $s \geq 2$, the matrix $\mathbf{D}_J^{(N)}$ is the $(s-1) \times s$ matrix whose i th row ($1 \leq i \leq s-1$) is defined as

$$\frac{1}{\tilde{N}_{J \setminus \{j_{i+1}\}}} \mathbf{N}_J [i+1; -\tilde{N}_{J \setminus \{j_{i+1}\}}]'$$

For example, when $l = 3$, it holds that

$$\begin{aligned} \mathbf{D}_{\{1\}}^{(N)} &= \mathbf{0}, & \mathbf{D}_{\{1,2\}}^{(N)} &= \mathbf{D}_{\{1,3\}}^{(N)} = (1 \quad -1), \\ \mathbf{D}_{\{1,2,3\}}^{(N)} &= \begin{pmatrix} \frac{N_1}{N_1+N_3} & -1 & \frac{N_3}{N_1+N_3} \\ \frac{N_1}{N_1+N_2} & \frac{N_2}{N_1+N_2} & -1 \end{pmatrix}. \end{aligned}$$

For simplicity, we often represent $\mathbf{D}_J^{(N)}$ as \mathbf{D}_J .

Furthermore, we define a function $\boldsymbol{\eta}_l^{(N)}$ from \mathbb{R}^l to $A^{(l)}$. For each vector $\mathbf{x} = (x_1, \dots, x_l)' \in \mathbb{R}^l$, $\boldsymbol{\eta}_l^{(N)}(\mathbf{x})$ is defined as

$$\boldsymbol{\eta}_l^{(N)}(\mathbf{x}) = \underset{\mathbf{y}=(y_1, \dots, y_l)' \in A^{(l)}}{\operatorname{argmin}} \sum_{i=1}^l N_i (x_i - y_i)^2. \tag{6}$$

In addition, let $\eta_i^{(N)}(\mathbf{x})[s]$ be the s th element ($1 \leq s \leq l$) of $\boldsymbol{\eta}_l^{(N)}(\mathbf{x})$. Note that well-definedness of $\boldsymbol{\eta}_l^{(N)}$ can be derived by using the Hilbert projection theorem (see, e.g., Rudin [15]). For simplicity, we often represent $\boldsymbol{\eta}_l^{(N)}(\mathbf{x})$ as $\boldsymbol{\eta}_l(\mathbf{x})$.

Finally, we provide the following lemma:

LEMMA 1. *The following three propositions hold:*

(1) *It holds that*

$$\mathbb{R}^l = \bigcup_{i=1}^l \bigcup_{J \in \mathcal{J}_i^{(l)}} \boldsymbol{\eta}_i^{-1}(A^{(l)}(J)),$$

$$\boldsymbol{\eta}_i^{-1}(A^{(l)}(J)) \cap \boldsymbol{\eta}_i^{-1}(A^{(l)}(J^*)) = \emptyset \quad (J \neq J^*).$$

(2) *For any integer i with $1 \leq i \leq l$ and for any set J in $\mathcal{J}_i^{(l)}$, it holds that*

$$\begin{aligned} &\boldsymbol{\eta}_i^{-1}(A^{(l)}(J)) \\ &= \{\mathbf{x} = (x_1, \dots, x_l)' \in \mathbb{R}^l \mid \mathbf{D}_J \mathbf{x}_J \geq \mathbf{0}, \forall t \in \mathbb{N}_l \setminus J, \bar{x}_J < x_t\}, \end{aligned} \tag{7}$$

where the inequality $\mathbf{s} \geq \mathbf{0}$ means that all elements of the vector \mathbf{s} are non-negative.

- (3) Let i be an integer with $1 \leq i \leq l$, and let J be a set with $J \in \mathcal{J}_i^{(l)}$. Let $\mathbf{x} = (x_1, \dots, x_l)'$ be an element of \mathbb{R}^l . Assume that \mathbf{x} satisfies

$$\mathbf{x} \in \boldsymbol{\eta}_l^{-1}(A^{(l)}(J)).$$

Then, it holds that

$$\forall s \in J, \quad \eta_l(\mathbf{x})[s] = \bar{x}_J, \quad \forall t \in \mathbb{N}_l \setminus J, \quad \eta_l(\mathbf{x})[t] = x_t.$$

In particular, for the case of $J = \mathbb{N}_l$, if \mathbf{x} satisfies

$$\mathbf{x} \in \boldsymbol{\eta}_l^{-1}(A^{(l)}(J)) = \{\mathbf{x} \in \mathbb{R}^l \mid \mathbf{D}_J \mathbf{x}_J \geq \mathbf{0}\},$$

then, the following proposition holds:

$$\forall s \in J, \quad \eta_l(\mathbf{x})[s] = \bar{x}_J.$$

The proof of Lemma 1 is given in Appendix 1.

2.3. Maximum likelihood estimators for unknown parameters. In this subsection, we derive MLEs for unknown parameters in the candidate model \mathcal{M} . First of all, we rewrite the candidate model. For any integer s with $1 \leq s \leq k$ and for all elements $q_1^{(s)}, \dots, q_v^{(s)}$ of \mathcal{Q}_s , let $\mathbf{X}_s = (\mathbf{Y}'_{q_1^{(s)}}, \dots, \mathbf{Y}'_{q_v^{(s)}})'$, where v is the number of elements in \mathcal{Q}_s , and let X_{st} be a t th element of \mathbf{X}_s . We put $\mathbf{X} = (\mathbf{X}'_1, \dots, \mathbf{X}'_k)'$,

$$\mu_{q_1^{(s)}} = \dots = \mu_{q_v^{(s)}} \equiv \theta_s,$$

and $\boldsymbol{\theta} = (\theta_1, \dots, \theta_k)'$. In addition, define $n_s = N_{q_1^{(s)}} + \dots + N_{q_v^{(s)}}$ and $\mathbf{n} = (n_1, \dots, n_k)'$. Note that $n_1 + \dots + n_k = N_1 + \dots + N_{k^*} = N$. Then, the candidate model can be rewritten as

$$X_{st} \sim N(\theta_s, \sigma^2), \quad t = 1, \dots, n_s,$$

with

$$\theta_1 \leq \theta_2, \dots, \theta_1 \leq \theta_k.$$

Here, a parameter space Θ for the candidate model is defined as follows:

$$\Theta = \{(a_1, \dots, a_k)' \in \mathbb{R}^k \mid \forall u \in \mathbb{N}_k \setminus \{1\}, a_1 \leq a_u\}.$$

Next, we consider the log-likelihood for the candidate model. Let

$$\bar{X}_s = \frac{1}{n_s} \sum_{v=1}^{n_s} X_{sv}, \quad s = 1, \dots, k,$$

and let $\bar{\mathbf{X}} = (\bar{X}_1, \dots, \bar{X}_k)'$. Then, since X_{st} 's are independently distributed as normal distribution, the log-likelihood function $l(\boldsymbol{\theta}, \sigma^2; \mathbf{X})$ is given by

$$\begin{aligned} l(\boldsymbol{\theta}, \sigma^2; \mathbf{X}) &= -\frac{N}{2} \log(2\pi\sigma^2) - \frac{1}{2\sigma^2} \sum_{s=1}^k \sum_{t=1}^{n_s} (X_{st} - \theta_s)^2 \\ &= -\frac{N}{2} \log(2\pi\sigma^2) - \frac{1}{2\sigma^2} \sum_{s=1}^k \sum_{t=1}^{n_s} (X_{st} - \bar{X}_s)^2 \\ &\quad - \frac{1}{2\sigma^2} \sum_{s=1}^k n_s (\bar{X}_s - \theta_s)^2. \end{aligned}$$

Hence, for any $\sigma^2 > 0$, the maximizer of $l(\boldsymbol{\theta}, \sigma^2; \mathbf{X})$ on $\boldsymbol{\Theta}$ is equal to the minimizer of

$$H(\boldsymbol{\theta}; \bar{\mathbf{X}}) = \sum_{s=1}^k n_s (\bar{X}_s - \theta_s)^2$$

on $\boldsymbol{\Theta}$. In other words, the MLE $\hat{\boldsymbol{\theta}} = (\hat{\theta}_1, \dots, \hat{\theta}_k)'$ of $\boldsymbol{\theta}$ is given by

$$\hat{\boldsymbol{\theta}} = \underset{\boldsymbol{\theta} \in \boldsymbol{\Theta}}{\operatorname{argmin}} H(\boldsymbol{\theta}; \bar{\mathbf{X}}). \quad (8)$$

We would like to note that the MLE $\hat{\boldsymbol{\theta}}$ can be written by using (6) as $\boldsymbol{\eta}_k^{(n)}(\bar{\mathbf{X}}) = \hat{\boldsymbol{\theta}}$. Here, we substitute $\bar{\mathbf{X}}$ for $\mathbf{x} = (x_1, \dots, x_k)'$. Then, from Lemma 1, there exists a unique integer α with $1 \leq \alpha \leq k$ and a unique set J with $J \in \mathcal{J}_\alpha^{(k)}$ such that

$$\mathbf{D}_J \mathbf{x}_J \geq \mathbf{0}, \quad \forall \beta \in \mathbb{N}_k \setminus J, \bar{x}_J < x_\beta.$$

For this set J , it holds that

$$\begin{aligned} \forall w \in J, \quad \hat{\theta}_w &= \bar{x}_J = \frac{\sum_{c \in J} n_c x_c}{\sum_{c \in J} n_c} = \frac{\sum_{c \in J} n_c \bar{X}_c}{\sum_{c \in J} n_c}, \\ \forall \beta \in \mathbb{N}_k \setminus J, \quad \hat{\theta}_\beta &= x_\beta = \bar{X}_\beta. \end{aligned} \quad (9)$$

Therefore, the MLE $\hat{\boldsymbol{\mu}} = (\hat{\mu}_1, \dots, \hat{\mu}_{k^*})'$ of $\boldsymbol{\mu} = (\mu_1, \dots, \mu_{k^*})'$ can be written as

$$\forall j \in Q_s, \quad \hat{\mu}_j = \hat{\theta}_s, \quad (s = 1, \dots, k). \quad (10)$$

On the other hand, the MLE $\hat{\sigma}^2$ of σ^2 can be written as

$$\begin{aligned} \hat{\sigma}^2 &= \frac{1}{N} \sum_{s=1}^k \sum_{t=1}^{n_s} (X_{st} - \bar{X}_s)^2 + \frac{1}{N} \sum_{s=1}^k n_s (\bar{X}_s - \hat{\theta}_s)^2 \\ &= \frac{1}{N} \sum_{s=1}^k \sum_{t=1}^{n_s} (X_{st} - \hat{\theta}_s)^2 = \frac{1}{N} \sum_{i=1}^{k^*} \sum_{j=1}^{N_i} (Y_{ij} - \hat{\mu}_i)^2, \end{aligned} \quad (11)$$

because the function $l(\hat{\boldsymbol{\theta}}, \sigma^2; \mathbf{X})$ is a concave function with respect to (w.r.t.) σ^2 .

3. C_p type criterion for the candidate model

In this section, we derive an unbiased C_p type criterion for the candidate model \mathcal{M} . Here, we assume the following condition:

(C1) The inequality $N - k^* - 2 > 0$ holds.

We do not need to assume that the true model is included in the candidate model. First, we consider the risk function based on the prediction mean squared error (PMSE). Let $\mathbf{Y}_* = (\mathbf{Y}'_{1,*}, \dots, \mathbf{Y}'_{k^*,*})'$ be a random vector, and let \mathbf{Y}_* be independent and identically distributed as \mathbf{Y} . Furthermore, for any integer s with $1 \leq s \leq k$ and for all elements $q_1^{(s)}, \dots, q_v^{(s)}$ of \mathcal{Q}_s , we define $\mathbf{X}_{s,*} = (\mathbf{Y}'_{q_1^{(s)},*}, \dots, \mathbf{Y}'_{q_v^{(s)},*})'$. In addition, we put $\mathbf{X}_* = (\mathbf{X}'_{1,*}, \dots, \mathbf{X}'_{k^*,*})'$. The risk function R based on the PMSE is given by

$$R = \mathbb{E} \left[\mathbb{E}_{\mathbf{Y}_*} \left[\frac{1}{\sigma_*^2} \sum_{i=1}^{k^*} \sum_{j=1}^{N_i} (Y_{ij,*} - \hat{\mu}_i)^2 \right] \right] = N + \mathbb{E} \left[\frac{1}{\sigma_*^2} \sum_{i=1}^{k^*} N_i (\mu_{i,*} - \hat{\mu}_i)^2 \right]. \quad (12)$$

Next, we define the following random variables:

$$\bar{Y}_i = \frac{1}{N_i} \sum_{j=1}^{N_i} Y_{ij} \quad (i = 1, \dots, k^*), \quad \bar{\sigma}^2 = \frac{1}{N} \sum_{i=1}^{k^*} \sum_{j=1}^{N_i} (Y_{ij} - \bar{Y}_i)^2. \quad (13)$$

Note that $\bar{Y}_1, \dots, \bar{Y}_{k^*}$ and $\bar{\sigma}^2$ are mutually independent, and $\bar{Y}_i \sim N(\mu_{i,*}, \sigma_*^2/N_i)$ and $N\bar{\sigma}^2/\sigma_*^2 \sim \chi_{N-k^*}^2$ because Y_{11}, \dots, Y_{kN_k} are independently distributed as normal distribution. Then, we estimate the risk function R by using

$$(N - k^* - 2) \frac{\hat{\sigma}^2}{\bar{\sigma}^2}. \quad (14)$$

Here, from (11) the MLE $\hat{\sigma}^2$ can be written as

$$\begin{aligned} \hat{\sigma}^2 &= \frac{1}{N} \sum_{i=1}^{k^*} \sum_{j=1}^{N_i} (Y_{ij} - \bar{Y}_i)^2 + \frac{1}{N} \sum_{i=1}^{k^*} N_i (\bar{Y}_i - \hat{\mu}_i)^2 \\ &= \bar{\sigma}^2 + \frac{1}{N} \sum_{i=1}^{k^*} N_i (\bar{Y}_i - \hat{\mu}_i)^2. \end{aligned} \quad (15)$$

Therefore, (14) can be expressed as

$$(N - k^* - 2) \frac{\hat{\sigma}^2}{\bar{\sigma}^2} = N - k^* - 2 + \left(\frac{N - k^* - 2}{N\bar{\sigma}^2/\sigma_*^2} \right) \frac{1}{\sigma_*^2} \sum_{i=1}^{k^*} N_i (\bar{Y}_i - \hat{\mu}_i)^2. \quad (16)$$

On the other hand, from (9) and (10), it can be seen that $\hat{\mu}_1, \dots, \hat{\mu}_{k^*}$ are functions of $\bar{X}_1, \dots, \bar{X}_k$. Moreover, for any integer s with $1 \leq s \leq k$, it holds that

$$\bar{X}_s = \frac{1}{n_s} \sum_{t=1}^{n_s} X_{st} = \frac{1}{\sum_{q \in Q_s} N_q} \sum_{q \in Q_s} \sum_{j=1}^{N_q} Y_{qj} = \frac{1}{\sum_{q \in Q_s} N_q} \sum_{q \in Q_s} N_q \bar{Y}_q. \quad (17)$$

Thus, $\bar{X}_1, \dots, \bar{X}_k$ are functions of $\bar{Y}_1, \dots, \bar{Y}_{k^*}$, and $\hat{\mu}_1, \dots, \hat{\mu}_{k^*}$ are also functions of $\bar{Y}_1, \dots, \bar{Y}_{k^*}$. Hence, noting that $\bar{Y}_1, \dots, \bar{Y}_{k^*}$ and $\bar{\sigma}^2$ are independent, and $N\bar{\sigma}^2/\sigma_*^2 \sim \chi_{N-k^*}^2$ and $E[(\chi_{N-k^*}^2)^{-1}] = (N - k^* - 2)^{-1}$, the expectation of (16) can be written as

$$\begin{aligned} & E \left[(N - k^* - 2) \frac{\hat{\sigma}^2}{\bar{\sigma}^2} \right] \\ &= N - k^* - 2 + E \left[\frac{1}{\sigma_*^2} \sum_{i=1}^{k^*} N_i \{ (\bar{Y}_i - \mu_{i,*}) + (\mu_{i,*} - \hat{\mu}_i) \}^2 \right] \\ &= N - 2 + 2E \left[\frac{1}{\sigma_*^2} \sum_{i=1}^{k^*} N_i (\bar{Y}_i - \mu_{i,*}) (\mu_{i,*} - \hat{\mu}_i) \right] \\ &\quad + E \left[\frac{1}{\sigma_*^2} \sum_{i=1}^{k^*} N_i (\mu_{i,*} - \hat{\mu}_i)^2 \right] \\ &= N - 2 - 2E \left[\frac{1}{\sigma_*^2} \sum_{i=1}^{k^*} N_i (\bar{Y}_i - \mu_{i,*}) \hat{\mu}_i \right] + E \left[\frac{1}{\sigma_*^2} \sum_{i=1}^{k^*} N_i (\mu_{i,*} - \hat{\mu}_i)^2 \right]. \quad (18) \end{aligned}$$

Therefore, by using (12) and (18), the bias B which is the difference between the expected value of (14) and R , is given by

$$\begin{aligned} B &= E \left[R - (N - k^* - 2) \frac{\hat{\sigma}^2}{\bar{\sigma}^2} \right] \\ &= 2 + 2E \left[\frac{1}{\sigma_*^2} \sum_{i=1}^{k^*} N_i (\bar{Y}_i - \mu_{i,*}) \hat{\mu}_i \right] \\ &= 2 + 2E \left[\frac{1}{\sigma_*^2} \sum_{s=1}^k \sum_{q \in Q_s} N_q (\bar{Y}_q - \mu_{q,*}) \hat{\mu}_q \right]. \quad (19) \end{aligned}$$

Here, for any integer s with $1 \leq s \leq k$, we put

$$\frac{\sum_{q \in Q_s} N_q \mu_{q,*}}{\sum_{q \in Q_s} N_q} = \frac{\sum_{q \in Q_s} N_q \mu_{q,*}}{n_s} \equiv \alpha_{s,*}. \quad (20)$$

Then, combining (10), (17) and (20), (19) can be expressed as

$$\begin{aligned}
B &= 2 + 2\mathbb{E}\left[\frac{1}{\sigma_*^2}\sum_{s=1}^k n_s(\bar{X}_s - \alpha_{s,*})\hat{\theta}_s\right] \\
&= 2 - 2\mathbb{E}\left[\frac{1}{\sigma_*^2}\sum_{s=1}^k n_s(\bar{X}_s - \alpha_{s,*})(\bar{X}_s - \hat{\theta}_s)\right] \\
&\quad + 2\mathbb{E}\left[\frac{1}{\sigma_*^2}\sum_{s=1}^k n_s(\bar{X}_s - \alpha_{s,*})\bar{X}_s\right].
\end{aligned}$$

Hence, noting that $\bar{X}_s \sim N(\alpha_{s,*}, \sigma_*^2/n_s)$, we have

$$B = 2(k+1) - 2\mathbb{E}\left[\frac{1}{\sigma_*^2}\sum_{s=1}^k n_s(\bar{X}_s - \alpha_{s,*})(\bar{X}_s - \hat{\theta}_s)\right]. \quad (21)$$

Next, we calculate the expectation in (21). Here, the following theorem holds:

THEOREM 1. *Let l be an integer with $l \geq 2$. Let n_1, \dots, n_l and τ^2 be positive numbers, and let ξ_1, \dots, ξ_l be real numbers. Let x_1, \dots, x_l be independent random variables, and let $x_s \sim N(\xi_s, \tau^2/n_s)$, ($s = 1, \dots, l$). Put $\mathbf{n} = (n_1, \dots, n_l)'$, $\boldsymbol{\xi} = (\xi_1, \dots, \xi_l)'$ and $\mathbf{x} = (x_1, \dots, x_l)'$. Then, it holds that*

$$\begin{aligned}
&\mathbb{E}\left[\frac{1}{\tau^2}\sum_{s=1}^l n_s(x_s - \xi_s)(x_s - \eta_l^{(n)}(\mathbf{x})[s])\right] \\
&= \sum_{i=2}^l (i-1)\mathbb{P}\left(\eta_l(\mathbf{x}) \in \bigcup_{J \in \mathcal{J}_i^l} A^{(l)}(J)\right).
\end{aligned}$$

Details of the proof of Theorem 1 are given in Appendix 2 and 3. Note that $\bar{X}_1, \dots, \bar{X}_k$ are mutually independent, and $\bar{X}_s \sim N(\alpha_{s,*}, \sigma_*^2/n_s)$ for any integer s with $1 \leq s \leq k$. Also note that from (8) the MLE $\hat{\boldsymbol{\theta}}$ is given by $\hat{\boldsymbol{\theta}} = \boldsymbol{\eta}_k^{(n)}(\bar{\mathbf{X}})$. Therefore, from Theorem 1, the expectation in (21) can be expressed as

$$\begin{aligned}
&\mathbb{E}\left[\frac{1}{\sigma_*^2}\sum_{s=1}^k n_s(\bar{X}_s - \alpha_{s,*})(\bar{X}_s - \hat{\theta}_s)\right] \\
&= \mathbb{E}\left[\frac{1}{\sigma_*^2}\sum_{s=1}^k n_s(\bar{X}_s - \alpha_{s,*})(\bar{X}_s - \eta_k^{(n)}(\bar{\mathbf{X}})[s])\right] \\
&= \sum_{u=2}^k (u-1)\mathbb{P}\left(\hat{\boldsymbol{\theta}} \in \bigcup_{J \in \mathcal{J}_u^k} A^{(k)}(J)\right) = L, \quad (\text{say}).
\end{aligned}$$

Hence, in order to correct the bias, it is sufficient to add $2(k+1) - 2L$ to (14). However, it is easily checked that L depends on the true parameters $\theta_{1,*}, \dots, \theta_{k,*}$ and σ_*^2 . For this reason, we must estimate L . Here, we define the following random variable \hat{m} :

$$\hat{m} = 1 + \sum_{a=2}^k 1_{\{\hat{\theta}_1 < \hat{\theta}_a\}}, \quad (22)$$

where $1_{\{\cdot\}}$ is an indicator function. It is clear that \hat{m} is a discrete random variable and its possible values are 1 to k . Incidentally, from the definitions of $A^{(k)}(J)$, \hat{m} and $\hat{\theta}$, it holds that

$$\hat{\theta} \in \bigcup_{J \in \mathcal{J}_u^k} A^{(k)}(J) \Leftrightarrow \hat{m} = k + 1 - u \Leftrightarrow k - \hat{m} = u - 1,$$

for any integer u with $1 \leq u \leq k$. Therefore, the random variable $k - \hat{m}$ satisfies

$$E[k - \hat{m}] = \sum_{u=2}^k (u - 1) P\left(\hat{\theta} \in \bigcup_{J \in \mathcal{J}_u^k} A^{(k)}(J)\right) = L.$$

Hence, in order to correct the bias, instead of $2(k+1) - 2L$, we add

$$2(k+1) - 2(k - \hat{m}) = 2(\hat{m} + 1)$$

to (14). In other words, it holds that

$$B = 2(k+1) - 2E[k - \hat{m}] = E[2(\hat{m} + 1)].$$

As a result, we obtain the C_p type criterion for the candidate model \mathcal{M} with the TO, called TOC_p .

THEOREM 2. *A C_p type criterion for the candidate model \mathcal{M} with the TO, called TOC_p is defined as*

$$\text{TOC}_p := (N - k^* - 2) \frac{\hat{\sigma}^2}{\bar{\sigma}^2} + 2(\hat{m} + 1),$$

where $\hat{\sigma}^2$, $\bar{\sigma}^2$ and \hat{m} are given by (11), (13) and (22), respectively. Moreover, for the risk function R given by (12), it holds that

$$E[\text{TOC}_p] = R.$$

REMARK 1. *The TOC_p is the unbiased estimator of R . Furthermore, unbiasedness of the TOC_p holds even if the true model is not included in the candidate model \mathcal{M} .*

In addition, for unbiasedness of the TOC_p , the following theorem holds:

THEOREM 3. *The TOC_p is the uniformly minimum-variance unbiased estimator (UMVUE) of R .*

PROOF. As we mentioned before, the random variable \hat{m} is a function of $\hat{\theta}_1, \dots, \hat{\theta}_k$, and $\hat{\theta}_1, \dots, \hat{\theta}_k$ are functions of $\bar{X}_1, \dots, \bar{X}_k$. Furthermore, $\bar{X}_1, \dots, \bar{X}_k$ are functions of $\bar{Y}_1, \dots, \bar{Y}_{k^*}$. Thus, \hat{m} is a function of $\bar{Y}_1, \dots, \bar{Y}_{k^*}$. On the other hand, since $\hat{\mu}_1, \dots, \hat{\mu}_{k^*}$ are functions of $\bar{Y}_1, \dots, \bar{Y}_{k^*}$, from (15), we can see that both $\hat{\sigma}^2$ and $\bar{\sigma}^2$ are functions of $\bar{Y}_1, \dots, \bar{Y}_{k^*}$. Therefore, from the definition of the TOC_p , the TOC_p is a function of $\bar{\sigma}^2$ and $\bar{Y}_1, \dots, \bar{Y}_{k^*}$. Incidentally, noting that $Y_{11}, \dots, Y_{k^*N_{k^*}}$ are mutually independent, and $Y_{ij} \sim N(\mu_{i,*}, \sigma_*^2)$ where $1 \leq i \leq k^*$ and $1 \leq j \leq N_i$, the joint distribution function $f(\mathbf{y}; \boldsymbol{\mu}_*, \sigma_*^2)$ can be written as

$$\begin{aligned} f(\mathbf{y}; \boldsymbol{\mu}_*, \sigma_*^2) &= C_1 \exp \left\{ -\frac{1}{2\sigma_*^2} \sum_{i=1}^{k^*} \left(N_i \bar{y}_i^2 + \sum_{j=1}^{N_i} (y_{ij} - \bar{y}_i)^2 \right) + \sum_{i=1}^{k^*} \frac{N_i \mu_{i,*}}{\sigma_*^2} \bar{y}_i - C_2 \right\}, \end{aligned}$$

where \bar{y}_i , C_1 and C_2 are given by

$$\bar{y}_i = \frac{1}{N_i} \sum_{j=1}^{N_i} y_{ij}, \quad C_1 = \frac{1}{(2\pi\sigma_*^2)^{N/2}}, \quad C_2 = \frac{1}{2\sigma_*^2} \sum_{i=1}^{k^*} N_i \mu_{i,*}^2.$$

Here, define

$$T_0 = \sum_{i=1}^{k^*} \left(N_i \bar{Y}_i^2 + \sum_{j=1}^{N_i} (Y_{ij} - \bar{Y}_i)^2 \right), \quad T_i = \bar{Y}_i, \quad (i = 1, \dots, k^*).$$

Then, $(T_0, T_1, \dots, T_{k^*})'$ is a complete sufficient statistic (see, e.g., Lehmann and Casella [12]). Moreover, since $\bar{\sigma}^2$ can be written by using $(T_0, T_1, \dots, T_{k^*})'$ as

$$\bar{\sigma}^2 = \frac{1}{N} \left(T_0 - \sum_{i=1}^{k^*} N_i T_i^2 \right),$$

$\bar{\sigma}^2$ is a function of the complete sufficient statistic $(T_0, T_1, \dots, T_{k^*})'$. Hence, the TOC_p which is a function of $\bar{\sigma}^2$ and $\bar{Y}_1, \dots, \bar{Y}_{k^*}$, is also a function of the complete sufficient statistic. Therefore, since the TOC_p is the unbiased estimator of R , from Lehmann-Scheffé theorem (see, e.g., Knight [10]), the TOC_p is the UMVUE of R . \square

REMARK 2. *We would like to note that Davies et al. [5] showed the bias-corrected C_p type criterion, MC_p (given by Fujikoshi and Satoh [6]) is the*

UMVUE of a risk function based on the prediction mean squared error for normal linear regression models without any order restriction.

4. Numerical experiments

In this section, we confirm the estimation accuracy for the TOC_p through numerical experiments. In addition, we also calculate the selection probability and the risk of the best model.

4.1. Estimation accuracy. Let $Y_{ij} \sim N(\theta_i, \sigma^2)$, where $i = 1, 2, 3, 4$ and $j = 1, \dots, N_i$ for each i . We set $N_1 = N_2 = N_3 = N_4$. Furthermore, we put $N = N_1 + N_2 + N_3 + N_4$. In this setting, we consider the ANOVA model with the following restriction:

$$\forall j \in \{3, 4\}, \quad \theta_1 = \theta_2 \leq \theta_j.$$

Hence, in this candidate model, the parameter space Θ is given by

$$\Theta \equiv \{\boldsymbol{\theta} = (\theta_1, \theta_2, \theta_3, \theta_4)' \in \mathbb{R}^4 \mid \forall j \in \{3, 4\}, \theta_1 = \theta_2 \leq \theta_j\}.$$

Here, for comparison, we define the following criterion:

$$fC_p = (N - k^* - 2) \frac{\hat{\sigma}^2}{\bar{\sigma}^2} + 2(k + 1),$$

where k is the number of independent mean parameters in the candidate model, and the notation “f” of fC_p is an abbreviation for “formal”. Thus, the penalty term of the fC_p is $2(3 + 1)$ in this candidate model. Note that under no order restrictions, the fC_p is equal to the usual unbiased C_p criterion. However, since the parameters are restricted, the fC_p is not necessarily (asymptotically) unbiased estimator of the risk function in general.

Next, in this numerical experiments, we consider the following true parameters:

$$\text{Case 1: } \theta_1 = 1, \quad \theta_2 = 1, \quad \theta_3 = 1.5, \quad \theta_4 = 1.8, \quad \sigma^2 = 1,$$

$$\text{Case 2: } \theta_1 = 1, \quad \theta_2 = 1, \quad \theta_3 = 1.05, \quad \theta_4 = 1.05, \quad \sigma^2 = 1,$$

$$\text{Case 3: } \theta_1 = 1, \quad \theta_2 = 1, \quad \theta_3 = 1, \quad \theta_4 = 1, \quad \sigma^2 = 1,$$

$$\text{Case 4: } \theta_1 = 1.2, \quad \theta_2 = 1, \quad \theta_3 = 0.8, \quad \theta_4 = 1.3, \quad \sigma^2 = 1.$$

We would like to note that the vector of true parameters $\boldsymbol{\theta} = (\theta_1, \dots, \theta_4)'$ is an interior point of Θ in Case 1. Similarly, in Case 2, $\boldsymbol{\theta}$ is an interior point of Θ , but $\boldsymbol{\theta}$ is very close to the boundary. On the other hand, $\boldsymbol{\theta}$ is a boundary point

Table 4.1. Risk of the candidate model, and estimation accuracies of each criterion in Case 1–2

N	Case 1					Case 2				
	Risk	TOC_p		fC_p		Risk	TOC_p		fC_p	
	$R - N$	Bias	MSE	Bias	MSE	$R - N$	Bias	MSE	Bias	MSE
12	2.49	0.00	4.71	-0.69	4.66	2.11	0.00	7.72	-1.69	10.46
36	2.79	0.00	2.61	-0.26	2.38	2.12	0.00	4.45	-1.62	6.89
100	2.96	0.00	2.14	-0.04	2.08	2.14	0.00	3.95	-1.50	5.95
200	3.00	0.00	2.04	0.00	2.03	2.16	0.00	3.72	-1.40	5.32
1000	3.00	0.00	2.02	0.00	2.02	2.34	0.00	3.17	-0.95	3.51
2000	3.00	0.00	2.00	0.00	2.00	2.50	0.00	2.87	-0.67	2.76

Table 4.2. Risk of the candidate model, and estimation accuracies of each criterion in Case 3–4

N	Case 3					Case 4				
	Risk	TOC_p		fC_p		Risk	TOC_p		fC_p	
	$R - N$	Bias	MSE	Bias	MSE	$R - N$	Bias	MSE	Bias	MSE
12	2.10	0.00	8.14	-1.79	11.35	2.32	0.00	10.25	-1.87	13.94
36	2.11	0.00	4.83	-1.78	8.00	2.78	0.00	7.84	-1.92	11.91
100	2.11	0.00	4.45	-1.78	7.63	4.03	0.00	12.31	-1.96	16.67
200	2.11	0.00	4.36	-1.79	7.56	6.01	-0.01	20.27	-1.99	24.65
1000	2.11	0.00	4.30	-1.78	7.49	22.00	0.00	84.89	-2.00	88.88
2000	2.11	0.00	4.27	-1.78	7.46	42.00	0.00	165.94	-2.00	169.94

of θ in Case 3. Moreover, in Case 4, θ is not included in Θ . Therefore, the true model is included in the candidate model when Case 1–3. However, in Case 4, it is not included. From 1,000,000 Monte Carlo simulation runs, we confirm estimation accuracies (bias and MSE) of the TOC_p and the fC_p . Obtained results are given in Table 4.1 and 4.2.

From Table 4.1, we can see that the TOC_p and the fC_p are unbiased and asymptotically unbiased estimators of R , respectively. Similarly, we can see that the biases of the TOC_p of Case 2 are similar to those of Case 1. On the other hand, the bias of the fC_p in Case 2 is still not small when the sample size N is 2000. Moreover, in Case 3, from Table 4.2 we can see that the TOC_p is the unbiased estimator of R and the fC_p has the asymptotic bias. In addition, from Table 4.2 we can see that the fC_p has asymptotic bias in Case 4. However, the TOC_p is the unbiased estimator of R . Furthermore,

for the MSEs, from Table 4.1 we can see that the MSEs of the fC_p are smaller than those of the TOC_p in Case 1 or Case 2 and large N . On the other hand, from Table 4.2 we can see that the MSEs of the TOC_p are smaller than those of the fC_p in both Case 3 and 4.

4.2. Selection probability and the risk of the best model. In this subsection, we calculate selection probabilities in cases of using the TOC_p and the fC_p , respectively. In addition, we also calculate the risk of the best model selected by minimizing each criterion. Let $Y_{ij} \sim N(\theta_i, \sigma^2)$, where $i = 1, 2, 3, 4$ and $j = 1, \dots, N_i$ for each i . We set $N_1 = N_2 = N_3 = N_4$. Moreover, we put $N = N_1 + N_2 + N_3 + N_4$. In this setting, we consider the following five candidate models:

- $\mathcal{M}1$: ANOVA model with $\theta_1 = \theta_2 = \theta_3 = \theta_4$,
- $\mathcal{M}2$: ANOVA model with $\theta_1 = \theta_2 = \theta_3 \leq \theta_4$,
- $\mathcal{M}3$: ANOVA model with $\theta_1 = \theta_2 \leq \theta_j$, ($j = 3, 4$),
- $\mathcal{M}4$: ANOVA model with $\theta_1 \leq \theta_j$, ($j = 2, 3, 4$),
- $\mathcal{M}5$: ANOVA model without any restriction.

Note that these five candidate models are nested. Furthermore, in this simulation we consider the following true models:

- Case 1: $\theta_1 = \theta_2 = 1$, $\theta_3 = \theta_4 = 1.5$, $\sigma^2 = 1$,
- Case 2: $\theta_1 = \theta_2 = 1$, $\theta_3 = 2.4$, $\theta_4 = 1.7$, $\sigma^2 = 1$.

From 10,000 Monte Carlo simulation runs, we calculate the selection probability and the risk of the best model for each criterion in both cases. Obtained results are given in Table 4.3–4.6.

Table 4.3. Selection probability (%) for the case of using each criterion in Case 1

N	TOC_p					fC_p				
	$\mathcal{M}1$	$\mathcal{M}2$	$\mathcal{M}3$	$\mathcal{M}4$	$\mathcal{M}5$	$\mathcal{M}1$	$\mathcal{M}2$	$\mathcal{M}3$	$\mathcal{M}4$	$\mathcal{M}5$
40	46.70	14.74	28.88	4.98	4.70	48.13	14.82	27.37	4.71	4.97
80	24.98	14.67	48.36	6.11	5.88	25.63	14.68	47.60	6.11	5.98
120	13.69	10.99	62.06	6.57	6.69	14.02	10.99	61.64	6.62	6.73
160	6.99	7.69	70.11	7.70	7.51	7.13	7.69	69.95	7.72	7.51
200	3.27	4.70	77.12	7.60	7.31	3.31	4.70	77.06	7.61	7.32

Table 4.4. Selection probability (%) for the case of using each criterion in Case 2

N	TOC_p					fC_p				
	$\mathcal{M}1$	$\mathcal{M}2$	$\mathcal{M}3$	$\mathcal{M}4$	$\mathcal{M}5$	$\mathcal{M}1$	$\mathcal{M}2$	$\mathcal{M}3$	$\mathcal{M}4$	$\mathcal{M}5$
40	3.24	0.22	80.98	7.76	7.80	3.50	0.22	80.39	7.91	7.98
80	0.04	0.00	84.72	7.74	7.50	0.04	0.00	84.64	7.78	7.54
120	0.00	0.00	84.29	7.30	8.41	0.00	0.00	84.27	7.32	8.41
160	0.00	0.00	84.32	7.98	7.70	0.00	0.00	84.32	7.98	7.70
200	0.00	0.00	84.50	7.49	8.01	0.00	0.00	84.50	7.49	8.01

Table 4.5. Risk for each candidate model, and the values of risks of best models ($R[TOC_p], R[fC_p]$) selected by minimizing the TOC_p and the fC_p in Case 1

N	$\mathcal{M}1$	$\mathcal{M}2$	$\mathcal{M}3$	$\mathcal{M}4$	$\mathcal{M}5$	$R[TOC_p]$	$R[fC_p]$
40	43.50	43.40	42.71	43.32	44.03	43.98	43.98
80	86.02	85.20	82.90	83.46	84.01	84.52	84.54
120	128.51	126.92	122.96	123.46	123.99	124.47	124.48
160	171.00	168.61	162.99	163.51	164.02	164.29	164.29
200	213.51	210.30	202.97	203.49	203.98	204.01	204.01

Table 4.6. Risk for each candidate model, and the values of risks of best models ($R[TOC_p], R[fC_p]$) selected by minimizing the TOC_p and the fC_p in Case 2

N	$\mathcal{M}1$	$\mathcal{M}2$	$\mathcal{M}3$	$\mathcal{M}4$	$\mathcal{M}5$	$R[TOC_p]$	$R[fC_p]$
40	54.46	54.71	42.94	43.48	44.01	43.82	43.85
80	107.94	107.86	82.99	83.50	83.99	83.55	83.55
120	161.44	161.02	123.02	123.51	124.02	123.59	123.59
160	214.90	214.10	163.01	163.53	164.02	163.59	163.59
200	268.39	267.22	203.01	203.50	204.01	203.57	203.57

From Table 4.3–4.6, we can see that the obtained results of using the TOC_p are very similar to those of using fC_p in both cases. This implies that using the criterion which has unbiasedness does not dramatically influence the performance of criteria such as the selection probability and the risk of the best model.

5. Conclusion

Under ANOVA model with the tree ordering, we derived the unbiased C_p type criterion, called TOC_p . In addition, the TOC_p is the unbiased estimator

even if the true model is not included in the candidate model. Moreover, we show that the TOC_p is the UMVUE. We confirmed the estimation accuracy and we also calculated the selection probability and the risk of the best model through numerical experiments.

We recall that the TOC_p is derived under the tree ordering which is the important restriction in applied statistics. Nevertheless, there are other important restrictions such as simple ordering and umbrella ordering. Hence, we should derive the unbiased C_p type criterion under above restrictions. Moreover, we should consider generalization of restrictions such as the restriction on a closed convex polyhedral cone and the restriction on closed convex set with a smooth boundary. Furthermore, we should investigate theoretical property of criteria derived under order restrictions. These are left for the future work.

Appendix 1: Proof of Lemma 1

In this section, we prove Lemma 1. First, we provide the following lemma.

LEMMA A. *The following three propositions hold:*

- (1) *Let A and B be non-empty subsets of \mathbb{N}_I , and let $A \cap B = \emptyset$. Then, it holds that*

$$\bar{x}_A < \bar{x}_B \Rightarrow \bar{x}_A < \bar{x}_{A \cup B} < \bar{x}_B.$$

- (2) *Let A and B_1, \dots, B_i be non-empty subsets of \mathbb{N}_I , and let A and B_1, \dots, B_i be disjoint. Then, it holds that*

$$\forall j \in \{1, \dots, i\}, \quad \bar{x}_A < \bar{x}_{B_j} \Rightarrow \bar{x}_A < \bar{x}_B, \quad (\text{A.1})$$

where B is given by

$$B = \bigcup_{j=1}^i B_j.$$

Similarly, it also holds that

$$\forall j \in \{1, \dots, i\}, \quad \bar{x}_{B_j} \leq \bar{x}_A \Rightarrow \bar{x}_B \leq \bar{x}_A. \quad (\text{A.2})$$

- (3) *Let A , B and C be non-empty subsets of \mathbb{N}_I , and let A , B and C be disjoint. Then, it holds that*

$$\bar{x}_A < \bar{x}_C, \quad \bar{x}_B \leq \bar{x}_C \Rightarrow \bar{x}_{A \cup B} < \bar{x}_C. \quad (\text{A.3})$$

The proof of Lemma A is omitted because it is easily obtained. Next, we prove Lemma 1.

PROOF. When $l = 2$, the statements of Lemma 1 are equivalent to Lemma C given by Inatsu [8], and it is already proved. Therefore, we prove the case of $l \geq 3$.

First, we prove (1) of Lemma 1. From (5) it holds that

$$\bigcup_{i=1}^l \bigcup_{J \in \mathcal{J}_i^{(l)}} A^{(l)}(J) = \{\mathbf{x} \in \mathbb{R}^l \mid x_1 \leq x_2, \dots, x_1 \leq x_l\} = A^{(l)},$$

and $A^{(l)}(J) \neq A^{(l)}(J^*)$ where $J \neq J^*$. Therefore, from the definition of the inverse image, it is clear that (1) holds because $\boldsymbol{\eta}_l$ is the function from \mathbb{R}^l to $A^{(l)}$.

Next, using mathematical induction we prove (2) and (3) of Lemma 1. Thus, assume that Lemma 1 is true when $l = 2, \dots, q-1$. In this assumption, we prove that Lemma 1 is also true when $l = q$. Here, in the case of $i = 1$, $\mathcal{J}_1^{(q)}$ has only one set $J = \{1\}$. First, for this set J , we show the inclusion relation \supset of (7). Let $\mathbf{x} = (x_1, \dots, x_q)'$ be an element of \mathbb{R}^q satisfying

$$\mathbf{D}_J \mathbf{x}_J \geq \mathbf{0}, \quad \forall t \in \mathbb{N}_q \setminus J, \bar{x}_J < x_t.$$

Here, note that $\bar{x}_J = x_1$. Hence, for any integer t with $2 \leq t \leq q$, the inequality $x_1 < x_t$ holds. This implies that $\mathbf{x} \in A^{(q)}(J) \subset A^{(q)}$. Meanwhile, let

$$H_q(\boldsymbol{\delta}; \mathbf{x}) = \sum_{u=1}^q N_u(x_u - \delta_u)^2.$$

Then, noting that $\mathbf{x} \in A^{(q)}$, we get

$$0 \leq \min_{\boldsymbol{\delta} \in A^{(q)}} H_q(\boldsymbol{\delta}; \mathbf{x}) \leq H_q(\mathbf{x}; \mathbf{x}) = 0.$$

Therefore, it holds that

$$\min_{\boldsymbol{\delta} \in A^{(q)}} H_q(\boldsymbol{\delta}; \mathbf{x}) = H_q(\mathbf{x}; \mathbf{x}) = 0.$$

This equality means that $\boldsymbol{\eta}_q(\mathbf{x}) = \mathbf{x} \in A^{(q)}(J)$. Thus, we obtain $\boldsymbol{\eta}_q(\mathbf{x}) \in A^{(q)}(J)$. Therefore, $\mathbf{x} \in \boldsymbol{\eta}_q^{-1}(A^{(q)}(J))$ holds. Hence, the inclusion relation \supset of (7) in the case of $J = \{1\}$ is proved. Next, we show \subset of (7). Let $\mathbf{y} = (y_1, \dots, y_q)'$ be an element of \mathbb{R}^q satisfying $\mathbf{y} \in \boldsymbol{\eta}_q^{-1}(A^{(q)}(J))$. In other words, we assume that

$$\boldsymbol{\eta}_q(\mathbf{y}) = \operatorname{argmin}_{\boldsymbol{\delta} \in A^{(q)}} H_q(\boldsymbol{\delta}; \mathbf{y}) \equiv \mathbf{a} = (\alpha_1, \dots, \alpha_q)' \in A^{(q)}(J).$$

Here, noting that $A^{(q)}(J)$ is an open set, there exists an ε -neighborhood $U(\mathbf{a}; \varepsilon)$ of \mathbf{a} such that $U(\mathbf{a}; \varepsilon) \subset A^{(q)}(J)$. Thus, for any element $\boldsymbol{\gamma} = (\gamma_1, \dots, \gamma_q)'$ of \mathbb{R}^q satisfying $\boldsymbol{\gamma} \in U(\mathbf{a}; \varepsilon) \subset A^{(q)}$, it holds that

$$H_q(\mathbf{a}; \boldsymbol{\gamma}) \leq H_q(\boldsymbol{\gamma}; \boldsymbol{\gamma}).$$

This implies that \mathbf{a} is a local minimizer of $H_q(\boldsymbol{\delta}; \boldsymbol{\gamma})$. In addition, since $H_q(\boldsymbol{\delta}; \boldsymbol{\gamma})$ is a strictly convex function on \mathbb{R}^q w.r.t. $\boldsymbol{\delta}$, the local minimizer \mathbf{a} is the unique global minimizer. Moreover, it is clear that the global minimizer is $\boldsymbol{\gamma}$ because $H_q(\boldsymbol{\delta}; \boldsymbol{\gamma})$ is non-negative and $H_q(\boldsymbol{\gamma}; \boldsymbol{\gamma}) = 0$. Therefore, we get $\mathbf{a} = \boldsymbol{\gamma}$ and it holds that

$$\boldsymbol{\eta}_q(\boldsymbol{\gamma}) = \mathbf{a} = \boldsymbol{\gamma} \in A^{(q)}(J).$$

Hence, for any s with $s \in \mathbb{N}_q \setminus J$, the inequality $y_1 < y_s$ holds. Consequently, the inclusion relation \subset of (7) in the case of $J = \{1\}$ is proved.

Next, for any i with $2 \leq i \leq q-1$, we prove the inclusion relation \supset of (7). Let i be an integer with $2 \leq i \leq q-1$, and let J be a set with $J \in \mathcal{J}_i^{(q)}$. Assume that $\mathbf{x} = (x_1, \dots, x_q)'$ is an element of \mathbb{R}^q satisfying $\mathbf{D}_J \mathbf{x}_J \geq \mathbf{0}$ and $\bar{x}_J < x_t$ for any $t \in \mathbb{N}_q \setminus J$. Here, the function $H_q(\mathbf{a}; \mathbf{x})$ can be expressed as

$$\begin{aligned} H_q(\mathbf{a}; \mathbf{x}) &= \sum_{d=1}^q N_d(x_d - \alpha_d)^2 = \sum_{s \in J} N_s(x_s - \alpha_s)^2 + \sum_{t \in \mathbb{N}_q \setminus J} N_t(x_t - \alpha_t)^2 \\ &= H_{\#J}(\mathbf{a}_J; \mathbf{x}_J) + H_{\#\mathbb{N}_q \setminus J}(\mathbf{a}_{\mathbb{N}_q \setminus J}; \mathbf{x}_{\mathbb{N}_q \setminus J}). \end{aligned}$$

Therefore, it is easily checked that

$$\min_{\mathbf{a} \in A^{(q)}} H_q(\mathbf{a}; \mathbf{x}) \geq \min_{\mathbf{a}_J \in A^{(\#J)}} H_{\#J}(\mathbf{a}_J; \mathbf{x}_J) + H_{\#\mathbb{N}_q \setminus J}(\mathbf{x}_{\mathbb{N}_q \setminus J}; \mathbf{x}_{\mathbb{N}_q \setminus J}). \quad (\text{A.4})$$

In addition, we put $\mathbf{x}_J = (y_1, \dots, y_{\#J})' = \mathbf{y}$, $\mathbf{a}_J = (\beta_1, \dots, \beta_{\#J})' = \boldsymbol{\beta}$, $\mathbf{N}_J = (n_1, \dots, n_{\#J})' = \mathbf{n}$ and $J^* = \mathbb{N}_{\#J}$. By using these notations, we obtain

$$H_{\#J}(\mathbf{a}_J; \mathbf{x}_J) = \sum_{s \in J} N_s(x_s - \alpha_s)^2 = \sum_{u=1}^{\#J} n_u(y_u - \beta_u)^2 = H_{\#J}(\boldsymbol{\beta}; \mathbf{y}),$$

and

$$\min_{\mathbf{a}_J \in A^{(\#J)}} H_{\#J}(\mathbf{a}_J; \mathbf{x}_J) = \min_{\boldsymbol{\beta} \in A^{(\#J)}} H_{\#J}(\boldsymbol{\beta}; \mathbf{y}).$$

Recall that Lemma 1 is true when $l = 2, \dots, q-1$ from the assumption of mathematical induction. Moreover, it also holds that $\mathbf{D}_J^{(N)} \mathbf{x}_J \geq \mathbf{0}$. This inequality is equal to $\mathbf{D}_{J^*}^{(n)} \mathbf{y}_{J^*} \geq \mathbf{0}$. Furthermore, noting that $J^* = \mathbb{N}_{\#J}$ and $2 \leq \#J \leq q-1$, from (3) of Lemma 1 we get

$$\begin{aligned}
\min_{\mathbf{a}_J \in A^{(\#J)}} H_{\#J}(\mathbf{a}_J; \mathbf{x}_J) &= \min_{\boldsymbol{\beta} \in A^{(\#J)}} H_{\#J}(\boldsymbol{\beta}; \mathbf{y}) \\
&= \sum_{u=1}^{\#J} n_u (y_u - \bar{y}_{J^*})^2 = \sum_{s \in J} N_s (x_s - \bar{x}_J)^2. \quad (\text{A.5})
\end{aligned}$$

Hence, from (A.4) and (A.5), it holds that

$$\min_{\mathbf{a} \in A^{(q)}} H_q(\mathbf{a}; \mathbf{x}) \geq \sum_{s \in J} N_s (x_s - \bar{x}_J)^2 + \sum_{t \in \mathbb{N}_q \setminus J} N_t (x_t - x_t)^2. \quad (\text{A.6})$$

Here, let $\boldsymbol{\gamma} = (\gamma_1, \dots, \gamma_q)'$ be a q -dimensional vector whose s th element ($s \in J$) is \bar{x}_J and t th element ($t \in \mathbb{N}_q \setminus J$) is x_t . Then, from the assumption, for any $t \in \mathbb{N}_q \setminus J$ it holds that $\bar{x}_J < x_t$. Thus, from the definition of $\boldsymbol{\gamma}$, we obtain $\boldsymbol{\gamma} \in A^{(q)}$. Hence, the following inequality holds:

$$\min_{\mathbf{a} \in A^{(q)}} H_q(\mathbf{a}; \mathbf{x}) \leq H_q(\boldsymbol{\gamma}; \mathbf{x}) = \sum_{s \in J} N_s (x_s - \bar{x}_J)^2 + \sum_{t \in \mathbb{N}_q \setminus J} N_t (x_t - x_t)^2. \quad (\text{A.7})$$

Therefore, from (A.6) and (A.7) we get

$$\min_{\mathbf{a} \in A^{(q)}} H_q(\mathbf{a}; \mathbf{x}) = H_q(\boldsymbol{\gamma}; \mathbf{x}).$$

This implies that

$$\boldsymbol{\eta}_q(\mathbf{x}) = \operatorname{argmin}_{\mathbf{a} \in A^{(q)}} H_q(\mathbf{a}; \mathbf{x}) = \boldsymbol{\gamma}.$$

Noting that from the definition of $\boldsymbol{\gamma}$, we get $\boldsymbol{\gamma} \in A^{(q)}(J)$, i.e., $\mathbf{x} \in \boldsymbol{\eta}_q^{-1}(A^{(q)}(J))$. Consequently, for any i with $2 \leq i \leq q-1$, the inclusion relation \supset of (7) is proved.

Next, we prove the inclusion relation \subset of (7). Let i be an integer with $2 \leq i \leq q-1$, and let J be a set with $J \in \mathcal{J}_i^{(q)}$. Also let $\mathbf{x} = (x_1, \dots, x_q)'$ be an element of \mathbb{R}^q satisfying $\mathbf{x} \in \boldsymbol{\eta}_q^{-1}(A^{(q)}(J))$. In other words, we assume that

$$\boldsymbol{\eta}_q(\mathbf{x}) = (\alpha_1, \dots, \alpha_q)' = \mathbf{a} \in A^{(q)}(J).$$

Here, from the definition of $A^{(q)}(J)$, for any $s \in J$ and for any $t \in \mathbb{N}_q \setminus J$, it holds that $\alpha_1 = \alpha_s$ and $\alpha_1 < \alpha_t$. Incidentally, from the definition of $\boldsymbol{\eta}_q$, we get

$$\begin{aligned}
\min_{\boldsymbol{\delta} \in A^{(q)}} \sum_{i=1}^q N_i (x_i - \delta_i)^2 &= \sum_{s \in J} N_s (x_s - \alpha_s)^2 + \sum_{t \in \mathbb{N}_q \setminus J} N_t (x_t - \alpha_t)^2 \\
&= \sum_{s \in J} N_s (x_s - \alpha_1)^2 + \sum_{t \in \mathbb{N}_q \setminus J} N_t (x_t - \alpha_t)^2.
\end{aligned}$$

In addition, for the subvector $\boldsymbol{\gamma}^* = (\gamma_1, \boldsymbol{\gamma}'_{\mathbb{N}_q \setminus J})'$, we consider the following function:

$$H(\boldsymbol{\gamma}^*; \mathbf{x}) = \sum_{s \in J} N_s(x_s - \gamma_1)^2 + \sum_{t \in \mathbb{N}_q \setminus J} N_t(x_t - \gamma_t)^2.$$

Noting that $\mathbf{a}^* = (\alpha_1, \boldsymbol{\alpha}'_{\mathbb{N}_q \setminus J})' \in A^{(q-\#J+1)}(\{1\})$ and $A^{(q-\#J+1)}(\{1\})$ is an open set, there exists an ε -neighborhood $U(\mathbf{a}^*; \varepsilon)$ of \mathbf{a}^* such that $U(\mathbf{a}^*; \varepsilon) \subset A^{(q-\#J+1)}(\{1\})$. Let $\boldsymbol{\zeta} = (\zeta_1, \dots, \zeta_q)'$, and let $\boldsymbol{\zeta}^* = (\zeta_1, \boldsymbol{\zeta}'_{\mathbb{N}_q \setminus J})' \in U(\mathbf{a}^*; \varepsilon)$. Moreover, let $\boldsymbol{\xi} = (\xi_1, \dots, \xi_q)'$ be a q -dimensional vector whose s th element ($s \in J$) is $\xi_s = \zeta_1$, and t th element ($t \in \mathbb{N}_q \setminus J$) is $\xi_t = \zeta_t$. Then, noting that $\boldsymbol{\xi} \in A^{(q)}$ we obtain

$$\begin{aligned} H(\boldsymbol{\zeta}^*; \mathbf{x}) &= \sum_{s \in J} N_s(x_s - \zeta_1)^2 + \sum_{t \in \mathbb{N}_q \setminus J} N_t(x_t - \zeta_t)^2 \\ &= \sum_{s \in J} N_s(x_s - \xi_s)^2 + \sum_{t \in \mathbb{N}_q \setminus J} N_t(x_t - \xi_t)^2 \\ &\geq \min_{\boldsymbol{\delta} \in A^{(q)}} \sum_{i=1}^q N_i(x_i - \delta_i)^2 \\ &= \sum_{s \in J} N_s(x_s - \alpha_1)^2 + \sum_{t \in \mathbb{N}_q \setminus J} N_t(x_t - \alpha_t)^2 = H(\mathbf{a}^*; \mathbf{x}). \end{aligned}$$

Thus, \mathbf{a}^* is a local minimizer of $H(\boldsymbol{\gamma}^*; \mathbf{x})$. In addition, since $H(\boldsymbol{\gamma}^*; \mathbf{x})$ is a strictly convex function on $\mathbb{R}^{q-\#J+1}$ w.r.t. $\boldsymbol{\gamma}^*$, the local minimizer \mathbf{a}^* is the unique global minimizer of $H(\boldsymbol{\gamma}^*; \mathbf{x})$. Moreover, the global minimizer can be obtained by differentiating $H(\boldsymbol{\gamma}^*; \mathbf{x})$ w.r.t. $\boldsymbol{\gamma}^*$ as

$$\alpha_1 = \bar{x}_J, \quad \alpha_t = x_t \quad (t \in \mathbb{N}_q \setminus J).$$

Therefore, noting that $\alpha_1 < \alpha_t$, we have $\bar{x}_J < x_t$.

Next, we prove $\mathbf{D}_J^{(N)} \mathbf{x}_J \geq \mathbf{0}$. We replace \mathbf{x}_J and N_J with $\mathbf{y} = (y_1, \dots, y_i)'$ and $\mathbf{n} = (n_1, \dots, n_i)'$, respectively. In addition, we put $J^* = \mathbb{N}_i$. Note that $\mathbf{x}_J = \mathbf{y} = \mathbf{y}_{J^*}$. Also note that \mathbf{y} is an i -dimensional vector and $2 \leq i \leq q-1$. Recall that from (1) of Lemma 1, it holds that

$$\mathbb{R}^i = \bigcup_{s=1}^i \bigcup_{J \in \mathcal{J}_s^{(i)}} \boldsymbol{\eta}_i^{-1}(A^{(i)}(J)),$$

$$\boldsymbol{\eta}_i^{-1}(A^{(i)}(J)) \cap \boldsymbol{\eta}_i^{-1}(A^{(i)}(J^*)) = \emptyset \quad (J \neq J^*).$$

In order to prove $\mathbf{D}_J^{(N)} \mathbf{x}_J \geq \mathbf{0}$, we show $\mathbf{y} \in \boldsymbol{\eta}_i^{-1}(A^{(i)}(\mathbb{N}_i))$ using proof by contradiction. Thus, we assume that there exists an integer s with $1 \leq s \leq$

$i - 1$ and a set J^{**} of $\mathcal{J}_s^{(i)}$ such that $\mathbf{y} \in \boldsymbol{\eta}_i^{-1}(A^{(i)}(J^{**}))$. Recall that from the assumption of mathematical induction, Lemma 1 is true when $l = 2, \dots, q - 1$. Furthermore, since $i \leq q - 1$, from (2) of Lemma 1, $\mathbf{y} \in \boldsymbol{\eta}_i^{-1}(A^{(i)}(J^{**}))$ is equivalent to

$$\mathbf{D}_{J^{**}}^{(n)} \mathbf{y}_{J^{**}} \geq \mathbf{0}, \quad \bar{y}_{J^{**}} < y_t \quad (t \in \mathbb{N}_i \setminus J^{**}).$$

Here, by using (2) of Lemma A, we get $\bar{y}_{J^{**}} < \bar{y}_{\mathbb{N}_i \setminus J^{**}}$. Moreover, using (1) of Lemma A we have $\bar{y}_{J^{**}} < \bar{y}_{\mathbb{N}_i} = \bar{x}_J$. Therefore, combining $\bar{x}_J < x_t$ ($t \in \mathbb{N}_q \setminus J$), we get

$$\bar{y}_{J^{**}} < x_r \quad (r \in \mathbb{N}_q \setminus J). \quad (\text{A.8})$$

Note that there exists a set J^{***} with $J^{***} \subsetneq J$ satisfies $\bar{y}_{J^{**}} = \bar{x}_{J^{***}}$ and

$$\mathbf{D}_{J^{***}}^{(n)} \mathbf{y}_{J^{**}} = \mathbf{D}_{J^{***}}^{(N)} \mathbf{x}_{J^{***}} \geq \mathbf{0}, \quad \bar{x}_{J^{***}} < x_v \quad (v \in J \setminus J^{***}). \quad (\text{A.9})$$

Hence, for the set J^{***} , from (A.8) and (A.9) it holds that

$$\mathbf{D}_{J^{***}}^{(N)} \mathbf{x}_{J^{***}} \geq \mathbf{0}, \quad \bar{x}_{J^{***}} < x_u \quad (u \in \mathbb{N}_q \setminus J^{***}).$$

As we proved before, this implies that $\mathbf{x} \in \boldsymbol{\eta}_q^{-1}(A^{(q)}(J^{***}))$. However, this result is a contradiction because $J \neq J^{***}$, $\mathbf{x} \in \boldsymbol{\eta}_q^{-1}(A^{(q)}(J))$ and $\boldsymbol{\eta}_q^{-1}(A^{(q)}(J)) \cap \boldsymbol{\eta}_q^{-1}(A^{(q)}(J^{***})) = \emptyset$. Therefore, we obtain $\mathbf{y} \in \boldsymbol{\eta}_i^{-1}(A^{(i)}(\mathbb{N}_i))$. From (2) of Lemma 1, this result is equivalent to $\mathbf{D}_{\mathbb{N}_i}^{(n)} \mathbf{y} \geq \mathbf{0}$. This inequality can be written by using N , J and \mathbf{x}_J as $\mathbf{D}_J^{(N)} \mathbf{x}_J \geq \mathbf{0}$. Thus, for any i with $2 \leq i \leq q - 1$, the inclusion relation \subset of (7) is proved.

Finally, in the case of $i = q$, i.e., $J = \mathbb{N}_q \in \mathcal{J}_q^{(q)}$, we prove (7). First, we prove the inclusion relation \supset of (7). Let $\mathbf{x} = (x_1, \dots, x_q)' \in \mathbb{R}^q$, and let $\mathbf{D}_J \mathbf{x}_J \geq \mathbf{0}$. Recall that the following relation holds:

$$\mathbb{R}^q = \bigcup_{s=1}^q \bigcup_{J \in \mathcal{J}_s^{(q)}} \boldsymbol{\eta}_q^{-1}(A^{(q)}(J)),$$

$$\boldsymbol{\eta}_q^{-1}(A^{(q)}(J)) \cap \boldsymbol{\eta}_q^{-1}(A^{(q)}(J^*)) = \emptyset \quad (J \neq J^*).$$

Again, we consider proof by contradiction. Hence, we assume that there exists an integer s with $1 \leq s \leq q - 1$ and a set J^* of $\mathcal{J}_s^{(q)}$ satisfying $\mathbf{x} \in \boldsymbol{\eta}_q^{-1}(A^{(q)}(J^*))$. Thus, as we mentioned before, it holds that

$$\mathbf{D}_{J^*} \mathbf{x}_{J^*} \geq \mathbf{0}, \quad \bar{x}_{J^*} < x_t \quad (t \in \mathbb{N}_q \setminus J^*).$$

We would like to recall that $1 \in J^*$ and the number of elements in J^* is s . Here, if $s = q - 1$, then $\mathbb{N}_q \setminus J^*$ has only one element a satisfying $a > 1$. Therefore, it holds that

$$\bar{x}_{\mathbb{N}_q \setminus \{a\}} < x_a.$$

However, this inequality is a contradiction because $\mathbf{D}_J \mathbf{x}_J \geq \mathbf{0}$. Hence, s satisfies $1 \leq s \leq q - 2$. Incidentally, there exists an element t^* of $\mathbb{N}_q \setminus J^*$ which satisfies

$$\forall t \in N_q \setminus (J^* \cup \{t^*\}), \quad x_t \leq x_{t^*}$$

Therefore, form (2) of Lemma A we get

$$\bar{x}_{N_q \setminus (J^* \cup \{t^*\})} \leq x_{t^*}$$

In addition, since $\bar{x}_J < x_{t^*}$, from (3) of Lemma A we obtain

$$\bar{x}_{\mathbb{N}_q \setminus \{t^*\}} < x_{t^*}$$

However, this inequality is also contradiction because $\mathbf{D}_J \mathbf{x}_J \geq \mathbf{0}$. Thus, we get $s = q$. This implies that $J^* = \mathbb{N}_q \in \mathcal{J}_q^{(q)}$ and $\mathbf{x} \in \boldsymbol{\eta}_q^{-1}(A^{(q)}(\mathbb{N}_q))$. Therefore, the inclusion relation \supset of (7) in the case of $i = q$ is proved. Next, we prove \subset . Assume that $\mathbf{x} \in \boldsymbol{\eta}_q^{-1}(A^{(q)}(\mathbb{N}_q))$. In other words, it holds that

$$\boldsymbol{\eta}_q(\mathbf{x}) \equiv \mathbf{a} \in A^{(q)}(\mathbb{N}_q).$$

From the definition of $A^{(q)}(\mathbb{N}_q)$, we get $\mathbf{a} = \mathbf{1}_q \alpha$, where $\mathbf{1}_q$ is a q -dimensional vector and every element of $\mathbf{1}_q$ is equal to one. Here, again we consider proof by contradiction. Therefore, we assume that there exists an integer s with $2 \leq s \leq q$ which satisfies

$$\bar{x}_{\mathbb{N}_q \setminus \{s\}} < x_s. \quad (\text{A.10})$$

Meanwhile, for the function $H_q(\boldsymbol{\delta}; \mathbf{x})$ given by

$$H_q(\boldsymbol{\delta}; \mathbf{x}) = \sum_{a=1}^q N_a (x_a - \delta_a)^2,$$

it is easily checked that

$$\min_{\boldsymbol{\delta} \in A^{(q)}} H_q(\boldsymbol{\delta}; \mathbf{x}) = H_q(\mathbf{a}; \mathbf{x}) = \sum_{a=1}^q N_a (x_a - \alpha)^2, \quad (\text{A.11})$$

because $\mathbf{x} \in \boldsymbol{\eta}_q^{-1}(A^{(q)}(\mathbb{N}_q))$ is true. Here, it is clear that the following inequality holds:

$$\sum_{a=1}^q N_a (x_a - \alpha)^2 \geq \min_{\beta \in \mathbb{R}} \sum_{a=1, a \neq s}^q N_a (x_a - \beta)^2 = \sum_{a=1, a \neq s}^q N_a (x_a - \bar{x}_{\mathbb{N}_q \setminus \{s\}})^2. \quad (\text{A.12})$$

Hence, combining (A.11) and (A.12) we get

$$\min_{\boldsymbol{\delta} \in A^{(q)}} H_q(\boldsymbol{\delta}; \mathbf{x}) \geq \sum_{a=1, a \neq s}^q N_a (x_a - \bar{x}_{\mathbb{N}_q \setminus \{s\}})^2. \quad (\text{A.13})$$

Let $\boldsymbol{\beta}$ be a q -dimensional vector whose s th and t th ($t \in \mathbb{N}_q \setminus \{s\}$) elements are x_s and $\bar{x}_{\mathbb{N}_q \setminus \{s\}}$, respectively. Then, the inequality (A.13) can be written by using $\boldsymbol{\beta}$ as

$$\min_{\boldsymbol{\delta} \in A^{(q)}} H_q(\boldsymbol{\delta}; \mathbf{x}) \geq H_q(\boldsymbol{\beta}; \mathbf{x}).$$

On the other hand, from the assumption (A.10), we obtain

$$\min_{\boldsymbol{\delta} \in A^{(q)}} H_q(\boldsymbol{\delta}; \mathbf{x}) \leq H_q(\boldsymbol{\beta}; \mathbf{x}),$$

because $\boldsymbol{\beta} \in A^{(q)}$. Thus, we have

$$\min_{\boldsymbol{\delta} \in A^{(q)}} H_q(\boldsymbol{\delta}; \mathbf{x}) = H_q(\boldsymbol{\beta}; \mathbf{x}),$$

and this means that $\boldsymbol{\eta}_q(\mathbf{x}) = \boldsymbol{\beta}$. However, this result is a contradiction because $\boldsymbol{\eta}_q(\mathbf{x}) = \mathbf{a}$ and $\mathbf{a} \neq \boldsymbol{\beta}$. Hence, for any integer s with $2 \leq s \leq q$, it holds that $\bar{x}_{\mathbb{N}_q \setminus \{s\}} \geq x_s$. This inequality is equivalent to $\mathbf{D}_{\mathbb{N}_q} \mathbf{x}_{\mathbb{N}_q} \geq \mathbf{0}$. Therefore, the inclusion relation \subset of (7) in the case of $i = q$ is proved. Consequently, (2) of Lemma 1 is proved.

Finally, we prove (3) of Lemma 1. When $J \neq \mathbb{N}_q$, we have already proved in the proof of (2) of Lemma 1. Thus, we prove the case of $J = \mathbb{N}_q$. Let $\mathbf{x} \in \boldsymbol{\eta}_q^{-1}(A^{(q)}(\mathbb{N}_q))$. Then, it holds that $\boldsymbol{\eta}_q(\mathbf{x}) \equiv \mathbf{a} \in A^{(q)}(\mathbb{N}_q)$ and \mathbf{a} can be written as $\mathbf{a} = \alpha \mathbf{1}_q$. Here, for the function $H_q(\boldsymbol{\delta}; \mathbf{x})$ defined by

$$H_q(\boldsymbol{\delta}; \mathbf{x}) = \sum_{a=1}^q N_a (x_a - \delta_a)^2,$$

we obtain

$$\begin{aligned} \min_{\boldsymbol{\delta} \in A^{(q)}} H_q(\boldsymbol{\delta}; \mathbf{x}) &= H_q(\mathbf{a}; \mathbf{x}) = \sum_{a=1}^q N_a (x_a - \alpha)^2 \\ &\geq \min_{\beta \in \mathbb{R}} \sum_{a=1}^q N_a (x_a - \beta)^2 = \sum_{a=1}^q N_a (x_a - \bar{x}_{\mathbb{N}_q})^2 \\ &= H_q(\bar{x}_{\mathbb{N}_q} \mathbf{1}_q; \mathbf{x}), \end{aligned} \tag{A.14}$$

because $\mathbf{x} \in \boldsymbol{\eta}_q^{-1}(A^{(q)}(\mathbb{N}_q))$ holds. On the other hand, since $\bar{x}_{\mathbb{N}_q} \mathbf{1}_q \in A^{(q)}$, we get

$$\min_{\boldsymbol{\delta} \in A^{(q)}} H_q(\boldsymbol{\delta}; \mathbf{x}) \leq H_q(\bar{x}_{\mathbb{N}_q} \mathbf{1}_q; \mathbf{x}).$$

By combining this inequality and (A.14), we have

$$\min_{\boldsymbol{\delta} \in A^{(q)}} H_q(\boldsymbol{\delta}; \mathbf{x}) = H_q(\bar{x}_{\mathbb{N}_q} \mathbf{1}_q; \mathbf{x}).$$

This implies $\boldsymbol{\eta}_q(\mathbf{x}) = \mathbf{a} = \bar{x}_{\mathbb{N}_q} \mathbf{1}_q$. Therefore, (3) of Lemma 1 is proved. \square

Appendix 2: Technical lemma

In this section, we provide two technical lemmas. Using Lemma 1 and provided two lemmas, we prove Theorem 1 in Appendix 3.

LEMMA B. *Let v_1, \dots, v_l be independent random variables, and let $v_s \sim N(\xi_s, \tau^2/N_s)$ where $1 \leq s \leq l$, $\tau^2 > 0$, $\xi_1, \dots, \xi_l \in \mathbb{R}$ and $N_1, \dots, N_l \in \mathbb{R}_{>0}$. Let $\mathbf{N} = (N_1, \dots, N_l)'$, $\mathbf{v} = (v_1, \dots, v_l)'$ and $\boldsymbol{\xi} = (\xi_1, \dots, \xi_l)'$. In addition, for any integer i with $1 \leq i \leq l$ and for any set J with $J \in \mathcal{J}_i^{(l)}$, define*

$$S(J) = \sum_{s \in J} N_s (v_s - \xi_s)(v_s - \bar{v}_J).$$

Then, the following two propositions hold:

- (1) *If $J \neq \mathbb{N}_l$, then $\mathbf{v}_{\mathbb{N}_l \setminus J}$, $((\mathbf{D}_J \mathbf{v}_J)', S(J))'$ and \bar{v}_J are mutually independent.*
- (2) *If $J = \mathbb{N}_l$, then $((\mathbf{D}_J \mathbf{v}_J)', S(J))'$ and \bar{v}_J are mutually independent.*

PROOF. First, we prove (1). From the assumption, \mathbf{v} is distributed as the multivariate normal distribution with a diagonal covariance matrix. Therefore, noting that the two sets J and $\mathbb{N}_l \setminus J$ are disjoint sets, it can be shown that the two subvectors \mathbf{v}_J and $\mathbf{v}_{\mathbb{N}_l \setminus J}$ are also distributed as (multivariate) normal distributions and these are mutually independent.

Next, we prove that $((\mathbf{D}_J \mathbf{v}_J)', S(J))'$ and \bar{v}_J are functions of \mathbf{v}_J , and these are mutually independent. Here, the case of $J = \{1\}$ is clear because $((\mathbf{D}_J \mathbf{v}_J)', S(J))' = (0, 0)'$. Thus, we consider the case of $J \neq \{1\}$. Since

$$\sum_{s \in J} N_s \bar{v}_J (v_s - \bar{v}_J) = 0,$$

it holds that

$$\begin{aligned} S(J) &= \sum_{s \in J} N_s (v_s - \xi_s)(v_s - \bar{v}_J) = \sum_{s \in J} N_s (v_s - \bar{v}_J - \xi_s)(v_s - \bar{v}_J) \\ &= \sum_{s \in J} N_s (v_s - \bar{v}_J)^2 - \sum_{s \in J} N_s \xi_s (v_s - \bar{v}_J). \end{aligned}$$

Here, let

$$\mathbf{A} = (\text{diag}(N_J))^{1/2} \left\{ \mathbf{I}_{\#J} - \frac{\mathbf{1}_{\#J}}{N_J} \mathbf{N}'_J \right\}, \quad (\text{B.1})$$

where $\text{diag}(N_J)$ means the diagonal matrix whose (a, a) element is the a th element of the vector N_J . Then, $S(J)$ can be expressed as

$$S(J) = (\mathbf{A}v_J)'(\mathbf{A}v_J) - (\boldsymbol{\zeta}'_J(\text{diag}(N_J))^{1/2})\mathbf{A}v_J.$$

Hence, $((\mathbf{D}_Jv_J)', S(J))'$ is the function of $((\mathbf{D}_Jv_J)', (\mathbf{A}v_J)')$. Therefore, it is sufficient to prove that $((\mathbf{D}_Jv_J)', (\mathbf{A}v_J)')$ and \bar{v}_J are independent. Note that the vector $((\mathbf{D}_Jv_J)', (\mathbf{A}v_J)', \bar{v}_J)'$ can be written as

$$\begin{pmatrix} \mathbf{D}_Jv_J \\ \mathbf{A}v_J \\ \bar{v}_J \end{pmatrix} = \begin{pmatrix} \mathbf{D}_J \\ \mathbf{A} \\ N'_J/\tilde{N}_J \end{pmatrix} v_J,$$

and v_J are distributed as multivariate normal distribution. Thus, it holds that $((\mathbf{D}_Jv_J)', (\mathbf{A}v_J)')$ and \bar{v}_J are distributed as (multivariate) normal distributions. Hence, in order to prove its independence, it is sufficient to prove that the covariance of $((\mathbf{D}_Jv_J)', (\mathbf{A}v_J)')$ and \bar{v}_J is the zero vector. Here, the covariance of \mathbf{D}_Jv_J and \bar{v}_J can be expressed as

$$\text{Cov}[\mathbf{D}_Jv_J, \bar{v}_J] = \mathbf{D}_J \text{Var}[v_J]N_J/\tilde{N}_J. \quad (\text{B.2})$$

Furthermore, noting that $\text{Var}[v_J] = \tau^2(\text{diag}(N_J))^{-1}$, (B.2) can be written as

$$\text{Cov}[\mathbf{D}_Jv_J, \bar{v}_J] = (\tau^2/\tilde{N}_J)\mathbf{D}_J(\text{diag}(N_J))^{-1}N_J = (\tau^2/\tilde{N}_J)\mathbf{D}_J\mathbf{1}_{\#J}.$$

In addition, from the definition of the matrix \mathbf{D}_J , it holds that $\mathbf{D}_J\mathbf{1}_{\#J} = \mathbf{0}$. Therefore, we get $\text{Cov}[\mathbf{D}_Jv_J, \bar{v}_J] = \mathbf{0}$. Similarly, the covariance of $\mathbf{A}v_J$ and \bar{v}_J is given by

$$\text{Cov}[\mathbf{A}v_J, \bar{v}_J] = (\tau^2/\tilde{N}_J)\mathbf{A}\mathbf{1}_{\#J},$$

and it holds that $\mathbf{A}\mathbf{1}_{\#J} = \mathbf{0}$ from (B.1). Thus, we have $\text{Cov}[\mathbf{A}v_J, \bar{v}_J] = \mathbf{0}$. Therefore, $((\mathbf{D}_Jv_J)', (\mathbf{A}v_J)')$ and \bar{v}_J are independent. This implies that $((\mathbf{D}_Jv_J)', S(J))'$ and \bar{v}_J are independent. Hence, (1) is proved. On the other hand, by using the same argument, we can also prove (2). \square

LEMMA C. Let v_1, \dots, v_l be independent random variables defined as in Lemma B, and let

$$A^{(l)}(\{1\}) = \{(x_1, \dots, x_l)' \in \mathbb{R}^l \mid x_1 < x_2, \dots, x_l < x_1\}.$$

Then, it holds that

$$\begin{aligned} & \mathbb{E} \left[\mathbf{1}_{\{v \in \eta^{-1}(A^{(l)}(\{1\}))\}} \times \frac{1}{\tau^2} \sum_{s=1}^l N_s v_s (v_s - \zeta_s) \right] \\ &= \mathbb{E} \left[\mathbf{1}_{\{v \in A^{(l)}(\{1\})\}} \times \frac{1}{\tau^2} \sum_{s=1}^l N_s v_s (v_s - \zeta_s) \right] \end{aligned}$$

$$\begin{aligned}
 &= I\mathbf{E}[1_{\{v \in A^{(l)}(\{1\})\}}] = I\mathbf{E}[1_{\{v \in \boldsymbol{\eta}_l^{-1}(A^{(l)}(\{1\}))\}}] \\
 &= I\mathbf{P}(v \in \boldsymbol{\eta}_l^{-1}(A^{(l)}(\{1\}))). \tag{C.1}
 \end{aligned}$$

PROOF. From the definition of the indicator function, it is clear that the fourth equality holds. On the other hand, for the first and third equalities, we must prove

$$v \in \boldsymbol{\eta}_l^{-1}(A^{(l)}(\{1\})) \Leftrightarrow v \in A^{(l)}(\{1\}).$$

However, we have already proved this relation in (7). Therefore, we prove the second equality. For any integer s with $1 \leq s \leq l$, we define

$$\frac{\sqrt{N_s}(v_s - \xi_s)}{\tau} = z_s, \quad b_s = \frac{\xi_s \sqrt{N_s}}{\tau}.$$

Note that z_1, \dots, z_l are independent and identically distributed as $N(0, 1)$. Furthermore, it holds that

$$\frac{1}{\tau^2} \sum_{s=1}^l N_s v_s (v_s - \xi_s) = \sum_{s=1}^l z_s (z_s + b_s). \tag{C.2}$$

In addition, for any integer t with $2 \leq t \leq l$, putting

$$\frac{\sqrt{N_t}}{\sqrt{N_1}} = a_t,$$

the following relation holds:

$$v \in A^{(l)}(\{1\}) \Leftrightarrow 2 \leq t \leq l, \quad v_1 < v_t \Leftrightarrow 2 \leq t \leq l, \quad a_t(z_1 + b_1) - b_t < z_t.$$

Here, define

$$E_l = \{(c_1, \dots, c_l) \in \mathbb{R}^l \mid 2 \leq t \leq l, a_t(c_1 + b_1) - b_t < c_t\}.$$

Then, for the vector $\mathbf{z} = (z_1, \dots, z_l)'$, it holds that $v \in A^{(l)}(\{1\}) \Leftrightarrow \mathbf{z} \in E_l$. Using this result and (C.2), we obtain

$$\begin{aligned}
 &\mathbf{E} \left[1_{\{v \in A^{(l)}(\{1\})\}} \times \frac{1}{\tau^2} \sum_{s=1}^l N_s v_s (v_s - \xi_s) \right] \\
 &= \mathbf{E} \left[1_{\{\mathbf{z} \in E_l\}} \times \sum_{s=1}^l z_s (z_s + b_s) \right] \\
 &= \int \dots \int_{E_l} \left\{ \sum_{s=1}^l z_s (z_s + b_s) \right\} \prod_{s=1}^l \phi(z_s) dz_1 \dots dz_l, \tag{C.3}
 \end{aligned}$$

where $\phi(x)$ is the probability density function of standard normal distribution. Here, when $l = 2$, Inatsu [8] proved that (C.3) is equal to $IE[1_{\{v \in A^{(l)}(\{1\})\}}]$. Hence, we prove the case of $l \geq 3$.

First, for any integer s with $2 \leq s \leq l$ we define

$$F_s(x) = \int_{a_s(x+b_1)-b_s}^{\infty} \phi(y) dy.$$

In addition, let

$$G_1 = \int_{-\infty}^{\infty} z_1(z_1 + b_1) \left(\prod_{s=2}^l F_s(z_1) \right) \phi(z_1) dz_1,$$

and let

$$G_s = \int_{-\infty}^{\infty} \left(\int_{a_s(z_1+b_1)-b_s}^{\infty} z_s(z_s + b_s) \phi(z_s) dz_s \right) \left(\prod_{2 \leq t \leq l, t \neq s} F_t(z_1) \right) \phi(z_1) dz_1, \quad (\text{C.4})$$

where $s = 2, \dots, l$. Then, (C.3) can be written as

$$\int \dots \int_{E_l} \left\{ \sum_{s=1}^l z_s(z_s + b_s) \right\} \prod_{s=1}^l \phi(z_s) dz_1 \dots dz_l = \sum_{s=1}^l G_s. \quad (\text{C.5})$$

Next, we calculate G_1 and G_s . Using the integration by parts, G_1 can be expressed as

$$\begin{aligned} G_1 &= \left[-\phi(z_1)(z_1 + b_1) \left(\prod_{s=2}^l F_s(z_1) \right) \right]_{-\infty}^{\infty} + \int_{-\infty}^{\infty} \phi(z_1) \left(\prod_{s=2}^l F_s(z_1) \right) dz_1 \\ &\quad + \int_{-\infty}^{\infty} \phi(z_1)(z_1 + b_1) \frac{d}{dz_1} \left(\prod_{s=2}^l F_s(z_1) \right) dz_1. \end{aligned} \quad (\text{C.6})$$

Here, noting that

$$\frac{d}{dz_1} F_s(z_1) = -a_s \phi(a_s(z_1 + b_1) - b_s)$$

and the first term of the right hand side of (C.6) is zero, (C.6) can be written as

$$\begin{aligned} G_1 &= \int_{-\infty}^{\infty} \phi(z_1) \left(\prod_{s=2}^l F_s(z_1) \right) dz_1 \\ &\quad + \int_{-\infty}^{\infty} \phi(z_1)(z_1 + b_1) \left\{ \sum_{s=2}^l \{-a_s \phi(a_s(z_1 + b_1) - b_s)\} \right. \\ &\quad \left. \left(\prod_{2 \leq t \leq l, t \neq s} F_t(z_1) \right) \right\} dz_1. \end{aligned} \quad (\text{C.7})$$

Next, we calculate G_s . Here, note that

$$\begin{aligned}
 & \int_{a_s(z_1+b_1)-b_s}^{\infty} z_s(z_s + b_s)\phi(z_s)dz_s \\
 &= [-\phi(z_s)(z_s + b_s)]_{a_s(z_1+b_1)-b_s}^{\infty} + \int_{a_s(z_1+b_1)-b_s}^{\infty} \phi(z_s)dz_s \\
 &= a_s(z_1 + b_1)\phi\{a_s(z_1 + b_1) - b_s\} + F_s(z_1). \tag{C.8}
 \end{aligned}$$

Hence, substituting (C.8) into (C.4) yields

$$\begin{aligned}
 G_s &= \int_{-\infty}^{\infty} \phi(z_1) \left(\prod_{s=2}^l F_s(z_1) \right) dz_1 \\
 &+ \int_{-\infty}^{\infty} \phi(z_1)(z_1 + b_1)\{a_s\phi(a_s(z_1 + b_1) - b_s)\} \left(\prod_{2 \leq t \leq l, t \neq s} F_t(z_1) \right) dz_1. \tag{C.9}
 \end{aligned}$$

Therefore, using (C.7) and (C.9) we get

$$\begin{aligned}
 \sum_{s=1}^l G_s &= l \int_{-\infty}^{\infty} \phi(z_1) \left(\prod_{s=2}^l F_s(z_1) \right) dz_1 = l \int \dots \int_{E_l} \prod_{s=1}^l \phi(z_s) dz_1 \dots dz_l \\
 &= l\mathbb{E}[1_{\{z \in E_l\}}] = l\mathbb{E}[1_{\{\mathbf{v} \in A^{(l)}(\{1\})\}}]. \tag{C.10}
 \end{aligned}$$

Thus, by substituting (C.10) into (C.5), we obtain (C.1). \square

Appendix 3: Proof of Theorem 1

In this section, we prove Theorem 1. First, we provide the following lemma.

LEMMA D. *Let n_1, n_2 and τ^2 be positive numbers, and let ξ_1 , and ξ_2 be real numbers. Put $\mathbf{n} = (n_1, n_2)'$. Let x_1 and x_2 be independent random variables distributed as $x_s \sim N(\xi_s, \tau^2/n_s)$, ($s = 1, 2$), and let $\mathbf{x} = (x_1, x_2)'$. Then, the following two propositions hold:*

(P1) *For any integer i with $1 \leq i \leq 2$, and for any set J with $J \in \mathcal{J}_i^{(2)}$, it holds that*

$$\begin{aligned}
 & \mathbb{E} \left[1_{\{\mathbf{D}_J^{(n)} \mathbf{x}_J \geq \mathbf{0}\}} \frac{1}{\tau^2} \sum_{s \in J} n_s (x_s - \xi_s)(x_s - \bar{x}_J^{(n)}) \right] \\
 &= (i-1)\mathbb{P}(\mathbf{D}_J^{(n)} \mathbf{x}_J \geq \mathbf{0}). \tag{D.1}
 \end{aligned}$$

(P2) *The following equality holds:*

$$\mathbb{E} \left[\frac{1}{\tau^2} \sum_{s=1}^2 n_s (x_s - \zeta_s) (x_s - \eta_2^{(n)}(\mathbf{x})[s]) \right] = \mathbb{P}(\boldsymbol{\eta}_2^{(n)}(\mathbf{x}) \in A^{(2)}(\mathbb{N}_2)). \quad (\text{D.2})$$

PROOF. First, we prove (D.1). When $i = 1$, i.e., $J = \{1\}$, noting that $\bar{x}_J = x_1$, the equality (D.1) is clear. On the other hand, when $i = 2$, i.e., $J = \mathbb{N}_2$, the equality (D.1) is equivalent to (P1) of Lemma F given by Inatsu [8], and it is already proved. Similarly, the proof of (D.2) is equivalent to the proof of (P2) of Lemma F given by Inatsu [8]. Therefore, lemma D is proved. \square

Next, we consider the following lemma:

LEMMA E. *Let l be an integer with $l \geq 2$. Assume that the following proposition (P) is true:*

(P) *Let N_1, \dots, N_l and ζ^2 be positive numbers, and let ζ_1, \dots, ζ_l be real numbers. Let y_1, \dots, y_l be independent random variables, and let $y_s \sim N(\zeta_s, \zeta^2/N_s)$ where $s = 1, \dots, l$. Put $\mathbf{N} = (N_1, \dots, N_l)'$, $\boldsymbol{\zeta} = (\zeta_1, \dots, \zeta_l)'$ and $\mathbf{y} = (y_1, \dots, y_l)'$. Then, for any integer i with $1 \leq i \leq l$ and for any set J with $J \in \mathcal{J}_i^{(l)}$, it holds that*

$$\begin{aligned} & \mathbb{E} \left[\mathbf{1}_{\{\mathbf{D}_J^{(N)} \mathbf{y}_J \geq \mathbf{0}\}} \frac{1}{\zeta^2} \sum_{s \in J} N_s (y_s - \zeta_s) (y_s - \bar{y}_J^{(N)}) \right] \\ &= (i-1) \mathbb{P}(\mathbf{D}_J^{(N)} \mathbf{y}_J \geq \mathbf{0}). \end{aligned} \quad (\text{E.1})$$

Under the assumption (P), the following proposition (P*) holds:

(P*) *Let n_1, \dots, n_{l+1} and τ^2 be positive numbers, and let $\zeta_1, \dots, \zeta_{l+1}$ be real numbers. Let x_1, \dots, x_{l+1} be independent random variables, and let $x_s \sim N(\zeta_s, \tau^2/n_s)$ where $s = 1, \dots, l+1$. Put $\mathbf{n} = (n_1, \dots, n_{l+1})'$, $\boldsymbol{\zeta} = (\zeta_1, \dots, \zeta_{l+1})'$ and $\mathbf{x} = (x_1, \dots, x_{l+1})'$. Then, for any integer i with $1 \leq i \leq l+1$ and for any set J with $J \in \mathcal{J}_i^{(l+1)}$, it holds that*

$$\begin{aligned} & \mathbb{E} \left[\mathbf{1}_{\{\mathbf{D}_J^{(n)} \mathbf{x}_J \geq \mathbf{0}\}} \frac{1}{\tau^2} \sum_{s \in J} n_s (x_s - \zeta_s) (x_s - \bar{x}_J^{(n)}) \right] \\ &= (i-1) \mathbb{P}(\mathbf{D}_J^{(n)} \mathbf{x}_J \geq \mathbf{0}). \end{aligned} \quad (\text{E.2})$$

Moreover, the following equality holds:

$$\begin{aligned} & \mathbb{E} \left[\frac{1}{\tau^2} \sum_{s=1}^{l+1} n_s (x_s - \zeta_s) (x_s - \eta_{l+1}^{(n)}(\mathbf{x})[s]) \right] \\ &= \sum_{i=2}^{l+1} (i-1) \mathbb{P} \left(\eta_{l+1}(\mathbf{x}) \in \bigcup_{J \in \mathcal{J}_i^{l+1}} A^{(l+1)}(J) \right). \end{aligned} \quad (\text{E.3})$$

Note that Lemma D and Lemma E yield Theorem 1. Hence, we prove Lemma E.

PROOF. First, we prove (E.2). Suppose that i is an integer satisfying $1 \leq i \leq l$ and suppose also that J is a set satisfying $J \in \mathcal{J}_i^{(l+1)}$. In this case, we replace \mathbf{n}_J , \mathbf{x}_J and ζ_J with $\mathbf{N} = (N_1, \dots, N_i)'$, $\mathbf{y} = (y_1, \dots, y_i)'$ and $\zeta = (\zeta_1, \dots, \zeta_i)'$, respectively. We put $J^* = \mathbb{N}_i$. Then, from the assumption (E.1), the left hand side of (E.2) can be expressed as

$$\begin{aligned} & \mathbb{E} \left[\mathbf{1}_{\{\mathbf{D}_J^{(n)} \mathbf{x}_J \geq \mathbf{0}\}} \frac{1}{\tau^2} \sum_{s \in J} n_s (x_s - \zeta_s) (x_s - \bar{x}_J^{(n)}) \right] \\ &= \mathbb{E} \left[\mathbf{1}_{\{\mathbf{D}_{J^*}^{(N)} \mathbf{y}_{J^*} \geq \mathbf{0}\}} \frac{1}{\tau^2} \sum_{t \in J^*} N_t (y_t - \zeta_t) (y_t - \bar{y}_{J^*}^{(N)}) \right] \\ &= (i-1) \mathbb{P}(\mathbf{D}_{J^*}^{(N)} \mathbf{y}_{J^*} \geq \mathbf{0}) = (i-1) \mathbb{P}(\mathbf{D}_J^{(n)} \mathbf{x}_J \geq \mathbf{0}). \end{aligned} \quad (\text{E.4})$$

Hence, we get (E.2). Therefore, it is sufficient to prove the case of $i = l+1$, i.e., $J = \mathbb{N}_{l+1} \in \mathcal{J}_i^{(l+1)}$. Here, the left hand side of (E.2) can be rewritten as

$$\mathbb{E} \left[\mathbf{1}_{\{\mathbf{D}_J^{(n)} \mathbf{x}_J \geq \mathbf{0}\}} \frac{1}{\tau^2} \sum_{s \in J} n_s (x_s - \zeta_s) (x_s - \bar{x}_J^{(n)}) \right] = X - Y, \quad (\text{E.5})$$

where X and Y are given by

$$\begin{aligned} X &= \mathbb{E} \left[\mathbf{1}_{\{\mathbf{D}_J^{(n)} \mathbf{x}_J \geq \mathbf{0}\}} \frac{1}{\tau^2} \sum_{s=1}^{l+1} n_s (x_s - \zeta_s) x_s \right], \\ Y &= \mathbb{E} \left[\mathbf{1}_{\{\mathbf{D}_J^{(n)} \mathbf{x}_J \geq \mathbf{0}\}} \frac{1}{\tau^2} \sum_{s=1}^{l+1} n_s (x_s - \zeta_s) \bar{x}_J^{(n)} \right]. \end{aligned}$$

First, we calculate Y . Noting that

$$\frac{1}{\tau^2} \sum_{s=1}^{l+1} n_s (x_s - \zeta_s) \bar{x}_J^{(n)} = \frac{\tilde{n}_J}{\tau^2} (\bar{x}_J^{(n)} - \bar{\zeta}_J^{(n)}) \bar{x}_J^{(n)}$$

and $\bar{x}_J^{(n)} \sim N(\bar{\xi}_J^{(n)}, \tau^2/\tilde{n}_J)$, from (2) of Lemma B we obtain

$$\begin{aligned} Y &= \mathbb{E} \left[\mathbf{1}_{\{\mathbf{D}_J^{(n)} \mathbf{x}_J \geq \mathbf{0}\}} \frac{1}{\tau^2} \sum_{s=1}^{l+1} n_s (x_s - \xi_s) \bar{x}_J^{(n)} \right] \\ &= \mathbb{E} [\mathbf{1}_{\{\mathbf{D}_J^{(n)} \mathbf{x}_J \geq \mathbf{0}\}}] \mathbb{E} \left[\frac{\tilde{n}_J}{\tau^2} (\bar{x}_J^{(n)} - \bar{\xi}_J^{(n)}) \bar{x}_J^{(n)} \right] \\ &= \mathbb{E} [\mathbf{1}_{\{\mathbf{D}_J^{(n)} \mathbf{x}_J \geq \mathbf{0}\}}] \times 1 = \mathbf{P}(\mathbf{D}_J^{(n)} \mathbf{x}_J \geq \mathbf{0}). \end{aligned} \quad (\text{E.6})$$

Next, we calculate X . From (1) of Lemma 1, it is easily checked that the following equality holds:

$$\mathbf{1}_{\{\mathbf{D}_J^{(n)} \mathbf{x}_J \geq \mathbf{0}\}} = 1 - \sum_{u=1}^l \sum_{J^* \in \mathcal{J}_u^{(l+1)}} \mathbf{1}_{\{x \in \eta_{l+1}^{-1}(A^{(l+1)}(J^*))\}}. \quad (\text{E.7})$$

Therefore, X can be expressed by using (E.7) as

$$\begin{aligned} X &= \mathbb{E} \left[\frac{1}{\tau^2} \sum_{s=1}^{l+1} n_s (x_s - \xi_s) x_s \right] \\ &\quad - \sum_{u=1}^l \sum_{J^* \in \mathcal{J}_u^{l+1}} \mathbb{E} \left[\mathbf{1}_{\{x \in \eta_{l+1}^{-1}(A^{(l+1)}(J^*))\}} \frac{1}{\tau^2} \sum_{s=1}^{l+1} n_s (x_s - \xi_s) x_s \right] \\ &= (l+1) \\ &\quad - \sum_{u=1}^l \sum_{J^* \in \mathcal{J}_u^{l+1}} \mathbb{E} \left[\mathbf{1}_{\{x \in \eta_{l+1}^{-1}(A^{(l+1)}(J^*))\}} \frac{1}{\tau^2} \sum_{s=1}^{l+1} n_s (x_s - \xi_s) x_s \right], \end{aligned} \quad (\text{E.8})$$

where the first term of the last equality in (E.8) is derived by $x_s \sim N(\xi_s, \tau^2/n_s)$. Next, for any integer u with $1 \leq u \leq l$ and for any set J^* with $J^* \in \mathcal{J}_u^{l+1}$, we calculate

$$\mathbb{E} \left[\mathbf{1}_{\{x \in \eta_{l+1}^{-1}(A^{(l+1)}(J^*))\}} \frac{1}{\tau^2} \sum_{s=1}^{l+1} n_s (x_s - \xi_s) x_s \right]. \quad (\text{E.9})$$

Here, recall that from (2) of Lemma 1, the following relation holds:

$$\mathbf{x} \in \eta_{l+1}^{-1}(A^{(l+1)}(J^*)) \Leftrightarrow \mathbf{D}_{J^*} \mathbf{x}_{J^*} \geq \mathbf{0}, \quad \forall t \in \mathbb{N}_{l+1} \setminus J^*, \bar{x}_{J^*} < x_t. \quad (\text{E.10})$$

Thus, noting that

$$\begin{aligned}
 & \frac{1}{\tau^2} \sum_{s=1}^{l+1} n_s (x_s - \zeta_s) x_s \\
 &= \frac{1}{\tau^2} \sum_{s \in J^*} n_s (x_s - \zeta_s) x_s + \frac{1}{\tau^2} \sum_{t \in \mathbb{N}_{l+1} \setminus J^*} n_t (x_t - \zeta_t) x_t \\
 &= \frac{1}{\tau^2} \sum_{s \in J^*} n_s (x_s - \zeta_s) (x_s - \bar{x}_{J^*} + \bar{x}_{J^*}) + \frac{1}{\tau^2} \sum_{t \in \mathbb{N}_{l+1} \setminus J^*} n_t (x_t - \zeta_t) x_t \\
 &= \frac{1}{\tau^2} \sum_{s \in J^*} n_s (x_s - \zeta_s) (x_s - \bar{x}_{J^*}) + \frac{\tilde{n}_{J^*}}{\tau^2} (\bar{x}_{J^*} - \bar{\zeta}_{J^*}) \bar{x}_{J^*} \\
 &\quad + \frac{1}{\tau^2} \sum_{t \in \mathbb{N}_{l+1} \setminus J^*} n_t (x_t - \zeta_t) x_t,
 \end{aligned}$$

the expectation (E.9) can be rewritten as

$$\mathbf{E} \left[\mathbf{1}_{\{x \in \eta_{l+1}^{-1}(A^{(l+1)}(J^*))\}} \frac{1}{\tau^2} \sum_{s=1}^{l+1} n_s (x_s - \zeta_s) x_s \right] = \mathbf{G} + \mathbf{H}, \quad (\text{E.11})$$

where G and H are given by

$$\begin{aligned}
 G &= \mathbf{E} \left[\mathbf{1}_{\{x \in \eta_{l+1}^{-1}(A^{(l+1)}(J^*))\}} \frac{1}{\tau^2} \sum_{s \in J^*} n_s (x_s - \zeta_s) (x_s - \bar{x}_{J^*}) \right], \\
 H &= \mathbf{E} \left[\mathbf{1}_{\{x \in \eta_{l+1}^{-1}(A^{(l+1)}(J^*))\}} \left(\frac{\tilde{n}_{J^*}}{\tau^2} (\bar{x}_{J^*} - \bar{\zeta}_{J^*}) \bar{x}_{J^*} + \frac{1}{\tau^2} \sum_{t \in \mathbb{N}_{l+1} \setminus J^*} n_t (x_t - \zeta_t) x_t \right) \right].
 \end{aligned}$$

By using (E.10), Lemma B and (E.4), G can be expressed as

$$\begin{aligned}
 G &= \mathbf{E}[\mathbf{1}_{\{\forall t \in \mathbb{N}_{l+1} \setminus J^*, \bar{x}_{J^*} < x_t\}}] \\
 &\quad \times \mathbf{E} \left[\mathbf{1}_{\{\mathbf{D}_{J^*} \mathbf{x}_{J^*} \geq \mathbf{0}\}} \frac{1}{\tau^2} \sum_{s \in J^*} n_s (x_s - \zeta_s) (x_s - \bar{x}_{J^*}) \right] \\
 &= \mathbf{E}[\mathbf{1}_{\{\forall t \in \mathbb{N}_{l+1} \setminus J^*, \bar{x}_{J^*} < x_t\}}] \times (u-1) \mathbf{E}[\mathbf{1}_{\{\mathbf{D}_{J^*} \mathbf{x}_{J^*} \geq \mathbf{0}\}}] \\
 &= (u-1) \times \mathbf{E}[\mathbf{1}_{\{\mathbf{D}_{J^*} \mathbf{x}_{J^*} \geq \mathbf{0}, \forall t \in \mathbb{N}_{l+1} \setminus J^*, \bar{x}_{J^*} < x_t\}}] \\
 &= (u-1) \times \mathbf{E}[\mathbf{1}_{\{x \in \eta_{l+1}^{-1}(A^{(l+1)}(J^*))\}}].
 \end{aligned}$$

On the other hand, using (E.10), Lemma B and Lemma C, H can be written as

$$\begin{aligned}
H &= \mathbb{E}[1_{\{\mathbf{D}_{J^*} \mathbf{x}_{J^*} \geq \mathbf{0}\}}] \\
&\quad \times \mathbb{E} \left[1_{\{\forall t \in \mathbb{N}_{l+1} \setminus J^*, \bar{x}_{J^*} < x_t\}} \right. \\
&\quad \left. \left(\frac{\tilde{n}_{J^*}}{\tau^2} (\bar{x}_{J^*} - \bar{\xi}_{J^*}) \bar{x}_{J^*} + \frac{1}{\tau^2} \sum_{t \in \mathbb{N}_{l+1} \setminus J^*} n_t (x_t - \xi_t) x_t \right) \right] \\
&= \mathbb{E}[1_{\{\mathbf{D}_{J^*} \mathbf{x}_{J^*} \geq \mathbf{0}\}}] \times (l+1-u+1) \mathbb{E}[1_{\{\forall t \in \mathbb{N}_{l+1} \setminus J^*, \bar{x}_{J^*} < x_t\}}] \\
&= (l+1-u+1) \times \mathbb{E}[1_{\{\mathbf{x} \in \eta_{l+1}^{-1}(A^{(l+1)}(J^*))\}}].
\end{aligned}$$

Hence, substituting G and H into (E.11) yields

$$\begin{aligned}
&\mathbb{E} \left[1_{\{\mathbf{x} \in \eta_{l+1}^{-1}(A^{(l+1)}(J^*))\}} \frac{1}{\tau^2} \sum_{s=1}^{l+1} n_s (x_s - \xi_s) x_s \right] \\
&= (l+1) \times \mathbb{E}[1_{\{\mathbf{x} \in \eta_{l+1}^{-1}(A^{(l+1)}(J^*))\}}]. \tag{E.12}
\end{aligned}$$

Furthermore, combining (E.12) and (E.8) we get

$$\begin{aligned}
X &= (l+1) - \sum_{u=1}^l \sum_{J^* \in \mathcal{J}_u^{l+1}} (l+1) \times \mathbb{E}[1_{\{\mathbf{x} \in \eta_{l+1}^{-1}(A^{(l+1)}(J^*))\}}] \\
&= (l+1) \mathbb{E} \left[1 - \sum_{u=1}^l \sum_{J^* \in \mathcal{J}_u^{l+1}} 1_{\{\mathbf{x} \in \eta_{l+1}^{-1}(A^{(l+1)}(J^*))\}} \right] \\
&= (l+1) \mathbb{E}[1_{\{\mathbf{x} \in \eta_{l+1}^{-1}(A^{(l+1)}(J))\}}] = (l+1) \mathbb{E}[1_{\{\mathbf{D}_J \mathbf{x}_J \geq \mathbf{0}\}}] \\
&= (l+1) \mathbb{P}(\mathbf{D}_J \mathbf{x}_J \geq \mathbf{0}). \tag{E.13}
\end{aligned}$$

Thus, substituting (E.6) and (E.13) into (E.5) yields

$$\mathbb{E} \left[1_{\{\mathbf{D}_J^{(n)} \mathbf{x}_J \geq \mathbf{0}\}} \frac{1}{\tau^2} \sum_{s \in J} n_s (x_s - \xi_s) (x_s - \bar{x}_J^{(n)}) \right] = l \mathbb{P}(\mathbf{D}_J \mathbf{x}_J \geq \mathbf{0}).$$

Hence, the expectation (E.2) for the case of $i = l+1$ (i.e., $J = \mathbb{N}_{l+1}$), is proved.

Finally, we prove (E.3). By using (1) and (3) of Lemma 1, the left hand side of (E.3) can be expressed as

$$\begin{aligned}
 & \mathbb{E} \left[\frac{1}{\tau^2} \sum_{s=1}^{l+1} n_s (x_s - \zeta_s) (x_s - \eta_{l+1}^{(n)}(\mathbf{x})[s]) \right] \\
 &= \mathbb{E} \left[\sum_{i=1}^{l+1} \sum_{J \in \mathcal{J}_i^{(l+1)}} \left(\mathbf{1}_{\{\mathbf{x} \in \eta_{i+1}^{-1}(A^{(l+1)}(J))\}} \frac{1}{\tau^2} \sum_{s=1}^{l+1} n_s (x_s - \zeta_s) (x_s - \eta_{l+1}^{(n)}(\mathbf{x})[s]) \right) \right] \\
 &= \sum_{i=2}^{l+1} \sum_{J \in \mathcal{J}_i^{(l+1)}} \mathbb{E} \left[\left(\mathbf{1}_{\{\mathbf{x} \in \eta_{i+1}^{-1}(A^{(l+1)}(J))\}} \frac{1}{\tau^2} \sum_{r \in J} n_r (x_r - \zeta_r) (x_r - \bar{x}_J) \right) \right]. \quad (\text{E.14})
 \end{aligned}$$

Here, using (E.2), Lemma B and (2) of Lemma 1, we obtain

$$\begin{aligned}
 & \mathbb{E} \left[\left(\mathbf{1}_{\{\mathbf{x} \in \eta_{i+1}^{-1}(A^{(l+1)}(J))\}} \frac{1}{\tau^2} \sum_{r \in J} n_r (x_r - \zeta_r) (x_r - \bar{x}_J) \right) \right] \\
 &= \mathbb{E}[\mathbf{1}_{\{u \in \mathbb{N}_{l+1} \setminus J, \bar{x}_J < x_u\}}] \times \mathbb{E} \left[\mathbf{1}_{\{\mathbf{D}_J \mathbf{x}_J \geq \mathbf{0}\}} \frac{1}{\tau^2} \sum_{r \in J} n_r (x_r - \zeta_r) (x_r - \bar{x}_J) \right] \\
 &= \mathbb{E}[\mathbf{1}_{\{u \in \mathbb{N}_{l+1} \setminus J, \bar{x}_J < x_u\}}] \times (i-1) \mathbb{E}[\mathbf{1}_{\{\mathbf{D}_J \mathbf{x}_J \geq \mathbf{0}\}}] \\
 &= (i-1) \mathbb{P}(\boldsymbol{\eta}_{l+1}(\mathbf{x}) \in A^{(l+1)}(J)). \quad (\text{E.15})
 \end{aligned}$$

Thus, substituting (E.15) into (E.14) yields

$$\begin{aligned}
 & \mathbb{E} \left[\frac{1}{\tau^2} \sum_{s=1}^{l+1} n_s (x_s - \zeta_s) (x_s - \eta_{l+1}^{(n)}(\mathbf{x})[s]) \right] \\
 &= \sum_{i=2}^{l+1} (i-1) \sum_{J \in \mathcal{J}_i^{(l+1)}} \mathbb{P}(\boldsymbol{\eta}_{l+1}(\mathbf{x}) \in A^{(l+1)}(J)) \\
 &= \sum_{i=2}^{l+1} (i-1) \mathbb{P} \left(\boldsymbol{\eta}_{l+1}(\mathbf{x}) \in \bigcup_{J \in \mathcal{J}_i^{l+1}} A^{(l+1)}(J) \right),
 \end{aligned}$$

because $A^{(l+1)}(J) \cap A^{(l+1)}(J^*) = \emptyset$ when $J \neq J^*$. Therefore, (E.3) is proved. \square

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