<Research Paper>

Journal of the Korean
Statistical Society
Vol. 17, No. 2, 1988

Slope-rotatable Designs for Estimating the Slope of Response Surfaces in Experiments with Mixtures

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ABSTRACT

In this paper a class of mixture designs for estimating the slope of second order Scheffe polynomial response surfaces for mixture experiments with q components is presented. The variance of the estimated directional slope at a point is a function of the direction of the slope and the design. If the variance is averaged over all possible directions in the (q-1)-dimensional simplex, the averaged variance is only a function of the point and the design. By choice of design, it is possible to make this variance constant for all points equidistant from the centroid point. This property is called "slope-rotatability over all directions in the simplex", and the necessary and sufficient conditions for mixture design to have this property are given and proved. The class of designs with this property is compared with other mixture designs and discussed.

1. Introduction

The special nature of mixture experiments can be expressed in the following set of constraints: If x_i denote the proportion of the ith component in the mixture, then

$$x_i \geqq 0 \quad \text{for all } i, \text{ and } \sum_{i=1}^{q} x_i = 1. \tag{1.1}$$

For fitting a mixture response surface over the simplex factor space, much attention has been given to the use of the canonical polynomials suggested by Scheffé (1958). Let us assume the surface can best be represented as a quadratic function in each of the q components. The second degree Scheffé polynomial in q components, $\underline{x}' = (x_1, x_2, \cdots, x_q)$, is

$$\eta(\underline{x}) = \sum_{i=1}^{q} \beta_i x_i + \sum_{i=1}^{q} \sum_{j>i}^{q} \beta_{ij} x_i x_j \tag{1.2}$$

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which may be written in matrix notation as

$$\eta(\underline{x}) = f(\underline{x})'\underline{\beta}$$

in which the 1 x m vector $\underline{f}(\underline{x})' = (x_1, x_2, \cdots, x_q, x_1x_2, \cdots, x_{q-1}x_q)$ and $\underline{\beta}$ is the m x 1 column vector of the corresponding coefficients with $m = q(q+1)/2$. It can be noted that the next substitution is used in the above equation(1.2).

$$x_j^2 = x_j\,(1-\sum_{\substack{i=1\\ i\neq j}}^{q} x_i) = x_j - \sum_{\substack{i=1\\ i\neq j}}^{q} x_i x_j .$$

The coefficients in the polynomial are to be estimated from observations on the response variable, $y(\underline{x}) = \eta(\underline{x}) + e$, where the observations are taken at n selected combinations of the x components. The e's are assumed to be uncorrelated random errors with zero means and constant variance, σ^2. The $\underline{\beta}$'s are then estimated by the method of least squares, $\underline{b} = (X'X)^{-1}X'\underline{y}$, in which X is the n x m matrix of values of the m elements of $\underline{f}(\underline{x})'$ taken at the design points and $\underline{y}$ is the n x 1 matrix of y observations.

If differences at points close together in the factor space are involved, the estimation of the local slopes(the rates of change) of the response surfaces becomes important. For instance, there are the cases in which we want to estimate rates of reaction in chemical experiments to various mixtures of blending components, rates of change in the yield of a crop to various component proportions of fertilizers, rates of change in thread elongation vlaues to various mixing ratios of fiber constituents, and so forth. The problem considered in this paper is, therefore, that of the choice of the mixture experimental design so as to achieve useful property on the estimated slope of the response surface in mixture experiments. Much of the literature on response surface analysis has dealt with the variance properties of the estimated response, $\hat{y}$. Some authors, however, have considered the estimation of partial derivatives of the response function with respect to the independent variables. Ott and Mendenhall (1972), Myers and Lahoda (1975), Hader and Park (1978), Box and Draper (1980), Huda and Mukerjee (1984), Mukerjee and Huda (1985), Park (1987) and others have focused attention on problems associated with estimation of derivatives of the expected response.

The variance of $\hat{y}$ depends on the particular values of the independent variables. Box and Hunter (1957) suggested that, subject to a suitable scaling of the independent variables with respect to each other it would be desirable to have equally reliable estimates of the expected response for all points $\underline{x}$ equidistant from the design origin, that is, to have the variance of $\hat{y}$ be a function of only $\rho = (x_1^2 + x_2^2 + \cdots\cdots)^{1/2}$. This requires X'X to be invariant under rotation and the designs having this property were called rotatable designs.

Hader and Park (1978) proposed an analogue of the Box-Hunter rotatability criterion, which requires that the variance of $\partial\hat{y}/\partial x_i$, the slope with respect to the axial direction of x_i, be constant on circles (q=2), spheres (q=3) or hyperspheres (q≧4) centered at the origin. Estimation of the slopes over axial directions would then be equally reliable for all points $\underline{x}$ equidistant from the design origin. Hader and Park referred to this property as slope-rotatability. They also presented slope-rotatable central composite designs.

In practice, it is often of interest to estimate the slope of the response surface at a point $\underline{x}$, not only over the axial directions, but over any specified direction. In this context, Park (1987) proposed an extended analogue of the Hader-Park slope-rotatability criterion, which requires that the averaged variance of the estimated slopes over all possible directions be constant for all points equidistant from the design origin. Park referred to this property as slope-rotatability over all directions.

However, very little attention has been given to the estimation of slope of the response function with respect to the mixture components in mixture experiments. In this paper, the concept of slope-rotatability over all directions in response surface experiments is extended to the design aspects in mixture experiments. Then it is possible to find designs for which the directional slope estimates are equally good (same averaged variance) at all combinations of the independent variables equidistant from the design center.

2. Estimation of Slopes in Simplex Factor Space

Suppose that estimation of slopes of $\eta(\underline{x})$ in the equation (1.2) at a point $\underline{x}$ is of interest. When the estimated response is denoted by $\hat{y}(\underline{x}) = \underline{f}(\underline{x})'\underline{b}$, where $\underline{b}' = (b_1, b_2, \cdots, b_q, b_{12}, \cdots, b_{q-1,q})$, the estimated slope of $\hat{y}(\underline{x})$ with respect to x_i is

$$\partial\hat{y}(\underline{x})/\partial x_i = b_i + \sum_{\substack{j=1 \\ j\neq i}}^{q} b^*_{ij} x_j \tag{2.1}$$

where $b^*_{ij} = b_{ij}$ if $i<j$ and $b^*_{ij} = b_{ji}$ if $i>j$. The variance of this slope is a function of the point $\underline{x}$ at which the slope is estimated, and also a function of the design through the relationship $V(\underline{b}) = (X'X)^{-1}\sigma^2$.

The vector of estimated slopes along the factor axes is given by

$$\underline{g}(\underline{x}) = (\partial y(\underline{x})/\partial x_1, \cdots, \partial y(\underline{x})/\partial x_q) = H(\underline{x})\ \underline{b} \tag{2.2}$$

where $H(\underline{x})$ is the matrix arising from the differentiation of $\underline{f}(\underline{x})'\ \underline{b}$ with respect to each of the q components. For instance, $H(\underline{x})$ becomes for the second degree Scheffé polynomial model in three components

$$H(\underline{x}) = \begin{bmatrix} 1 & 0 & 0 & x_2 & x_3 & 0 \\ 0 & 1 & 0 & x_1 & 0 & x_3 \\ 0 & 0 & 1 & 0 & x_1 & x_2 \end{bmatrix}.$$

The estimated slope at any point $\underline{x}$ in the direction specified by the q x 1 vector of direction cosines

$$\underline{\alpha} = (\alpha_1, \cdots, \alpha_q)'$$

is $\underline{\alpha}'\underline{g}(\underline{x})$ where $\underline{\alpha}'\underline{\alpha} = 1$, and the variance of this slope is

$$\begin{aligned} V(\underline{x}) &= \text{var}\,[\underline{\alpha}'\underline{g}(\underline{x})] = \underline{\alpha}'V[\underline{g}(\underline{x})]\underline{\alpha} \\ &= \underline{\alpha}'H(\underline{x})V(\underline{b})H(\underline{x})'\underline{\alpha} = \sigma^2\underline{\alpha}'H(\underline{x})(X'X)^{-1}H(\underline{x})'\underline{\alpha}. \end{aligned}$$

However, in the mixture experiments, all possible directions of $\underline{\alpha}$ are subject to additional condition $\underline{1}'\underline{\alpha} = \underline{\alpha}'\underline{1} = 0$ for q x 1 vector $\underline{1} = (1, \cdots, 1)'$, because the predictor variables are constrainde by (1.1) and the resulting factor space is a regular (q-1) - dimensional simplex only on which the direction cosines should be considered.

Now, we call $\underline{\alpha}'\underline{g}(\underline{x})$ as the directional slope to the direction $\underline{\alpha}$ at $\underline{x}$. If we are interested in all possible directions in the simplex, then we consider the average of $V(\underline{x})$ over all possible directions. The following lemma can be obtained.

Lemma 1. The average of $V(\underline{x})$ over all possible directions in a (q-1)-dimensional simplex in such a way that the distribution over all possible directions is uniform is

$$\overline{V}(\underline{x}) = \sigma^2\{\text{tr}[H(\underline{x})(X'X)^{-1}H(\underline{X})'] - \underline{1}'H(\underline{x})(X'X)^{-1}H(\underline{x})'\underline{1}/q\}/(q-1). \tag{2.3}$$

Proof. The proof of this equality is given in Appendix(A.1). ∎

Note that $\overline{V}(\underline{x})$ is a function of the point $\underline{x}$ at which the slope is being estimated, and depends on the design through the matrix $(X'X)^{-1}$. By the choice of design it is possible to make this averaged variance $\overline{V}(\underline{x})$ constant for all points in the simplex equdistant from the center point. This property will hereafter be called "slope-rotatability over all directions in the simplex".

3. Slope-Rotatability over All Directions

In this section, the necessary and sufficient conditions for a design to have the slope-rotatability over all directions are given for the second degree Scheffé polynomial model (1.2). Let us denote the averaged variance $\overline{V}(\underline{x})$ as

$$\overline{V}(\underline{x}) = a + \sum_{j=1}^{q} c(j)x_j + \sum_{\substack{j=1 \\ j \neq k}}^{q}\sum_{k=1}^{q} d(j,k)x_jx_k$$

Theorem 1. The necessary and sufficient conditions for a design to be slope-rotatable over all directions in the simplex for the second degree Scheffé polynomial model (1.2) are

1) c(j) are constant for all j
2) d(j,k) are constant for all $j \neq k$

where

$$c(j) = \sum_{\substack{i=1 \\ i \neq j}}^{q} \{2\,\mathrm{cov}(b_i, b^*_{ij}) + \mathrm{var}(b^*_{ij})\}/q$$

$$-\{2\sum_{\substack{i=1 \\ i \neq j}}^{q} \mathrm{cov}(b_i, b^*_{ij}) + \sum_{\substack{h=1 \\ h \neq j}}^{q} \sum_{\substack{i=1 \\ i \neq h,j}}^{q} (2\,\mathrm{cov}(b_i, b^*_{hj}) + \mathrm{cov}(b^*_{hj}, b^*_{ij}))\}/q(q-1)$$

$$d(j,k) = \{\sum_{\substack{i=1 \\ i \neq j,k}}^{q} \mathrm{cov}(b^*_{ij}, b^*_{ik}) - \sum_{\substack{i=1 \\ i \neq j}}^{q} \mathrm{var}(b^*_{ij})\}/q$$

$$-\{\mathrm{var}(b^*_{jk}) + \sum_{\substack{i=1 \\ i \neq j,k}}^{q} (\mathrm{cov}(b^*_{ij}, b^*_{jk}) + \mathrm{cov}(b^*_{ik}, b^*_{jk}))$$

$$+ \sum_{\substack{h=1 \\ h \neq j,k}}^{q} \sum_{\substack{i=1 \\ i \neq h,j,k}}^{q} \mathrm{cov}(b^*_{hj}, b^*_{ik})$$

$$- \sum_{\substack{h=1 \\ h \neq j}}^{q} \sum_{\substack{i=1 \\ i \neq h,k}}^{q} \mathrm{cov}(b^*_{hj}, b^*_{ij})\}/q(q-1)$$

Proof. The proof of this theorem is given in Appendix (A.2) ■

As shown by Box and Hunter (1957) and Khuri and Cornell (1987), let us use the notations such as [ii], [iiii], and [iijj] to denote the pure second order moments, the pure fourth order mements, and the mixed fourth order moments, respectively. A useful sufficient condition to find slope-rotatability over all directions is stated as follows.

Corollary 1. If the symmetric moment conditions described in Murty and Das (1968) such as

(1) $[ii] = A$ for all i
(2) $[ij] = B$ for all $i \neq j$
(3) $[iij] = C$ for all $i \neq j$
(4) $[ijk] = D$ for all $i \neq j \neq k$
(5) $[iijj] = E$ for all $i \neq j$
(6) $[iijk] = F$ for all $i \neq j \neq k$
(7) $[ijkl] = G$ for all $i \neq j \neq k \neq l$

are satisfied for some constants A, B, C, D, E, F, and G, for the second degree Scheffé model (1.2), then the design is slope-rotatable over all directions in the mixture experiments.

Proof The proof of this corollary can be found in Appendix (A.3) ■

4. Slope-Rotatable Designs over All Directions in the Simplex

Now it is desirable to compare the class of slope-rotatable designs over all directions in the simplex with other classes of mixture designs. We need the following definition of the symmetric simplex design which can be found in Murty and Das (1968) in order to compare mixture designs over all simplex factor space.

Definition. A symmetric simplex design for experiments with mixtures consists of some or all the groups G_d, $d = 1 \cdots, q$, where every group G_d is obtained by permuting the different fractions over the q components in a dth ordered mixture with d_1 components taking a proportion p_1, d_2 of them taking a proportion p_2, and so on, d_h of them taking a proportion p_h such that

$$d_1 + \cdots + d_h \text{ and } d_1p_1 + \cdots + d_hp_h = 1.$$

Murty and Das showed that the simplex-lattice design, the simplex-centroid design and the radial-lattice and the radial-centroid designs cited in Scheffé (1963) are symmetric simplex designs.

The following mixture designs are slope-rotatable over all directions, and they are also symmetric simplex designs.

(1) The simplex-lattice design, the simplex-centroid design and the radial-lattice and the radial-cenroid designs.

(2) The simplex screening design proposed by Snee and Marquardt (1976) and the Lambrakis design suggested by Lambrakis (1969).

(3) The design in q components with the three group G_d; $d= 1,2,3$, where the components in each group G_d take the proportion $1/d$. Such design thus consists of the q points of the type $(1,0, \cdots,0)$, the $q(q-1)/2$ points of the type $(\frac{1}{2}, \frac{1}{2}, 0, \cdots, 0)$, and the $q(q-1)(q-2)/6$ points of the type $(1/3, 1/3, 1/3, 0, \cdots, 0)$.

(4) The design with the q groups, G_d, $d = 1,2,\cdots,q$, such that any particular group G_d has design points with each of the nonzero fractions equal to $1/d$.

It seems that the slope-rotatable design over all directions is identical to the symmetric simplex design. However, this is not the case. We can find a class of design which is not the symmertic simplex design but the slope-rotatable design over all directions.

Consider the following equiradial design in three component mixture experiments such that n design points are equally spaced on a circle centered at the centroid(1 / 3, 1 / 3, 1 / 3) with radious ρ. If θ denotes the angle between the x_1 axis and the line which connects a design point to the centroid, then the coordinates of each point are given by (x_{1u}, x_{2u}, x_{3u}), u= 0,1,⋯,n-1, where

$$x_{1u} = 1/3 + \sqrt{6}\rho\cos(\theta + 2u\pi/n)/3$$
$$x_{2u} = 1/3 + \sqrt{6}\rho\cos(2\pi/3 - \theta - 2u\pi/n)/3$$
$$x_{3u} = 1/3 + \sqrt{6}\rho\cos(\pi/3 - \theta - 2u\pi/n)/3.$$

Using the relations explained in detail in Myers (1971) such that

$$\sum\cos(2u\pi/n) = \sum\sin(2u\pi/n) = 0,$$
$$\sum\cos(2u\pi/n)\sin(2u\pi/n) = \sum\cos^2(2u\pi/n)\sin(2u\pi/n)$$
$$= \sum\cos(2u\pi/n)\sin^2(2u\pi/n) = 0,$$
$$\sum\cos^2(2u\pi/n) = \sum\sin^2(2u\pi/n) = n/2,$$
$$\sum\cos^2(2u\pi/n)\sin^2(2u\pi/n) = n/8,$$

the values of the constants in Corollary 1 can be obtained as follows:

$$A = n/9 + n\rho^2/3,\ B = n/9 - n\rho^2/6,\ C = n/27,$$
$$D = n/27 - n\rho^2/6,\ E = n/81 - n\rho^2/18,$$
$$F = n/81 + n\rho^4/12,\ G = 0.$$

Hence, this design is slope-rotatable over all directions. Now consider the case n = 5, θ= 0, $\rho = \sqrt{6}/6$, $\sigma^2 = 1$, then we can obtain 5 design points equally spaced on a circle. A design which consists of such 5 points and a center point such as

(.0000, .5000, .5000), (.2303, .1103, .6594), (.6030, .0288,. 3682)

(.6030, .3682, .0288), (.2303, .6594, .1103), (.3333, .3333, .3333)

will be an example which is not a symmetric simplex design but has the slope rotatability, since the design points are not permutations of fractions in each group G_d. The value of $\overline{V}(\underline{x})$ for this design is 26.41 for all 5 points equally spaced on a circle with $\rho = \sqrt{6}/6$ and 2.40 for the centroid.

From the preceding illustrations, it is clear that the most often used designs in mixture experiments in the whole simplex factor space belong to the class of slope-rotatable designs over all directions. It was shown that the symmetric simplex designs proposed by Murty and Das(1986) satisfy the symmetric moment conditions in Corollary 1. Hence, we can conclude that the class of symmetric simplex designs is a subset of the class of designs which satisfy the symmetric moment conditions, which in turn is a subset of the class of slope-rotatable designs over all directions in the simplex.

5. Concluding Remarks

In this paper, "slope-rotatability over all directions" in the regular simplex has been proposed as a desirable property of designs for mixture experiments.This concept is an analogue of "slope-rotatability" which was proposed for the response surface analysis by Park (1987).

The necessary and sufficient conditions for a design to have slope-rotatability over all directions in the simplex, that is, to have equal averaged variance of slopes, $\overline{V}(\underline{x})$, for each point $\underline{x}$ in the same distance from the centroid, have been derived for the second degree Scheffé polynomial model in q components. Moreover, the symmetric moment conditions which are sufficient to have such slope-rotatability have been found.

Though the slope-rotatability over all directions in the regular simplex is desirable in construction of mixture designs, this property may not be appropriate when the factor space is constrained and the resulting type of design region is an irregular hyperpolyhedron. The problem to construct a mixture design which has a desirable property similar to the slope-rotatability for this general type of design region will be considered in later study.

Appendix

A.1. Proof of Lemma 1.

The average of $\overline{V}(\underline{x})$ over all directions in the (q-1)-dimensional simplex in such a way that the distribution (or probability measure), v, over all possible directions is uniform will be calculated as follws:

$$\begin{aligned}\overline{V}(\underline{x}) &= \int_A \underline{\alpha}' V[\underline{g}(\underline{x})]\underline{\alpha}\, dv = \int_A tr(\underline{\alpha}' V[\underline{g}(\underline{x})]\underline{\alpha})dv \\ &= \int_A tr(V[\underline{g}(\underline{x})]\underline{\alpha}\underline{\alpha}')\, dv = tr(\int_A V[\underline{g}(\underline{x})]\underline{\alpha}\underline{\alpha}' dv) \\ &= tr(V[\underline{g}(\underline{x})] \int_A \underline{\alpha}\underline{\alpha}' dv)\end{aligned}$$

where $A = \{\underline{\alpha}: \underline{\alpha}'\underline{\alpha} = 1$, and $\underline{1}'\underline{\alpha} = \underline{\alpha}'\underline{1} = 0\}$, that is, a (q-2)-dimensional sphere with unit radius. By the symmetry of A,

$$\int_A \alpha_1^2 \, dv = \cdots = \int_A \alpha_q^2 \, dv$$

and

$$\int_A \alpha_1 \alpha_2 \, dv = \cdots = \int_A \alpha_{q-1} \alpha_q \, dv.$$

Since

$$1 = \int_A 1 \, dv = \int_A \underline{\alpha}'\underline{\alpha} \, dv = \int_A \mathrm{tr}(\underline{\alpha}\underline{\alpha}') \, dv$$
$$= \mathrm{tr}\left(\int_A \underline{\alpha}\underline{\alpha}' \, dv\right) = \sum_{i=1}^{q} \int_A \alpha_i^2 \, dv = q\int_A \alpha_i^2 \, dv$$

and

$$0 = \int_A 0 \, dv = \int_A \underline{1}'\underline{\alpha}\underline{\alpha}'\underline{1} \, dv = \underline{1}'\left(\int_A \underline{\alpha}\underline{\alpha}' \, dv\right)\underline{1}$$
$$= \sum_{i=1}^{q} \int_A \alpha_i^2 \, dv + 2\sum_{i=1}^{q} \sum_{j>i}^{q} \int_A \alpha_i \alpha_j \, dv$$
$$= 1 + q(q-1)\int_A \alpha_i \alpha_j \, dv,$$

we can obtain

$$\int_A \alpha_i^2 \, dv = 1/q \quad 1 \leqq i \leqq q$$

and

$$\int_A \alpha_i \alpha_j \, dv = -1/q(q-1), \quad 1 \leqq i < j \leqq q.$$

Therefore,

$$\int_A \underline{\alpha}\underline{\alpha}' \, dv = I_q/(q-1) - \underline{1}\,\underline{1}'/q(q-1).$$

From the above, we can derive the form of $\overline{V}(\underline{x})$ as

$$\begin{aligned}\overline{V}(\underline{x}) &= \int_A \underline{\alpha}' V[\underline{g}(\underline{x})]\underline{\alpha}\, dv \\ &= tr(V[\underline{g}(\underline{x})])/(q-1) - \underline{1}' V[\underline{g}(\underline{x})]\underline{1}/q(q-1) \\ &= \sigma^2 \{ tr[H(\underline{x})(X'X)^{-1}H(\underline{x})'] \\ &\quad -\underline{1}'H(\underline{x})(X'X)^{-1}H(\underline{x})'\underline{1}/q\}/(q-1) \quad \blacksquare\end{aligned}$$

A.2. Proof of Theorem 1.

For the second degree Scheffé polynomial mdoel (1.2), the vector of estimated slopes along the factor axes is obtained in (2.2). After some tedious algebaic calculations, it can be shown that

$$\begin{aligned} tr(H(\underline{x})V(\underline{b})H(\underline{x})') &= \sum_{i=1}^{q} var(\partial\hat{y}(\underline{x})/\partial x_i) \\ &= \sum_{i=1}^{q} var(b_i) + \sum_{j=1}^{q} x_j \sum_{\substack{i=1 \\ i\neq j}}^{q} (2cov(b_i, b^*_{ij}) \\ &\quad + var(b^*_{ij}) + \sum_{\substack{j=1 \\ j\neq k}}^{q} \sum_{k=1}^{q} x_j x_k (\sum_{\substack{i=1 \\ i\neq j,k}}^{q} cov(b^*_{ij}, b^*_{ik}) \\ &\quad - \sum_{\substack{i=1 \\ i\neq j}}^{q} var(b^*_{ij})) \end{aligned}$$

and

$$\begin{aligned} \underline{1}'H(\underline{x})V(\underline{b})H(\underline{x})'\underline{1} &= \sum_{h=1}^{q} \sum_{j=1}^{q} cov(\partial\hat{y}(\underline{x})/\partial x_h, \partial\hat{y}(\underline{x})/\partial x_j) \\ &= tr(H(\underline{x})V(\underline{b})H(\underline{x})') + \sum_{i=1}^{q} \sum_{j=i}^{q} cov(b_i, b_j) + \sum_{j=1}^{q} x_j \{2\sum_{\substack{i=1 \\ i\neq j}}^{q} cov(b_i, b^*_{ij}) \\ &\quad + \sum_{\substack{h=1 \\ h\neq j}}^{q} \sum_{\substack{i=1 \\ i\neq h,j}}^{q} (2cov(b_i, b^*_{hj}) + cov(b^*_{hj}, b^*_{ij}))\} + \sum_{\substack{j=1 \\ j\neq k}}^{q} \sum_{i=1}^{q} x_j x_k \{var(b^*_{jk}) \\ &\quad + \sum_{\substack{i=1 \\ i\neq j,k}}^{q} (cov(b^*_{ij}, b^*_{jk}) + cov(b^*_{ik}, b^*_{ik}) \\ &\quad - \sum_{\substack{h=1 \\ h\neq j}}^{q} \sum_{\substack{i=1 \\ i\neq h,j}}^{q} cov(b^*_{hj}, b^*_{ij})\} \end{aligned}$$

From (2.3), the average of $V(\underline{x})$ over all possible directions can be written as follows:

$$\bar{V}(\underline{x}) = \{ tr\,(H(\underline{x})V(\underline{b})H(\underline{x})') - \underline{1}'H(\underline{x})V(\underline{b})H(\underline{x})'\underline{1}/q\}/(q-1)$$

$$= a + \sum_{j=1}^{q} c(j)x_j + \sum_{\substack{j=1 \\ j\neq k}}^{q} \sum_{k=1}^{q} d(j,k)\, x_j x_k$$

where

$$a = \{ \sum_{i=1}^{q} var(b_i) - 2\sum_{i=1}^{q} \sum_{j>i}^{q} cov(b_i, b_j)/(q-1) \}/q$$

and $c(j)$, $d(j,k)$ are defined as in Theorem 1. If the two conditions stated in the theorem are satisfied, then

$$c(j) = c \text{ for all } j \text{ and } d(j,k) = d \text{ for all } j \neq k,$$

where c and d are some constants, so that

$$\bar{V}(\underline{x}) = a + c\sum_{i=1}^{q} x_i + d\sum_{\substack{i=1 \\ i\neq j}}^{q} \sum_{j=1}^{q} x_i x_j$$

$$= a + c + d\,(1 - \sum_{i=1}^{q} x_i^2)$$

$$= (a + c + d) - d\rho^2$$

which ensures that $\bar{V}(\underline{x})$ is a function only of $\rho^2 = \sum_{i=1}^{q} x_i^2$ If any of the two conditions are not satisfied, then $\bar{V}(\underline{x})$ may be written as

$$\bar{V}(\underline{x}) = a + \sum_{i=1}^{q} c_i x_i + \sum_{\substack{i=1 \\ i\neq j}}^{q} \sum_{j=1}^{q} d_{ij}\, x_i x_j$$

where a, c_i and d_{ij} are arbitrary constants. In such case $\bar{V}(\underline{x})$ can not be a function only of ρ, which denotes the distance from the center point, and there exist two points at the same distance from the center point which yield different values of $\bar{V}(\underline{x})$. Hence the two conditions are necessary. ■

A.3. Proof of Corollary 1.

When the given symmetric moment conditions are satisfied, Murty and Das (1968) showed that the variances and covariances

$var(b_i)$ = v1(A,B,C,D,E,F,G) for all i,
$var(b_{ij})$ = v2(A,B,C,D,E,F,G) for all $i \neq j$,
$cov(b_i, b_j)$= v3(A,B,C,D,E,F,G) for all $i \neq j$,
$cov(b_i, b_{ij}^*)$= v4(A,B,C,D,E,F,G) for all $i \neq j$,
$cov(b_i, b_{jk}^*)$= v5(A,B,C,D,E,F,G) for all $i \neq j \neq k$,
$dov(b_{ij}^*, b_{jk}^*)$= v6(A,B,C,D,E,F,G) for all $i \neq j \neq k$,
$cov(b_{ij}^*, b_{kl}^*)$= v7(A,B,C,D,E,F,G) for all $i \neq j \neq k \neq l$,

where vi(A,B,C,D,E,F,G) denotes a function of constants A, B, C, D, E, F, and G which are given in Corollary 1. Substituting these expressions in c(j) and d(j,k), we can show that

$c(j) = \{(q-1)v2 + 2(q-2)v4 - 2(q-2)v5 - (q-2)v6\} / q$ for all j,
$d(j,k) = \{2(q-2)^2 v6 - (q^2-2q+2)v2 - (q-2)(q-3)v7\} / q(q-1)$ for all $j \neq k$,

where vi is an abbreviation of vi(A,B,C,D,E,F,G). Hence the conditions 1 and 2 of Theorem 1 are all satisfied. ■

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