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ON RESPONSES TO THE SIMPLEX CENTROID DESIGN

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A modification is made to the Simplex-Centroid Design, introduced by Scheffé (1963) and it is applied to the polynomial of third degree.

1. Introduction. This paper is related to the Simplex-Centroid Design introduced by Scheffé [4]. The main features of this design in a q-component mixture in which the proportions $x_1, x_2, \ldots, x_q$ are in the simplex

$$\sum_{i=1}^{q} x_i = 1, \quad x_i \geq 0, \tag{1.1}$$

are the Centroid Polynomial

$$u = \sum_{i=1}^{q} a_i x_i + \sum_{1\leq i<j\leq q} a_{ij} x_i x_j + \sum_{1\leq i<j<k\leq q} + \cdots + \sum_{1\leq i_1<\ldots<i_n\leq q} a_{i_1 i_2 \ldots i_n} x_{i_1} x_{i_2} \cdots x_{i_n} \tag{1.2}$$

as a regression function and the mixtures of one, two, three, ..., q components of equal proportions.

These mixtures are to be used to estimate the coefficients in the polynomial (1.2). The purpose of this design is the empirical prediction of the response to any mixture of the components when the response depends only on the proportions of the components present but not on the total amount of the mixture. D. P. Lambrakis [2] introduced the idea of modificating this design. The modification consists in replacing the mixtures of one component — pure mixtures — by mixtures of $q-1$ components of equal proportions $(q-1)$-nary mixtures.

In this paper the responses $g_{\bar{i}}, f_{\overline{ij}}, w_{\overline{ijk}}$ are used for the estimation of the coefficients of the regration function (1.2) of degree three.

2. Case of $g_{\bar{i}}, f_{\overline{ij}}, w_{\overline{ijk}}$. The polynomial of third degree is

$$u = \sum_{1\leq i\leq q} a_i x_i + \sum_{1\leq i<j\leq q} a_{ij} x_i x_j + \sum_{1\leq i<j<k\leq q} a_{ijk} x_i x_j x_k. \tag{2.1}$$

The mixtures to be used to estimate the coefficients in (2.1) are

a) $(q-1)$-nary $g_{\bar{i}}$ $(1\leq i\leq q)$ with proportions $x_1 = x_2 = \cdots = x_q = 1/(q-1)$, $x_r = 0$, for $r = i$ (total number equal to q);

b) $(q-2)$-nary $f_{\overline{ij}}$ $(1\leq i<j\leq q)$ with proportions $x_1 = x_2 = \cdots = x_q = 1/(q-2)$, $x_r = 0$ for $r = i, j$, (total number equal to $\binom{q}{2}$);

c) $(q-3)$-nary $w_{\overline{ijk}}$ $(1\leq i<j<k\leq q)$ with proportions $x_1 = x_2 = \cdots = x_q = 1/(q-3)$, $x_r = 0$ for $r = i, j, k$, total number equal to $\binom{q}{3}$.

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Taking $r_{\bar{i}}, r_{\overline{ij}}, r_{\overline{ijk}}$ observations for $g_{\bar{i}}, f_{\overline{ij}}$ $w_{\overline{ijk}}$, respectively, and substituting their observed means $\widehat{g}_{\bar{i}}, \widehat{f}_{\overline{ij}}, \widehat{w}_{\overline{ijk}}$ into (2.1) we have the system of normal equations

(2.2)
$$\widehat{g}_{\bar{i}} = \frac{1}{(q-1)} \sum_{r \neq i} \widehat{a}_r + \frac{1}{(q-1)^2} \sum_{r,\, s \neq i} \widehat{a}_{rs} + \frac{1}{(q-1)^3} \sum_{r,\, s,\, t \neq i} \widehat{a}_{rst},$$

(2.3)
$$\widehat{f}_{\overline{ij}} = \frac{1}{(q-2)} \sum_{r \neq i,\, j} \widehat{a}_r + \frac{1}{(q-2)^2} \sum_{r,\, s \neq i,\, j} \widehat{a}_{rs} + \frac{1}{(q-2)^3} \sum_{r,\, s,\, t \neq i,\, j} \widehat{a}_{rst},$$

(2.4)
$$\widehat{w}_{\overline{ijk}} = \frac{1}{(q-3)} \sum_{r \neq i,\, j,\, k} \widehat{a}_r + \frac{1}{(q-3)^2} \sum_{r,\, s \neq i,\, j,\, k} \widehat{a}_{rs} + \frac{1}{(q-3)^3} \sum_{r,s,t \neq i,j,k} \widehat{a}_{rst}.$$

The main problem is the determination of the estimates $\widehat{a}_i, \widehat{a}_{ij}, \widehat{a}_{ijk}$ by solving the system (2.2)—(2.4).

We receive the estimates of a_i, a_{ij}, a_{ijk} from the expressions

(2.5)
$$\widehat{a}_i = \Sigma \widehat{a}_r - \sum_{r \neq i} \widehat{a}_r,$$

(2.6)
$$\widehat{a}_{ij} = \Big(\Sigma \widehat{a}_{rs} + \sum_{r,\, s \neq i,\, j} \widehat{a}_{rs} \Big) - \Big(\sum_{r,\, s \neq i} \widehat{a}_{rs} + \sum_{r,\, s \neq i} \widehat{a}_{rs} \Big),$$

(2.7)
$$\widehat{a}_{ijk} = \Big(\Sigma \widehat{a}_{rst} + \sum_{r,\, s,\, t \neq i,\, j} \widehat{a}_{rst} + \sum_{r,\, s,\, t \neq j,k} \widehat{a}_{rst} + \sum_{r,\, s,\, t \neq i,\, k} \widehat{a}_{rst} \Big)$$
$$- \Big(\sum_{r,\, s,\, t \neq i} \widehat{a}_{rst} + \sum_{r,\, s,\, t \neq j} \widehat{a}_{rst} + \sum_{r,\, s,\, t \neq k} \widehat{a}_{rst} + \sum_{r,\, s,\, t \neq i,\, j,\, k} \widehat{a}_{rst} \Big).$$

3. Solution of the system (2.2)—(2.5). Equation (2.2) is actually a system of q equations. If we write down explicitly all these equations we observe that each element $\widehat{a}_r (1 \leq r \leq q)$ appears in the system $(q-1)$ times, $\widehat{a}_{rs} (1 \leq r < s \leq q)$ and $\widehat{a}_{rst} (1 \leq r < s < t \leq q)$ respectively $(q-2)$ and $(q-3)$ times. If we add all the equations mentioned above we have the equation

(A.1)
$$\Sigma \widehat{g} = \Sigma \widehat{a}_r + \frac{(q-2)}{(q-1)^2} \Sigma \widehat{a}_{rs} + \frac{(q-3)}{(q-1)^2} \Sigma \widehat{a}_{rst}.$$

Equation (2.3) is actually a system of $\binom{q}{q-2} = \binom{q}{2}$ equations. If we write all of them we observe that each element $\widehat{a}_r$ $(1 \leq r \leq q)$ appears in the system $(q-1)(q-2)/2$ times, $\widehat{a}_{rs}$ $(1 \leq r < s \leq q)$ appears $(q-2)$ $(q-3)/2$ times and $\widehat{a}_{rst}$ $(1 \leq r < s < t \leq q)$ appears $(q-3)(q-4)/2$ times. If we add all these equations we receive the equation

(A.2)
$$\Sigma \widehat{f} = \frac{(q-1)}{2} \Sigma \widehat{a}_r + \frac{(q-3)}{2(q-2)} \Sigma \widehat{a}_{rs} + \frac{(q-3)(q-4)}{2(q-2)^3} \Sigma \widehat{a}_{rst}.$$

Similarly, equation (2.4) is actually a system of $\binom{q}{q-3} = \binom{q}{3}$ equations. If we write all of them we observe that each element $\widehat{a}_r (1 \leq r \leq q)$ appears in the system $(q-1)(q-2)(q-3)/6$ times, $\widehat{a}_{rs} (1 \leq r < s \leq q)$ appears $(q-2)(q-3)(q-4)/6$ times and $\widehat{a}_{rst}$ $(1 \leq r < s < t \leq q)$ appears $(q-3)(q-5)(q-4)/6$ times. If we add all these equations we get the new equation

(A.3) $$\Sigma\widehat{w}=\frac{(q-1)(q-2)}{6}\Sigma\widehat{a}_r+\frac{(q-2)(q-4)}{}\Sigma\widehat{a}_{rs}+\frac{(q-4)(q-5)}{6(q-3)^2}\Sigma\widehat{a}_{rst}.$$

From (2.3) we can form a system of $(q-1)$ equations where the left side of each equation is a mixture of $q-2$ components of equal proportions and not containing one component x_i $(1\leq i\leq q)$.

If we write all these equations we observe that the elements $\widehat{a}_r$ $(r\neq i)$, $\widehat{a}_{rs}$ $(r, s\neq i)$, $\widehat{a}_{rst}$ $(r, s, t\neq i)$ are contained in the system, resp. $q-2$, $q-3$ and $q-4$ times. If we add all these equations we get the equation

(A.4) $$\Sigma\widehat{f}=\sum_{r\neq i}\widehat{a}_r+\frac{(q-3)}{(q-2)^2}\sum_{r,s\neq i}\widehat{a}_{rs}+\frac{(q-4)}{(q-3)^3}\sum_{r,s,t\neq i}\widehat{a}_{rst}.$$

From equation (2.4) we can form a system of $(q-1)$ equations, where the left side of each equation is a mixture of $q-3$ components of equal proportions and not containing one component x_i $(1\leq i\leq q)$. If we write all these equations we observe that the elements $\widehat{a}_r$ $(r\neq i)$, $\widehat{a}_{rs}$, $(r, s\neq i)$, $\widehat{a}_{rst}$ $(r, s, t\neq i)$ are contained in the system resp. $q-3$, $(q-3)(q-4)/(q-2)$ and $(q-4)(q-5)/(q-2)$ times. If we add all these equations we receive the equation

(A.5) $$\Sigma\widehat{w}=\sum_{r\neq i}\widehat{a}_r+\frac{(q-4)}{(q-2)(q-3)}\sum_{r,s\neq i}\widehat{a}_{rs}+\frac{(q-4)(q-5)}{(q-2)(q-3)^3}\sum_{r,s,t\neq i}\widehat{a}_{rst}.$$

We already have the equation (2.2)

$$\widehat{g}_i=\frac{1}{(q-1)}\sum_{r\neq i}\widehat{a}_r+\frac{1}{(q-1)^2}\sum_{r,s\neq i}\widehat{a}_{rs}+\frac{1}{(q-1)^3}\sum_{r,s,t\neq i}\widehat{a}_{rst}.$$

If we solve the system of (A.1) — (A.3) we receive $\Sigma\widehat{a}_r$, $\Sigma\widehat{a}_{rs}$, $\Sigma\widehat{a}_{rst}$, where by solving the system of (2.2), (A.4), (A.5) we get the

$$\sum_{r\neq i}\widehat{a}_r,\quad\sum_{r,s\neq i}\widehat{a}_{rs},\quad\sum_{r,s,t\neq i}\widehat{a}_{rst}.$$

Thus, we have (2.5) — (2.7).

REFERENCES

1. E. G. Konstantelos. Experiments with mixtures, another extension of the modification to the simplex-centroid design. *Sci. Ann., Fac. Phys. Math., Univ. Thessaloniki*, **15**, 1975, 213—221.
2. D. P. Lambrakis. Designs for experiments with mixtures. *Ph. D. Thesis*, University of Aberteen, 1966.
3. M. H. Quenouille. Experiments with mixtures. *J. Roy. Statist. Soc., B*, **21**, 1959, 201—202.
4. H. Scheffe. Experiments with mixtures. *J. Roy. Statist. Soc., B*, **20**, 1958, 344—360.

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