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Model Robust Optimal Designs for Kronecker Model for Mixture Experiments

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Abstract

In comparison to Scheffè's canonical polynomial models (S-models), the Kronecker models (K-models) for mixture experiments are symmetric, compact in notation, and based on the Kronecker algebra of vectors and matrices. Further, there is a corresponding transition from S-models to K-models in the form of model re-parameterization. In the literature, it has been recommended to use second-degree K-models in practice compared to the widely used second-degree S-models especially when the moment matrix is of an ill-conditioning type. The motivation of the present article is to discriminate between K-models and S-models in terms of the model-robust D- and A-optimality criteria. These optimality criteria are discussed when there is uncertainty in selecting an appropriate model out of two rival models for a mixture experiment.

Keywords and Phrases: Canonical polynomial model, Kronecker model, Mixture experiment, Ill-conditioning, D-optimality, A-optimality.

AMS Classification: 62K05.

1. Introduction

The optimal design for a mixture experiment continues to receive significant attention from many scholars in the statistical literature. Recently, several articles have been published on this particular topic e.g., Pal et al. (2023), Pal and Mandal (2021), Panda (2021), Panda and Sahoo (2022a, 2022b, 2024).

In a mixture experiment having q number of mixture components, a response to a mixture is a function of the relative proportion, x_i, of each of the components only. Here the response of interest does not depend upon the absolute amount of the components. The proportion of each of the q components must satisfy both a summation constraint and a non-negativity constraint:

$$x_i \geq 0,\ i = 1, 2, ..., q \text{ and} \sum_{i=1}^{q} x_i = 1 .$$

As a result, the experimental region is a $(q-1)-$dimensional simplex given by

$$S_{q-1} = \left\{ \boldsymbol{x} = (x_1, x_2, ... x_q)' : \sum_{i=1}^{q} x_i = 1,\ x_i \geq 0,\ 1 \leq i \leq q \right\}.$$

To analyze mixture data, several models have been introduced in the literature *e.g.* Scheffè's canonical polynomial model (S-model), Becker's model, Kronecker model (K-model), etc. Among the several mixture models discussed in the literature, S-models are the most widely used models for analyzing data related to mixture experiments. The expected responses of the first- and second-degree canonical polynomial models are of the following form:

$$\eta_1(\boldsymbol{x}) = \boldsymbol{f}_1'(\boldsymbol{x})\boldsymbol{\theta} = \sum_{i=1}^{q} \theta_i x_i, \tag{1.1}$$

$$\eta_2(\boldsymbol{x}) = \boldsymbol{f}_2'(\boldsymbol{x})\boldsymbol{\beta} = \sum_{i=1}^{q} \beta_i x_i + \sum_{\substack{i,j=1 \\ i<j}}^{q} \beta_{ij} x_i x_j, \tag{1.2}$$

where

$$\boldsymbol{f}_1 : S_{q-1} \to R^{m_1},\ \boldsymbol{x} \to \boldsymbol{x},$$

$$\boldsymbol{f}_2 : S_{q-1} \to R^{m_2},\ \boldsymbol{x} = (x_1, x_2, ..., x_q)' \to (\boldsymbol{x}',\ (x_i x_j)_{1 \leq i < j \leq q})'$$

with $m_1 = q$ and $m_2 = {}^{q+1}C_2$. Here the unknown parameter vectors $\boldsymbol{\theta} = (\theta_1, \theta_2, ... \theta_q)' \in R^q$ and $\boldsymbol{\beta} = (\beta_1, ... \beta_q, \beta_{12}, ..., \beta_{q-1q})' \in R^{{}^{q+1}C_2}$ respectively where R^n denote the n-dimensional Euclidean space. The information matrix of a design ξ for models given by Equations (1.1) and (1.2) is as follows

$$\boldsymbol{M}_i(\xi) = \int_{S_{q-1}} \boldsymbol{f}_i(\boldsymbol{x}) \boldsymbol{f}_i'(\boldsymbol{x}) d\xi(\boldsymbol{x}) \text{ for i = 1, 2.}$$

The information matrix contains the amount of information that the design ξ contains about the unknown parameters associated with the model of interest.

Draper and Pukelsheim (1998) proposed a new form of model of mixture experiments known as the K-model for mixture experiments as an alternative to the canonical polynomial models. The model form of the first-degree is the same as that of the Equation (1.1) and the second-degree K-model is of the following form:

$$\eta_2(\boldsymbol{x}) = \boldsymbol{f}_2'(\boldsymbol{x})\boldsymbol{\theta} = \sum_{i=1}^{q} \mu_{ii} x_i^2 + \sum_{\substack{i,j=1 \\ i<j}}^{q} (\mu_{ij} + \mu_{ji}) x_i x_j \tag{1.3}$$

where

$$\boldsymbol{f}_2 : S_{q-1} \to R^{q^2},\ \boldsymbol{x} = (x_1, x_2, ..., x_q)' \to \boldsymbol{x} \otimes \boldsymbol{x} = \underbrace{(x_i x_j)_{i,j=1,2,...q}}_{\text{Ordered lexicographically}}$$

and with $\boldsymbol{\mu} = (\mu_{11}, \mu_{12}, ..., \mu_{qq})' \in R^{q^2}$ is the vector of unknown parameters. Here we assume that the observations are uncorrelated and have common unknown finite variance σ^2. These latter models have some special features as compared to the former models such as: (a) K-models are based on the Kronecker algebra of vectors and matrices; (b) they are symmetric, and (c) involve compact notation. The use of ridge analysis becomes simple if an experimenter utilizes the K-model instead of the S-model *see* Draper and Pukelsheim (2000). The objective of reducing the maximum eigenvalue of the information matrix can be achieved by using the second-degree K model for mixture experiments as compared to that of Scheffé's quadratic polynomial model or any other quadratic mixture model. Additionally, the same model can be used in practice for shrinking the ill-conditioning. For further details, one can refer to the work of Prescott et al. (2002).

The main focus of this article lies in the discussion of model robust designs. In the design and analysis of the experiment, generally, an experimenter assumes the model for analyzing the data with a belief that the assumed model shall be roughly close to the true model. However, if the model chosen is not an adequate one then the optimal design obtained for the assumed model provides considerably biased information about the true response. In this sense, the design can be considered as a bad design *i.e.* it is no more a model robust design. In the literature, three important characteristics are cited for a model to be considered a good model-robust design. These characteristics are: (i) allow the experimenter to fit the assumed model, (ii) detect the model inadequacy when the model fitted one is not an appropriate approximation to the true model, and (iii) reasonable efficient inferences can be made based on the assumed model when it is an appropriate one.

Further, in an experiment, an experimenter frequently requires the detection of model inadequacy in the design of an experiment that is again highly dependent upon the true response. However, in general, the true model is unknown often. Thus, the assumed model can perceive the model inadequacy if it occurs, whenever the design points are located at representative locations of the true model. On the other hand, the design may not even detect the model inadequacy, if the design points are badly located. Hence, it can be concluded that the best way to identify the model inadequacy can be made when the true model is known. This leads to the fact that the selection of a model robust design depends on the selection of the optimality criterion as well as the true and assumed model. For further details, one can refer to the work by Stigler (1971), Studden (1982), Chang and Notz (1996), Mandal et al. (2015), Ai et al. (2023), etc. In this backdrop, Huang et al. (2009) obtained model-robust D- and A-optimal designs when there is uncertainty in choosing an appropriate model out of two given rival models with a mixture experiment *i.e.* Scheffè's canonical polynomial models given by Equations (1.1) and (1.2). In the present work, we wish to extend the idea of model robust D- and A-optimality of Huang et al. (2009) to K- Models. The basic motivation of this article is to discriminate between S-models and K-models in terms of model robust D- and A-optimality. This model distinction also makes sense since there is a corresponding transition from S-models to K-models in the form of model re-parameterization.

The rest of the paper is organized as follows. Section 2 gives the preliminaries. In Section 3, we discuss the main result. Finally, we conclude with some discussion and conclusions in Section 4.

2. Preliminaries

Draper and Pukelshiem (1999) and Draper et al. (2000) obtained complete class results for first- and second-degree K-models for the Kiefer ordering based on elementary centroid designs. The advantage of the complete class results is that any design not of a mixture of the elementary centroid designs can be further improved upon by using a suitable combination of the elementary centroid designs. In this aspect, we restrict our consideration to weighted centroid designs defined below, see Klein (2004b).

Definition 2.1. Let us denote the canonical unit vectors in R^q by $\boldsymbol{e}_1, \ldots, \boldsymbol{e}_q$ and set $\boldsymbol{e}_{ij} = \boldsymbol{e}_i \otimes \boldsymbol{e}_j$ for $i, j = 1, 2, ..., q$. The canonical unit vectors in $R^{\binom{q}{2}}$ are denoted by $\boldsymbol{E}_{ij}$ with $1 \le i < j \le q$ in lexicographic order. For $q \ge 2$ and $j \in \{1, 2, ..., q\}$, the jth elementary centroid design η_j is the uniform distribution on the centroids of depth j, that is, on all points taking the form

$$\frac{1}{j}\sum_{i=1}^{j} \boldsymbol{e}_{k_i} \in S_{q-1} \text{ with } 1 \le k_1 < k_2 < ... < k_j \le q .$$

A weighted centroid design with a weight vector $\boldsymbol{\alpha} = (\alpha_1, \alpha_2, ..., \alpha_q)'$ is a convex combination $\eta(\boldsymbol{\alpha}) = \sum_{j=1}^{q} \alpha_j \eta_j$ such that $\alpha_j \ge 0$, $\sum_{j=1}^{q} \alpha_j = 1$. Let the set of all weighted centroid designs is denoted by W.

We use the following two lemmas from Klein (2004a) for deriving our main results.

Lemma 2.1. Let $\boldsymbol{1}_q = (1, 1, ..., 1)' \in R^q$. Define $\boldsymbol{U}_1 = \boldsymbol{I}_q$, $\boldsymbol{W}_1 = \boldsymbol{I}_{{}^qC_2}$ and $\boldsymbol{U}_2 = \boldsymbol{1}_q \boldsymbol{1}_q' - \boldsymbol{I}_q \in Sym(q)$ and

$$\boldsymbol{V}_1 = \sum_{\substack{i,j=1\\ i<j}}^{q} \boldsymbol{E}_{ij}(\boldsymbol{e}_i + \boldsymbol{e}_j)', \qquad \boldsymbol{V}_2 = \sum_{\substack{i,j=1\\ i<j}}^{q} \sum_{\substack{k=1\\ k\notin\{i,j\}}}^{q} E_{ij}\boldsymbol{e}_k' \quad \in R^{{}^qC_2 \times q}$$

$$\boldsymbol{W}_2 = \sum_{\substack{i,j=1\\ i<j}}^{q} \sum_{\substack{k,l=1\\ k<l\\ |\{i,j\}\cap\{k,l\}|=1}}^{q} \boldsymbol{E}_{ij}\boldsymbol{E}_{kl}', \qquad \boldsymbol{W}_3 = \sum_{\substack{i,j=1\\ i<j}}^{q} \sum_{\substack{k,l=1\\ k<l\\ \{i,j\}\cap\{k,l\}=\phi}}^{q} \boldsymbol{E}_{ij}\boldsymbol{E}_{kl}' \quad \in Sym({}^qc_2)$$

Then any matrix $\boldsymbol{C} \in Sym(n_1, \mathrm{H}_1)$ can be uniquely represented as $\boldsymbol{C} = \omega_1 \boldsymbol{U}_1 + \omega_2 \boldsymbol{U}_2$ with coefficients $\omega_1, \omega_2 \in \mathrm{R}$. Similarly, any matrix $\boldsymbol{C} \in Sym(n_2, \mathrm{H}_2)$ is of the form

$$\boldsymbol{C} = \begin{pmatrix} \omega_3 \boldsymbol{U}_1 + \omega_4 \boldsymbol{U}_2 & \omega_5 \boldsymbol{V}_1' + \omega_6 \boldsymbol{V}_{21}' \\ \omega_5 \boldsymbol{V}_1 + \omega_6 \boldsymbol{V}_2 & \omega_7 \boldsymbol{W}_1 + \omega_8 \boldsymbol{W}_2 + \omega_9 \boldsymbol{W}_3 \end{pmatrix}$$

with unique coefficients $\omega_3, \ldots, \omega_9 \in R$. Here $Sym(q)$ and $Sym({}^qc_2)$ represents the set of symmetric matrices of order q and ${}^qc_2$ respectively. Note that $\boldsymbol{V}_2 = \boldsymbol{0}$, $\boldsymbol{W}_2 = \boldsymbol{W}_3 = \boldsymbol{0}$ for $q = 2$, and $\boldsymbol{W}_3 = \boldsymbol{0}$ for $q = 3$. For the definition of $Sym\,(n_i, \mathrm{H}_i)$ for i = 1, 2, one can refer to the work of Huang et al. (2009), and Klein (2004a). The following Lemma provides a multiplication table for the above-mentioned matrices.

Lemma 2.2. For any $q \geq 2$, the matrices $\boldsymbol{U}_1$, $\boldsymbol{U}_2$, $\boldsymbol{V}_1$, $\boldsymbol{V}_2$, $\boldsymbol{W}_1$, $\boldsymbol{W}_2$, and $\boldsymbol{W}_3$ satisfy the following equations:

(i) $\boldsymbol{U}_2^2 = (q-1)\boldsymbol{U}_1 + (q-2)\boldsymbol{U}_2$,

$\boldsymbol{V}_1'\boldsymbol{V}_2 = \boldsymbol{V}_2'\boldsymbol{V}_1 = (q-2)\boldsymbol{U}_2$

$\boldsymbol{V}_1'\boldsymbol{V}_1 = (q-1)\boldsymbol{U}_1 + \boldsymbol{U}_2$,

$\boldsymbol{V}_2'\boldsymbol{V}_2 = {}^{q-1}C_2\boldsymbol{U}_1 + {}^{q-2}C_2\boldsymbol{U}_2$

(ii) $\boldsymbol{V}_1\boldsymbol{U}_2 = \boldsymbol{V}_1 + 2\boldsymbol{V}_2$,

$\boldsymbol{V}_2\boldsymbol{U}_2 = (q-2)\boldsymbol{V}_1 + (q-3)\boldsymbol{V}_2$,

$\boldsymbol{W}_2\boldsymbol{V}_1 = (q-2)\boldsymbol{V}_1 + 2\boldsymbol{V}_2$,

$\boldsymbol{W}_2\boldsymbol{V}_2 = (q-2)\boldsymbol{V}_1 + 2(q-3)\boldsymbol{V}_2$,

$\boldsymbol{W}_3\boldsymbol{V}_1 = (q-3)\boldsymbol{V}_2$,

$\boldsymbol{W}_3\boldsymbol{V}_2 = {}^{q-2}C_2\boldsymbol{V}_1 + {}^{q-3}C_2\boldsymbol{V}_2$

(iii) $\boldsymbol{V}_1\boldsymbol{V}_1' = 2\boldsymbol{W}_1 + \boldsymbol{W}_2$,

$\boldsymbol{V}_1\boldsymbol{V}_2' = \boldsymbol{V}_2\boldsymbol{V}_1' = \boldsymbol{W}_2 + 2\boldsymbol{W}_3$,

$\boldsymbol{V}_2\boldsymbol{V}_2' = (q-2)\boldsymbol{W}_1 + (q-3)\boldsymbol{W}_2 + (q-4)\boldsymbol{W}_3$,

$\boldsymbol{W}_2^2 = 2(q-2)\boldsymbol{W}_1 + (q-2)\boldsymbol{W}_2 + 4\boldsymbol{W}_3$,

$$\boldsymbol{W}_3^2 = \binom{q-2}{2}\boldsymbol{W}_1 + \binom{q-3}{2}\boldsymbol{W}_2 + \binom{q-4}{2}\boldsymbol{W}_3,$$

$\boldsymbol{W}_2\boldsymbol{W}_3 = \boldsymbol{W}_3\boldsymbol{W}_2 = (q-3)\boldsymbol{W}_2 + 2(q-4)\boldsymbol{W}_3$. □

Next, we focus on the design problem for the K-models especially when the maximum number of unknown parameters is estimable. In this regard, Klein (2004b) discussed that the full parameter vector $\boldsymbol{\mu} \in R^{q^2}$ is not estimable and thus a maximum parameter subsystem $\boldsymbol{K}'\boldsymbol{\mu}$ can be defined such that the span of the regression range $S = \{f(\boldsymbol{x}):\ \boldsymbol{x} \in S_{q-1}\}$. He further defined the canonical maximum parameter subsystem which is as follows:

Let us denote the canonical unit vectors in R^q by $\boldsymbol{e}_1$, …, $\boldsymbol{e}_q$ and set $\boldsymbol{e}_{ij} = \boldsymbol{e}_i \otimes \boldsymbol{e}_j$ for $i, j = 1, 2, ..., q$. The canonical unit vectors in $R^{\binom{q}{2}}$ are denoted by $\boldsymbol{E}_{ij}$ with $1 \leq i < j \leq q$ in lexicographic order. We write $t = \binom{q+1}{2}$, and define the matrix $\boldsymbol{K} = (\boldsymbol{K}_1,\ \boldsymbol{K}_2) \in R^{q^2 \times t}$ by

$$\boldsymbol{K}_1 = \sum_{i=1}^{q} \boldsymbol{e}_{ii}\boldsymbol{e}_i', \ \boldsymbol{K}_2 = \frac{1}{2}\sum_{\substack{i,j=1 \\ i<j}}^{q} (\boldsymbol{e}_{ij} + \boldsymbol{e}_{ji})\boldsymbol{E}_{ij}'. \tag{2.1}$$

In this case, the span set of S shall be equal to the range set of $\boldsymbol{K}$, and the maximum parameter subsystem has the form which is as follows:

$$\boldsymbol{K}'\boldsymbol{\mu} = \begin{pmatrix} (\mu_{ii})_{1\le i\le q} \\ \left(\frac{1}{2}(\mu_{ij} + \mu_{ji})\right)_{1\le i<j\le q} \end{pmatrix} \in R^t \quad \text{for all } \boldsymbol{\mu} \in R^{q^2}. \tag{2.2}$$

Our investigation on model robust optimality is based on the first- and maximum-parameter subsystem of the second-degree K model given by Equations (1.1) and (2.2) respectively. The information matrices for the model Equation (1.1) based on elementary centroid designs η_1 and η_2 (see Klein, 2004b) are as follows:

$$\boldsymbol{M}_1(\eta_1) = \frac{\boldsymbol{U}_1}{q}, \quad \boldsymbol{M}_1(\eta_2) = \frac{1}{2q}\boldsymbol{U}_1 + \frac{1}{2q(q-1)}\boldsymbol{U}_2$$

and for model Equation (2.2) based on the same are

$$\boldsymbol{M}_2(\eta_1) = \begin{pmatrix} \frac{\boldsymbol{U}_1}{q} & \boldsymbol{0} \\ \boldsymbol{0} & \boldsymbol{0} \end{pmatrix},$$

$$\boldsymbol{M}_2(\eta_2) = \begin{pmatrix} \frac{1}{8q}\boldsymbol{U}_1 + \frac{1}{8q(q-1)}\boldsymbol{U}_2 & \frac{1}{4q(q-1)}\boldsymbol{V}_1' \\ \frac{1}{4q(q-1)}\boldsymbol{V}_1 & \frac{1}{2q(q-1)}\boldsymbol{W}_1 \end{pmatrix}.$$

In the next section, we provide the main results of the article i.e., to obtain model robust D- and A-optimal designs for the K-models.

3. Main Results

3.1 Model Robust D-optimal Designs

The re-parameterization from S-models to K-models through a linear transformation is already discussed in Section 1. The D-criterion is invariant under the linear re-parameterization of the space of regression polynomials *see* Gaftke (1981). Therefore, the model-robust D-optimal designs of K-models remain identical to that of S-models.

Next, we derive the model robust A-optimal designs of the K-models.

3.2 Model Robust A-optimal Designs

Let ξ_1^A and ξ_2^A are the A-optimal designs of the first K-model and maximum parameter subsystem of the second-degree K-model respectively. Then $\xi_1^A = \eta_1$ and $\xi_2^A = \alpha_1\eta_1 + \alpha_2\eta_2$ with weights

$$\alpha_1 = \frac{2(q-1)\sqrt{q+3}-q-3}{4q^2-9q+1}, \text{ and } \alpha_2 = \frac{2(q-1)[2(q-1)-\sqrt{q+3}]}{4q^2-9q+1}$$

[see pg. 124, Klein (2004b)]. The model-robust A-criterion is defined as a convex combination of the A-criteria in the first- and second-degree K-models

$$\tilde{\Phi}^A_{\tilde{r}}(\xi) = \tilde{r}\,\frac{tr\,\boldsymbol{M}_1^{-1}(\xi)}{tr\,\boldsymbol{M}_1^{-1}(\xi_1^A)} + (1-\tilde{r})\,\frac{tr\,\boldsymbol{M}_2^{-1}(\xi)}{tr\,\boldsymbol{M}_2^{-1}(\xi_2^A)} \text{ for } \tilde{r} \in [0, 1] .$$

Let us further define a bijective function $\tilde{r} \to r(\tilde{r})$ from [0, 1] to itself by setting

$$r = r(\tilde{r}) = \frac{\tilde{r}/tr\,\boldsymbol{M}_1^{-1}(\xi_1^A)}{\tilde{r}/tr\,\boldsymbol{M}_1^{-1}(\xi_1^A) + (1-\tilde{r})/tr\,\boldsymbol{M}_2^{-1}(\xi_2^A)} \in [0, 1] \tag{3.1}$$

then we may rewrite $\Phi^A_{\tilde{r}}(\xi)$ in the following form

$$\tilde{\Phi}^A_{\tilde{r}}(\xi) = \left(\frac{\tilde{r}}{tr\,\boldsymbol{M}_1^{-1}(\xi_1^A)} + \frac{1-\tilde{r}}{tr\,\boldsymbol{M}_2^{-1}(\xi_2^A)}\right)\left(r\,tr\,\boldsymbol{M}_1^{-1}(\xi) + (1-r)\,tr\,\boldsymbol{M}_2^{-1}(\xi)\right).$$

We have $tr\,\boldsymbol{M}_1^{-1}(\xi_1^A) = q^2$ and $tr\,\boldsymbol{M}_2^{-1}(\xi_2^A) = \left(8/(q\,\alpha_1)\right) + \left({}^qC_2\left(4/\alpha_1 + 2q(q-1)/\alpha_2\right)\right)$.

Thus eliminating the standardizing constants, we may write $\tilde{\Phi}^A_{\tilde{r}}(\xi)$ as

$$\Phi^A_r(\xi) = r\,tr\,\mathbf{M}_1^{-1}(\xi) + (1-r)\,tr\,\mathbf{M}_2^{-1}(\xi) \text{ with } r \in [0, 1]. \tag{3.2}$$

Now our design criterion is given by minimizing Equation (3.2) which is equivalent to $\tilde{\Phi}^A_{\tilde{r}}(\boldsymbol{\xi})$. For given $r \in [0, 1]$, a design $\boldsymbol{\xi}^A$ with $\boldsymbol{M}_2(\xi^A) \in PD(m_2)$ is called model-robust A-optimal if and only if it satisfies

$$\Phi^A_r(\boldsymbol{\xi}^A) = \min\left\{\Phi^A_r(\boldsymbol{\xi}) \,\middle|\, \boldsymbol{\xi} \in \Omega \text{ with } \boldsymbol{M}_2(\boldsymbol{\xi}) \in PD(m_2)\right\}.$$

We restrict our consideration to the class W of weighted centroid designs following Lemma 4.1 of Huang et al. (2009). Due to complete class results for K-models, this lemma also holds for K-models. The lemma is as follows:

Lemma 3.1. The set W from Definition 2.1 is an essentially complete class of designs relative to the model-robust A-criterion $\Phi^A_r, r \in [0, 1]$, defined in Equation (3.2). Then a design ξ^A_r with $\boldsymbol{M}_2(\xi^A_r) \in PD(m_2)$ (for given $r \in [0, 1]$) is model-robust A-optimal if and only if

$$r\,tr\,\boldsymbol{M}_1^{-2}(\boldsymbol{\xi}_r^A)\boldsymbol{M}_1(\boldsymbol{\eta}_j) + (1-r)\,tr\,\boldsymbol{M}_2^{-2}(\xi_r^A)\boldsymbol{M}_2(\boldsymbol{\eta}_j) \le r\;tr\,\boldsymbol{M}_1^{-1}(\boldsymbol{\xi}_r^A) + (1-r)\boldsymbol{M}_2^{-1}(\boldsymbol{\xi}_r^A)$$

for all $1 \le j \le q$. □

To obtain model-robust A-optimal designs, we consider designs that are convex combinations of the two optimal designs in the first- and second-degree model, and among these designs, we find that design which minimizes the Equation (3.2).

Definition 3.1. Let the set Ξ_A be defined as

$$\Xi_A = \{\xi_\phi = \phi\xi_1^A + (1-\phi)\xi_2^A,\ \phi \in [0, 1]\}.$$

The set Ξ_A is a subset of W.

Lemma 3.2. For a given prior $r \in [0, 1]$, there doesn't exist a unique weight $\phi_r^A \in [\varepsilon, 1]$ such that the design $\boldsymbol{\xi}_{\phi_r^A}$ is model-robust A-optimal design among all designs in Ξ_A, where $\varepsilon \in [0, 1)$.

Proof: For the elementary centroid designs $\boldsymbol{\eta}_1$ and $\boldsymbol{\eta}_2$ we have

$$\boldsymbol{M}_1(\boldsymbol{\eta}_1) = \frac{1}{q}\mathbf{U}_1, \quad \boldsymbol{M}_1(\boldsymbol{\eta}_2) = \frac{1}{2q}\boldsymbol{U}_1 + \frac{1}{2q(q-1)}\boldsymbol{U}_2,$$

$$\boldsymbol{M}_2(\boldsymbol{\eta}_1) = \begin{pmatrix} \frac{1}{q}\boldsymbol{U}_1 & \boldsymbol{0} \\ \boldsymbol{0} & \boldsymbol{0} \end{pmatrix}, \quad \mathbf{M}_2(\boldsymbol{\eta}_2) = \begin{pmatrix} \frac{1}{8q}\boldsymbol{U}_1 + \frac{1}{8q(q-1)}\boldsymbol{U}_2 & \frac{1}{4q(q-1)}\boldsymbol{V}_1' \\ \frac{1}{4q(q-1)}\boldsymbol{V}_1 & \frac{1}{2q(q-1)}\boldsymbol{W}_1 \end{pmatrix}.$$

For given $\phi \in [0, 1]$, we have

$$\begin{aligned}
\boldsymbol{M}_1(\boldsymbol{\xi}_\phi) &= \phi \boldsymbol{M}_1(\boldsymbol{\xi}_1^A) + (1-\phi)\boldsymbol{M}_1(\boldsymbol{\xi}_2^A) \\
&= \phi \boldsymbol{M}_1(\boldsymbol{\eta}_1) + (1-\phi)\left(\alpha_1 \boldsymbol{M}_1(\boldsymbol{\eta}_1) + \alpha_2 \boldsymbol{M}_1(\boldsymbol{\eta}_2)\right) \\
&= \phi \frac{\boldsymbol{U}_1}{q} + (1-\phi)\left[\left(\frac{\alpha_1}{q} + \frac{\alpha_2}{2q}\right)\boldsymbol{U}_1 + \frac{\alpha_2}{2q(q-1)}\boldsymbol{U}_2\right] \\
&= \left[\frac{1}{q}(\phi + (1-\phi)\alpha_1) + \frac{\alpha_2}{2q}(1-\phi)\right]\boldsymbol{U}_1 + \left[\frac{\alpha_2(1-\phi)}{2q(q-1)}\right]\boldsymbol{U}_2 \\
&= \left[r_1 + r_2\right]\boldsymbol{U}_1 + \left[\frac{r_2}{q-1}\right]\boldsymbol{U}_2
\end{aligned} \tag{3.3}$$

where

$$r_1 = r_1(\phi) = \frac{1}{q}\left[\phi + (1-\phi)\alpha_1\right], \text{ and } r_2 = r_2(\phi) = \frac{\alpha_2(1-\phi)}{2q}.$$

Similarly, we can find

$$\boldsymbol{M}_2(\boldsymbol{\xi}_\phi) = \phi \boldsymbol{M}_2(\boldsymbol{\xi}_1^A) + (1-\phi)\boldsymbol{M}_2(\boldsymbol{\xi}_2^A)$$

$$= \phi \begin{bmatrix} \frac{\boldsymbol{U}_1}{q} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} \end{bmatrix} + (1-\phi) \begin{bmatrix} \left(\frac{\alpha_1}{q} + \frac{\alpha_2}{8q}\right)\boldsymbol{U}_1 + \frac{\alpha_2}{8q(q-1)}\boldsymbol{U}_2 & \frac{\alpha_2}{4q(q-1)}\boldsymbol{V}_1' \\ \frac{\alpha_2}{4q(q-1)}\boldsymbol{V}_1 & \frac{\alpha_2}{2q(q-1)}\boldsymbol{W}_1 \end{bmatrix}$$

$$= \begin{bmatrix} e\boldsymbol{U}_1 + f\boldsymbol{U}_2 & g\boldsymbol{V}_1' \\ g\boldsymbol{V}_1 & h\boldsymbol{W}_1 \end{bmatrix} \tag{3.4}$$

where

$$e = r_1 + \frac{r_2}{4}, \quad f = \frac{r_2}{4(q-1)}, \quad g = \frac{r_2}{2(q-1)}, \text{ and } h = \frac{r_2}{(q-1)}.$$

Next, using the multiplication table from Lemma 2.2, we get

$$\boldsymbol{M}_1^{-2}(\boldsymbol{\xi}_\phi) = s_1\boldsymbol{U}_1 + t_1\boldsymbol{U}_2 \tag{3.5}$$

where

$$s_1 = \frac{\left[(q-1)(r_1+r_2)+(2q-3)r_2\right]^2}{\left[(q-1)r_1+(q-2)r_2\right]^2\left[r_1+2r_2\right]^2},$$

and

$$t_1 = \frac{r_2^{\,2}}{\left[(q-1)r_1+(q-2)r_2\right]^2\left[r_1+2r_2\right]^2}.$$

The detailed derivation of Equation (3.5) is mentioned in Appendix A.I. Similarly, using the multiplication table from Lemma 2.2 we can find

$$\boldsymbol{M}_2^{-2}(\boldsymbol{\xi}_\phi) = \begin{pmatrix} a_2\boldsymbol{U}_1 + b_2\boldsymbol{U}_2 & c_2\boldsymbol{V}_1' \\ c_2\boldsymbol{V}_1 + d_2\boldsymbol{V}_2 & e_2\boldsymbol{W}_1 + f_2\boldsymbol{W}_2 + g_2\boldsymbol{W}_3 \end{pmatrix}. \tag{3.6}$$

The detailed derivation of Equation (3.6) is mentioned in Appendix A. II. Next using the principle of maxima and minima we set $\frac{d}{d\phi}\Phi_r^A(\phi) = 0$ and get

$$r\sigma_1(\phi) + (1-r)\sigma_2(\phi) = 0,$$

where

$$\sigma_1(\phi) = s_1\left(\alpha_1 - 1 + \frac{\alpha_2}{2}\right) + \frac{t_1\alpha_2}{2},$$

$$\sigma_2(\phi) = a_2(\alpha_1 - 1) + \frac{\alpha_2}{8}\left(a_2 + b_2 + 2c_2\right) + \frac{1}{4}\alpha_2(c_2 + e_2).$$

Then we solve for r and get

$$r = h^{-1}(\phi) = \frac{\sigma_2(\phi)}{\sigma_2(\phi) - \sigma_1(\phi)}. \tag{3.7}$$

It can be shown that $\lim_{\phi\to\varepsilon} h^{-1}(\phi) = 0$, $\lim_{\phi\to 1} h^{-1}(\phi) = 1$, and $\frac{d}{d\phi}h^{-1}(\phi) \geq 0$ for all $\phi \in [\varepsilon, 1]$ where $\varepsilon \in (0, 1)$. Figure 1 gives the behavior of the weight $\phi^A_{r(\tilde{r})}$ as a function of $\tilde{r}$. Here the weight $\phi^A_{r(\tilde{r})}$ is found as the numerical solution of Equation (3.7). From Figure 1, it is seen that $\phi^A_{r(\tilde{r})}$ is not a one-to-one function of $\tilde{r}$, hence $\phi^A_{r(\tilde{r})}$ cannot be a unique weight for different values of the prior. □

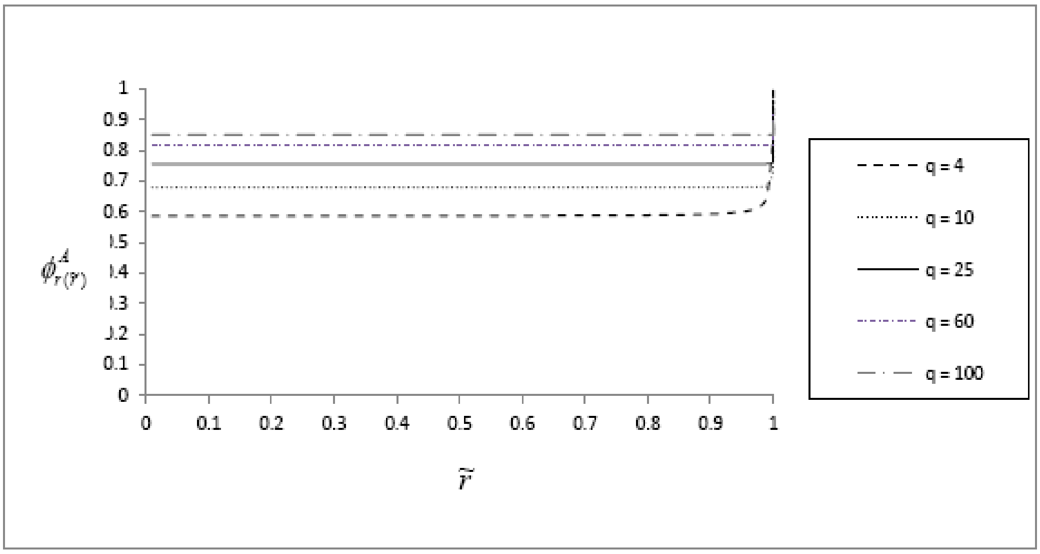

Figure 1. The A-optimal weight $\phi^{A}_{r(\tilde{r})}$ as a function of $\tilde{r} \in$ [0, 1]

Lemma 3.3. For a given $p \in [0, 1]$, the design $\xi_{\phi_p{}^A} \in \Xi_A$ with the weight $\phi_p{}^A = h(p)$ (*see* Lemma 3.2) is not a model-robust A-optimal design.

Proof: The necessary and sufficient conditions of model robust A-optimality follow from Lemma 3.2. To check these conditions, using Lemma A.3 [pg. 130, Klein (2004b)], we evaluate the following moment matrices *i.e.*

$$\boldsymbol{M}_1(\eta_j) = a_{1,j}\boldsymbol{U}_1 + b_{1,j}\boldsymbol{U}_2$$

with $a_{1,j} = \dfrac{1}{jq}$, $b_{1,j} = \dfrac{j-1}{jq(q-1)}$

and

$$\boldsymbol{M}_2(\eta_j) = \begin{pmatrix} a_{2,j}\boldsymbol{U}_1 + b_{2,j}\boldsymbol{U}_2 & c_{2,j}\boldsymbol{V}_1' + d_{2,j}\boldsymbol{V}_2' \\ c_{2,j}\boldsymbol{V}_1 + d_{2,j}\boldsymbol{V}_2 & e_{2,j}\boldsymbol{W}_1 + f_{2,j}\boldsymbol{W}_2 + g_{2,j}\boldsymbol{W}_3 \end{pmatrix}$$

with $a_{2,j} = \dfrac{1}{j^3 q}$, $b_{2,j} = \dfrac{1}{j^3 q}\dfrac{j-1}{q-1}$

$$c_{2,j} = \frac{2}{j^3 q}\frac{j-1}{q-1}, d_{2,j} = \frac{2}{j^3 q}\frac{j-1}{q-1}\frac{j-2}{q-2}$$

$$e_{2,j} = \frac{4}{j^3 q}\frac{j-1}{q-1}, f_{2,j} = \frac{4}{j^3 q}\frac{j-1}{q-1}\frac{j-2}{q-2}, g_{2,j} = \frac{4}{j^3 q}\frac{j-1}{q-1}\frac{j-2}{q-2}\frac{j-3}{q-3}.$$

Using the multiplication table in Lemma 2.2, we obtain the following quantities

$\mathrm{N}_{1,j} = tr\,\boldsymbol{M}_1^{-2}(\xi_\phi)\boldsymbol{M}_1(\eta_j)$, $\mathrm{N}_{2,j} = tr\,\boldsymbol{M}_2^{-2}(\xi_\phi)\boldsymbol{M}_2(\eta_j)$ for $1 \le j \le q$.

As $tr\,\boldsymbol{U}_2 = tr\,\boldsymbol{W}_2 = tr\,\boldsymbol{W}_3 = 0,$ hence we get

$$\mathrm{N}_{1,j} = tr\left[\left\{s_1.\frac{1}{jq} + (q-1)t_1.\frac{j-1}{jq(q-1)}\right\}\boldsymbol{U}_1 + \left\{t_1.\frac{1}{jq} + s_1.\frac{j-1}{jq(q-1)} + (q-2)t_1\frac{j-1}{jq(q-1)}\right\}\boldsymbol{U}_2\right]$$

$$= q\left[s_1.\frac{1}{jq} + (q-1)t_1.\frac{j-1}{jq(q-1)}\right]$$

$$= \frac{1}{j}(s_1 - t_1) + t_1$$

$$\mathrm{N}_{2,j} = q.\left\{a_2.a_{2,j} + (q-1)b_2.b_{2,j} + (q-1)c_2.c_{2,j} + \binom{q-1}{2}d_2.d_{2,j}\right\}$$

$$+\binom{q}{2}\left\{2.c_2.c_{2,j} + (q-2)d_2.d_{2,j} + e_2.e_{2,j} + 2(q-2)f_2.f_{2,j} + \binom{q-2}{2}g_2.g_{2,j}\right\}$$

$$= q.\left\{a_2.\frac{1}{j^3q} + (q-1)b_2.\frac{1}{j^3q}\frac{j-1}{q-1} + (q-1)c_2.\frac{2}{j^3q}\frac{j-1}{q-1} + \binom{q-1}{2}d_2.\frac{2}{j^3q}\frac{j-1}{q-1}\frac{j-2}{q-2}\right\}$$

$$+\binom{q}{2}\left\{2.c_2.\frac{2}{j^3q}\frac{j-1}{q-1} + (q-2)d_2.\frac{2}{j^3q}\frac{j-1}{q-1}\frac{j-2}{q-2} + e_2.\frac{4}{j^3q}\frac{j-1}{q-1}\right.$$

$$\left. + 2(q-2)f_2.\frac{4}{j^3q}\frac{j-1}{q-1}\frac{j-2}{q-2} + \binom{q-2}{2}g_2.\frac{4}{j^3q}\frac{j-1}{q-1}\frac{j-2}{q-2}\frac{j-3}{q-3}\right\}$$

$$= \left\{a_2.\frac{1}{j^3} + (j-1)b_2.\frac{1}{j^3} + (j-1)c_2.\frac{2}{j^3} + (j-1)(j-2).\frac{d_2}{j^3}\right\} + \left\{2.(j-1).\frac{c_2}{j^3}\right.$$

$$\left. + (j-1)(j-2).\frac{d_2}{j^3} + 2(j-1).\frac{e_2}{j^3} + 4(j-1)(j-2).\frac{f_2}{j^3} + (j-1)(j-2)(j-3).\frac{g_2}{j^3}\right\}$$

$$= \frac{1}{j^3}\{a_2 - b_2 - 2c_2 + 2d_2 - 2c_2 + 2d_2 - 2e_2 + 8f_2 - 6g_2\}$$

$$+ \frac{1}{j^2}\{b_2 + 2c_2 - 3d_2 + 2c_2 - 3d_2 + 2e_2 - 12f_2 + 11g_2\} + \frac{1}{j}\{2d_2 + 4f_2 - 6g_2\} + const.$$

$$= \frac{1}{j^3}\{a_2 - b_2 - 4c_2 + 4d_2 - 2e_2 + 8f_2 - 6g_2\} + \frac{1}{j^2}\{b_2 + 4c_2 - 6d_2 + 2e_2 - 12f_2 + 11g_2\}$$

$$+ \frac{1}{j}\{2d_2 + 4f_2 - 6g_2\} + const.$$

with s_1, t_1, a_2, b_2, c_2, d_2, e_2, f_2, and g_2 as mentioned in the proof of Lemma 3.2 and Appendix A.II. As $s_1 - t_1 > 0$, hence the term $N_{1,j}$ is decreasing in j. Next to prove $N_{2,j}$ is decreasing in j, we evaluate

$$N_{2,j} - N_{2,j+1} = \frac{1}{j^3}\{a_2 - b_2 - 4c_2 + 4d_2 - 2e_2 + 8f_2 - 6g_2\} + \frac{1}{j^2}\{b_2 + 4c_2 - 6d_2 + 2e_2 - 12f_2 + 11g_2\} + \frac{1}{j}\{2d_2 + 4f_2 - 6g_2\} - \frac{1}{(j+1)^3}\{a_2 - b_2 - 4c_2 + 4d_2 - 2e_2 + 8f_2 - 6g_2\} - \frac{1}{(j+1)^2}\{b_2 + 4c_2 - 6d_2 + 2e_2 - 12f_2 + 11g_2\} - \frac{1}{j}\{2d_2 + 4f_2 - 6g_2\}$$

$$= \left[\frac{1}{j^3} - \frac{1}{(j+1)^3}\right]\{a_2 - b_2 - 4c_2 + 4d_2 - 2e_2 + 8f_2 - 6g_2\} + \left[\frac{1}{j^2} - \frac{1}{(j+1)^2}\right]\{b_2 + 4c_2 - 6d_2 + 2e_2 - 12f_2 + 11g_2\} + \left[\frac{1}{j} - \frac{1}{j+1}\right]\{2d_2 + 4f_2 - 6g_2\}$$

$$= \left[\frac{3j^2 + 3j + 1}{j^3(j+1)^3}\right]\{a_2 - b_2 - 4c_2 + 4d_2 - 2e_2 + 8f_2 - 6g_2\} + \left[\frac{2j+1}{j^2(j+1)^2}\right]\{b_2 + 4c_2 - 6d_2 + 2e_2 - 12f_2 + 11g_2\} + \left[\frac{1}{j(j+1)}\right]\{2d_2 + 4f_2 - 6g_2\}$$

for $2 \le j \le q-1$. As $3j^2 + 3j + 1 \le j(j+1)(2j+1) \le j^2(j+1)^2$ for $j \ge 2$, we obtain

$$N_{2,j} - N_{2,j+1} \ge \frac{3j^2 + 3j + 1}{j^3(j+1)^3}(a_2 - g_2) = \frac{(3j^2 + 3j + 1)}{j^3(j+1)^3}\frac{(q+2)(4r_1 + 7r_2)^2}{64} > 0$$

for all $q \ge 2$ and $\phi \in [0,1]$.

Again, we have

$$p\, tr\, \boldsymbol{M}_1^{-2}(\xi_\phi)\boldsymbol{M}_1(\eta_1) + (1-p) tr\, \boldsymbol{M}_2^{-2}(\xi_\phi)\boldsymbol{M}_2(\eta_1)$$
$$= p.\{(s_1 - t_1) + t_1\} + (1-p)a_2$$
$$= p.s_1 + (1-p)a_2 \tag{3.8}$$

and

$$p\, tr\, \boldsymbol{M}_1^{-1}(\xi_\phi) + (1-p) tr\, \boldsymbol{M}_2^{-1}(\xi_\phi)$$
$$= p\frac{q^2[3 + 4q + \sqrt{3+q} - (2 + \sqrt{3+q})\phi + q(-11 + 2\phi)]}{1 + q[-7 + \sqrt{3+q} - (2 + \sqrt{3+q})\phi + 2q(1+\phi)]}$$

$$+(1-p)\left[\frac{q^3}{\left(\phi+\frac{(1-\phi)\left(2(q-1)\sqrt{q+3}-3-q\right)}{1+q(4q-9)}\right)^2}\right.$$

$$\left.+\frac{1}{2}q(q-1)\left(\frac{q(1+q(4q-9))}{(2-2q+\sqrt{3+q})(\phi-1)}+\frac{q^2}{2\left(\phi+\frac{(1-\phi)(2(q-1)\sqrt{3+q}-3-q)}{1+q(4q-9)}\right)^2}\right)\right] \quad (3.9)$$

Substituting $\phi=\phi_p^A$, a numerical solution of $p=\frac{\sigma_2(\phi)}{\sigma_2(\phi)-\sigma_1(\phi)}$ from Equation (3.7) in Equations (3.8), and (3.9), it can be checked that the R.H.S of both Equations (3.8) and (3.9) are not equal. Hence, the equality of model robust A-optimality does not hold. This completes the proof. □

4. Discussion and Conclusions

The current work discusses the aspect of the model robust A-optimality criterion for the K-models. From the above discussion, it is seen that the support points of the simplex centroid designs are D- and A-optimal designs for both K- and S-models (first- and second-degree models) with appropriate weights assigned to these points. Further, it is observed that an appropriately defined convex combination of these D-optimal designs is model-robust D-optimal designs for both K- and S-models. However, in the case of the model-robust A-optimality criterion, it holds only for the S-models and not for the K-models. Thus, it can be concluded that, for K-models, the A-optimal designs may not be able to detect the model inadequacy at the support points whereas the A-optimal designs could be able to detect the model inadequacy at the same support points for the S-models. This can be attributed to the fact of re-parameterization from S-models to K-models through a linear transformation *i.e.* the design points of the A-optimal designs are badly located w.r.t model-robust A-optimality concerning the K-models.

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Appendix A

A. I. Derivation of $\boldsymbol{M}_1^{-2}(\boldsymbol{\xi}_\phi)$

Using Equation (3.3), we get the inverse of the matrix $\boldsymbol{M}_1(\boldsymbol{\xi}_\phi)$ as

$$\boldsymbol{M}_1^{-1}(\boldsymbol{\xi}_\phi) = \kappa_1 \boldsymbol{U}_1 + \kappa_2 \boldsymbol{U}_2 \tag{A1}$$

where

$$\kappa_1 = \frac{(q-1)(r_1+r_2)+(q-2)r_2}{(q-1)(r_1+r_2)^2+(q-2)(r_1+r_2)r_2 - r_2^2},$$

$$\kappa_2 = \frac{r_2}{(q-1)(r_1+r_2)^2+(q-2)(r_1+r_2)r_2 - r_2^2}.$$

Subsequently, using the multiplication table from Lemma 2.2 for the matrix and after performing some little algebra we get

$$\boldsymbol{M}_1^{-2}(\xi_\phi) = s_1\boldsymbol{U}_1 + t_1\boldsymbol{U}_2$$

where

$$s_1 = \frac{\left[(q-1)(r_1+r_2)+(2q-3)r_2\right]^2}{\left[(q-1)r_1+(q-2)r_2\right]^2\left[r_1+2r_2\right]^2}, \text{ and}$$

$$t_1 = \frac{r_2^2}{\left[(q-1)r_1+(q-2)r_2\right]^2\left[r_1+2r_2\right]^2}.$$

A. II. Derivation of $\boldsymbol{M}_2^{-2}(\boldsymbol{\xi}_\phi)$

Next, we obtain the inverse matrix $\boldsymbol{M}_2^{-2}(\xi_\phi)$ using the formula of inverse for partitioned matrices *i.e.* for a non-singular matrix $\boldsymbol{\Delta} = \begin{bmatrix} \boldsymbol{A} & \boldsymbol{B} \\ \boldsymbol{C} & \boldsymbol{D} \end{bmatrix}$ the inverse matrix is

$$\Delta^{-1} = \begin{bmatrix} \boldsymbol{K}^{-1} & -\boldsymbol{K}^{-1}\boldsymbol{B}\boldsymbol{D}^{-1} \\ \boldsymbol{D}^{-1}\boldsymbol{C}\boldsymbol{K}^{-1} & \boldsymbol{D}^{-1} + \boldsymbol{D}^{-1}\boldsymbol{C}\boldsymbol{K}^{-1}\boldsymbol{B}\boldsymbol{D}^{-1} \end{bmatrix}, \tag{A2}$$

where $\boldsymbol{K} = \boldsymbol{A} - \boldsymbol{B}\boldsymbol{D}^{-1}\boldsymbol{C}$ provided $\boldsymbol{D}$ is a non-singular matrix [*see* Rao and Bhimasankaram (2000)].

Using Equation (A2) for the matrix given in Equation (3.4) we get the following

(i) $\boldsymbol{K} = (e\boldsymbol{U}_1 + f\boldsymbol{U}_2) - g\boldsymbol{V}_1'(h\boldsymbol{W}_1)^{-1}g\boldsymbol{V}_1$

$$= e\boldsymbol{U}_1 + f\boldsymbol{U}_2 - \frac{g^2}{h}\boldsymbol{V}_1'\boldsymbol{V}_1$$

$$= e\boldsymbol{U}_1 + f\boldsymbol{U}_2 - \frac{g^2}{h}\{(q-1)\boldsymbol{U}_1 + \boldsymbol{U}_2\}$$

$$= e\boldsymbol{U}_1 + f\boldsymbol{U}_2 - \frac{g^2}{h}\{(q-1)\boldsymbol{U}_1 + \boldsymbol{U}_2\}$$

$$= \left\{e - \frac{g^2}{h}(q-1)\right\}\boldsymbol{U}_1 + \left\{f - \frac{g^2}{h}\right\}\boldsymbol{U}_2$$

$= k_1\boldsymbol{U}_1 + l_1\boldsymbol{U}_2$, where $k_1 = e - \frac{g^2}{h}(q-1)$ and $l_1 = f - \frac{g^2}{h}$

and subsequently, we get

$$\boldsymbol{K}^{-1} = \frac{[k_1 + (q-2)l_1]^2}{(k_1 - l_1)^2[k_1 + (q-1)l_1]^2}\boldsymbol{U}_1 + \frac{l_1^2}{(k_1 - l_1)^2[k_1 + (q-1)l_1]^2}\boldsymbol{U}_2$$

$$= a_1\boldsymbol{U_1} + b_1\boldsymbol{U_2}$$

(ii) $-\boldsymbol{D}^{-1}\boldsymbol{C}\boldsymbol{K}^{-1} = -(h\boldsymbol{W}_1)^{-1}g\boldsymbol{V}_1(a_1\boldsymbol{U}_1 + b_1\boldsymbol{U}_2)$

$$= -\frac{1}{h_1}\boldsymbol{W}_1 g\boldsymbol{V}_1(a_1\boldsymbol{U}_1 + b_1\boldsymbol{U}_2)$$

$$= -\frac{ga_1}{h}\boldsymbol{V}_1\boldsymbol{U}_1 - \frac{gb_1}{h}\boldsymbol{V}_1\boldsymbol{U}_2$$

$$= -\frac{ga_1}{h}\boldsymbol{V}_1 - \frac{gb_1}{h}(\boldsymbol{V}_1 + 2\boldsymbol{V}_2)$$

$$= -\frac{g}{h}(a_1 + b_1)\boldsymbol{V}_1 - \frac{2gb_1}{h}\boldsymbol{V}_2$$

$= c_1\boldsymbol{V}_1 + d_1\boldsymbol{V}_2$, where $c_1 = -\frac{g}{h}(a_1 + b_1)$ and $d_1 = -\frac{2gb_1}{h}$

(iii) $-\boldsymbol{K}^{-1}\boldsymbol{B}\boldsymbol{D}^{-1} = -(a_1\boldsymbol{U}_1 + b_1\boldsymbol{U}_2)g\boldsymbol{V}_1'\left(\frac{1}{h}\boldsymbol{W}_1\right)$

$$= -\frac{ga_1}{h}\boldsymbol{V_1'} - \frac{gb_1}{h}\boldsymbol{U_2V_1'}$$

$$= -\frac{ga_1}{h}\boldsymbol{V}_1' - \frac{gb_1}{h}\boldsymbol{V}_1'\boldsymbol{U}_2$$

$$= -\frac{ga_1}{h}\boldsymbol{V}_1' - \frac{gb_1}{h}(\boldsymbol{V}_1' + 2\boldsymbol{V}_2')$$

$$= -\frac{ga_1}{h}\boldsymbol{V}_1' - \frac{gb_1}{h}\boldsymbol{V}_1' - 2\frac{gb_1}{h}\boldsymbol{V}_2'$$

$$= -\frac{g}{h}(a_1 + b_1)\boldsymbol{V}_1' - \frac{2g}{h}b_1\boldsymbol{V}_2'$$

$$= c_1\boldsymbol{V}_1' + d_1\boldsymbol{V}_2'$$

(*iv*) $\boldsymbol{D}^{-1} + \boldsymbol{D}^{-1}\boldsymbol{C}\boldsymbol{K}^{-1}\boldsymbol{B}\boldsymbol{D}^{-1} = \frac{1}{h}\boldsymbol{W}_1 + \frac{1}{h}\boldsymbol{W}_1.g\boldsymbol{V}_1.(a_1\boldsymbol{U}_1 + b_1\boldsymbol{U}_2).g\boldsymbol{V}_1'.\frac{1}{h}\boldsymbol{W}_1$

$$= \frac{1}{h}\boldsymbol{W}_1 + \left(\frac{g}{h}a_1.\boldsymbol{V}_1 + \frac{g}{h}b_1.\boldsymbol{V}_1\boldsymbol{U}_2\right)\frac{g}{h}\boldsymbol{V}_1'.\boldsymbol{W}_1$$

$$= \frac{1}{h}\boldsymbol{W}_1 + \frac{g^2}{h^2}a_1.\boldsymbol{V}_1\boldsymbol{V}_1' + \frac{g^2}{h^2}b_1.\boldsymbol{V}_1\boldsymbol{U}_2\boldsymbol{V}_1'$$

$$= \frac{1}{h}\boldsymbol{W}_1 + \frac{g^2}{h^2}a_1.(2\boldsymbol{W}_1 + \boldsymbol{W}_2) + \frac{g^2}{h^2}b_1.(\boldsymbol{V}_1 + 2\boldsymbol{V}_2)\boldsymbol{V}_1'$$

$$= \frac{1}{h}\boldsymbol{W}_1 + \frac{g^2}{h^2}a_1.(2\boldsymbol{W}_1 + \boldsymbol{W}_2) + \frac{g^2}{h^2}b_1.\boldsymbol{V}_1.\boldsymbol{V}_1' + 2\frac{g^2}{h^2}b_1.\boldsymbol{V}_2.\boldsymbol{V}_1'$$

$$= \frac{1}{h}\boldsymbol{W}_1 + \frac{g^2}{h^2}a_1.(2\boldsymbol{W}_1 + \boldsymbol{W}_2) + \frac{g^2}{h^2}b_1.(2\boldsymbol{W}_1 + \boldsymbol{W}_2) + 2\frac{g^2}{h^2}b_1.(\boldsymbol{W}_2 + 2\boldsymbol{W}_3)$$

$$= \left(\frac{1}{h} + 2\frac{g^2}{h^2}a_1 + 2\frac{g^2}{h^2}b_1\right).\boldsymbol{W}_1 + \left(\frac{g^2}{h^2}a_1 + 3\frac{g^2}{h^2}b_1\right).\boldsymbol{W}_2 + 4\frac{g^2}{h^2}b_1.\boldsymbol{W}_3$$

$$= e_1.\boldsymbol{W}_1 + f_1.\boldsymbol{W}_2 + g_1.\boldsymbol{W}_3$$

where $e_1 = \frac{1}{h} + 2\frac{g^2}{h^2}(a_1 + b_1)$, $f_1 = \frac{g^2}{h^2}(a_1 + 3b_1)$ and $g_1 = 4\frac{g^2}{h^2}b_1$.

So

$$\boldsymbol{M}_2^{-1}(\xi_\phi) = \begin{bmatrix} a_1\boldsymbol{U}_1 + b_1\boldsymbol{U}_2 & c_1\boldsymbol{V}_1' + d_1\boldsymbol{V}_2' \\ c_1\boldsymbol{V}_1 + d_1\boldsymbol{V}_2 & e_1\boldsymbol{W}_1 + f_1\boldsymbol{W}_2 + g_1\boldsymbol{W}_3 \end{bmatrix}$$

Again taking the inverse of the $\boldsymbol{M}_2^{-1}(\xi_\phi)$, we get

$$\boldsymbol{M}_2^{-2}(\xi_\phi) = \begin{bmatrix} a_2\boldsymbol{U}_1 + b_2\boldsymbol{U}_2 & c_2\boldsymbol{V}_1' + d_2\boldsymbol{V}_2' \\ c_2\boldsymbol{V}_1 + d_2\boldsymbol{V}_2 & e_2\boldsymbol{W}_1 + f_2\boldsymbol{W}_2 + g_2\boldsymbol{W}_3 \end{bmatrix}$$

where $a_2 = a_1^2 + (q-1)(b_1^2 + c_1^2) + \binom{q-1}{2} d_1^2$

$$b_2 = (q-2)b_1^2 + c_1^2 + 2a_1b_1 + 2(q-2)c_1d_1 + \binom{q-2}{2} d_1^2$$

$$c_2 = c_1(a_1 + b_1 + e_1) + (q-2)(b_1d_1 + c_1f_1 + d_1f_1) + \binom{q-2}{2} d_1g_1$$

$$d_2 = d_1(a_1 + e_1) + 2c_1(b_1 + f_1) + (q-3)(b_1d_1 + c_1g_1 + 2d_1f_1) + \binom{q-3}{2} d_1g_1$$

$$e_2 = 2c_1^2 + (q-2)d_1^2 + e_1^2 + 2(q-2)f_1^2 + \binom{q-2}{2} g_1^2$$

$$f_2 = c_1^2 + 2c_1d_1 + (q-3)d_1^2 + 2e_1f_1 + (q-2)f_1^2 + \binom{q-3}{2} g_1^2 + 2(q-3)f_1g_1$$

$$g_2 = 4c_1d_1 + (q-4)d_1^2 + 4f_1^2 + 2e_1g_1 + \binom{q-4}{2} g_1^2 + 4(q-4)f_1g_1$$