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Response Surface Fitting Using a Generalization of the Bradley–Terry Paired Comparison Model

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Summary

A paired comparison technique is presented for fitting response surfaces. This is especially useful when subjective responses are involved, where it is often difficult to justify the basic assumptions of the classical procedure.

This report discusses aspects of the estimation of parameters and their properties, tests of relevant hypotheses and the selection of experimental designs. The method is applied to an example in food testing.

Keywords: PAIRED-COMPARISON; RESPONSE SURFACE

1. Introduction

Paired comparison techniques have been used for many years for the subjective comparison of several treatments (David, 1963), and extensions are available for the comparison of factorial treatment combinations. This report presents a further extension of the paired comparison method, the analogue of multiple regression analysis. Although it is possible to formulate a general paired comparison regression model this report will concentrate on the analogue of multiple linear regression mainly because of its application to response surface fitting.

In the field of sensory assessment, it is frequently required to determine the effect of varying product composition. The classical response surface approach is useful here, despite many of its basic assumptions being invalid in the sensory situation, but occasionally it becomes virtually impossible to implement the classical method, particularly when carry-over and sensory organ fatigue effects are present. The degree to which these affect the results depends on the sense used, taste and smell being usually the more prone. Classical response surface designs, even with blocking, frequently require more units than may be reliably assessed in one sensory assessment session. Further, the assessors may not, due to the above effects—and others—be able reliably to score their impressions on a continuous scale. If any of these factors is present, the method of paired comparisons becomes extremely useful.

A number of models have been proposed for the analysis of paired comparison data in the analogue of one-way analysis of variance. The specific analogue one-way ANOVA paired comparison model which this paper adapts to analogue multiple regression is that due to Rao and Kupper (1967), itself a generalization of the Bradley–Terry model (1952). A parallel generalization of the Bradley–Terry model, due to Davidson (1970), could also be extended for the present purpose in an exactly similar manner.

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2. The Model

In the method of paired comparisons, t items are presented to assessors in pairs. Each assessor gives his judgement concerning which one of the pair possesses more of the particular attribute under study. We assume that the judgements are located along a single dimension and that the actual response perceived by an assessor comes from a logistic distribution having the "true" score as its mean.

Let V_i be the perceived response of the assessors and μ_i the "true" score. For the Bradley–Terry model

$$p_{ij} = \Pr\{V_i > V_j\} = \frac{1}{4}\int_{-(\mu_i-\mu_j)}^{\infty} \operatorname{sech}^2(y/2)\,dy. \tag{2.1}$$

It will be noticed that no assumptions have been made concerning the structure, if any, of the "true" scores μ_i. For the purpose of this report we shall assume that they are functions of continuous independent variables, $x_1, \ldots, x_s$, measurable without error, i.e. $\mu_i = f(x_{1i}, x_{2i}, \ldots, x_{si}) = f(\mathbf{x}_i)$.

By analogy with the classical regression situation, the form of $f(\mathbf{x}_i)$ which is most useful is that which is linear in the unknown parameters, i.e.

$$f(\mathbf{x}_i) = \sum \beta_k x_{ki}. \tag{2.2}$$

We can fit a large range of surface types by allowing some of the x_{ki}'s to be functions of the others, e.g.

(i) $f(\mathbf{x}_i) = \beta_1 x_{1i} + \beta_2 x_{1i}^2$, where $s = 2$, $x_{1i} = x_{1i}$ and $x_{2i} = x_{1i}^2$,

(ii) $f(\mathbf{x}_i) = \beta_1 x_{1i} + \beta_2 x_{2i} + \beta_3 x_{1i}^2 + \beta_4 x_{2i}^2 + \beta_5 x_{1i} x_{2i}$, where $s = 5$, $x_{1i} = x_{1i}$, $x_{2i} = x_{2i}$, $x_{3i} = x_{1i}^2$, $x_{4i} = x_{2i}^2$ and $x_{5i} = x_{1i} x_{2i}$,

(iii) $f(\mathbf{x}_i) = \beta_1 x_{1i} + \beta_2 e^{x_{1i}}$, where $s = 2$, $x_{1i} = x_{1i}$ and $x_{2i} = e^{x_{1i}}$.

Notice that a constant has not been included since it would be inestimable.

Rao and Kupper (1967) have proposed an extension of the Bradley–Terry model which allows for ties and in combination with (2.2) this gives

$$p_{i.ij} = \Pr\{V_i > V_j\} = \frac{1}{4}\int_{-\Sigma\beta_k(x_{ki}-x_{kj})+\eta}^{\infty} \operatorname{sech}^2(y/2)\,dy, \quad i,j = 1, \ldots, t, \quad i \neq j$$

$$p_{0.ij} = \Pr\{V_i = V_j\} = \frac{1}{4}\int_{-\Sigma\beta_k(x_{ki}-x_{kj})-\eta}^{-\Sigma\beta_k(x_{ki}-x_{kj})+\eta} \operatorname{sech}^2(y/2)\,dy, \tag{2.3}$$

where η is the threshold of perception for the judges. The parameter $\theta = e^{\eta}$ will be used extensively throughout the rest of this paper.

3. Point Estimation of θ and β_i ($i = 1, \ldots, s$)

θ and β_i can be estimated by the method of maximum likelihood. The experimental design compares t treatments, each generating s independent variables $x_1, \ldots, x_s$. Each of the $\binom{t}{2}$ paired comparisons is replicated r_{ij} times where (i,j) are the treatments for that pair. The following notation will be used:

$n_{i.ij}$ is the number of times treatment combination i is thought to possess more of the target property than treatment combination j.

$n_{0.ij}$ is the number of times treatment combinations i and j are thought to possess equal values of the target property. Clearly $r_{ij} = n_{i.ij} + n_{0.ij} + n_{j.ij}$. Let

$$m_{ij} = n_{0.ij} + n_{i.ij}, \quad m_i = \sum_{j \neq i} m_{ij}, \quad n_0 = \sum\sum_{i<j} n_{0.ij} \quad \text{and} \quad N = \sum\sum_{i<j} r_{ij}.$$

The log-likelihood of the observed experiment is

$$\ln \mathscr{L} = n_0 \ln(\theta^2-1) + \sum_i m_i \sum_k x_{ki} \ln \pi_k - \sum\sum_{i\neq j} m_{ij} \ln(p_i + \theta p_j) \tag{3.1}$$

where

$$p_i = \prod_k \pi_k^{x_{ki}}, \quad \pi_k = e^{\beta_k}, \quad i,j = 1,\ldots,t, \quad k = 1,\ldots,s.$$

The traditional way of maximizing $\ln \mathscr{L}$ is to differentiate with respect to the parameters and solve the resulting equations iteratively. In this case, the equations to be solved are

$$\sum\sum_{i\neq j} \{m_{ij} p_j(x_{ri}-x_{rj})/(p_i+\theta p_j)\} = 0, \quad r = 1,\ldots,s, \tag{3.2}$$

$$2n_0\, \theta/(\theta^2-1) - \sum\sum_{i\neq j} m_{ij} p_j/(p_i+\theta p_j) = 0. \tag{3.3}$$

The estimates obtained from these equations, however, converge extremely slowly and, in the absence of an alternative method, resort must be made to more general maximization procedures. The author has found the Rosenbrock constrained method (1960), with starting values $\hat{\beta}_k = 0$ $(k = 1,\ldots,s)$ and $\hat{\theta} = (N+n_0)/(N-n_0)$, quite satisfactory for this purpose. Problems involving six parameters and nine design points have been found to take about 1 minute on an IBM 360/50 and no problems involving local maxima have been encountered.

4. Asymptotic Variance–Covariance Matrix of the Parameters

This matrix is required in order to place confidence limits on the parameters and to examine the properties of possible experimental designs. Using a method similar to that of Rao and Kupper (1967) the following result may readily be obtained: $(\hat{\theta}-\theta), (\hat{\pi}_1-\pi_1), \ldots, (\hat{\pi}_r-\pi_r), \ldots, (\hat{\pi}_s-\pi_s)$ have the asymptotic $(s+1)$-variate normal distribution with zero means and variance–covariance matrix $(\lambda_{ij})^{-1}$ $(i,j = 0,1,2,\ldots,s)$, where

$$\lambda_{00} = 2n_0(\theta^2+1)/(\theta^2-1)^2 - \sum\sum_{i<j} r_{ij}\,\phi_{ij}\,\theta^{-1}, \tag{4.1}$$

$$\lambda_{0r} = \frac{1}{\pi_r}\sum\sum_{i<j} r_{ij}\,\phi_{ij}\,\theta^{-1}(x_{rj}-x_{ri}), \tag{4.2}$$

$$\lambda_{lr} = \frac{1}{\pi_r\pi_l}\sum\sum_{i<j} r_{ij}\,\phi_{ij}(x_{rj}-x_{ri})(x_{lj}-x_{li}), \tag{4.3}$$

$$\lambda_{rr} = \frac{1}{\pi_r^2}\sum\sum_{i<j} r_{ij}\,\phi_{ij}(x_{rj}-x_{ri})^2, \tag{4.4}$$

where

$$\phi_{ij} = \theta^2 p_i p_j\{\theta(p_i^2+p_j^2)+2p_ip_j\}/\{(p_i+\theta p_j)(\theta p_i+p_j)\}^2. \tag{4.5}$$

A more directly useful result is the following:

$(\hat{\theta}-\theta), (\hat{\beta}_1-\beta_1), \ldots, (\hat{\beta}_s-\beta_s)$ have the asymptotic $(s+1)$-variate normal distribution with zero means and variance–covariance matrix $(\lambda'_{ij})^{-1}$ $(i,j = 0,1,\ldots,s)$, where

$$\lambda'_{00} = \lambda_{00}, \quad \lambda'_{0r} = \lambda_{0r}/\pi_r, \quad \lambda'_{lr} = \lambda_{lr}/(\pi_l\pi_r), \quad \lambda'_{rr} = \lambda_{rr}/\pi_r^2.$$

This follows from the previous result using Hald (1952, p. 164).

5. Experimental Designs

Designs having properties based on the elements of the variance–covariance matrix of the parameters $\theta, \beta_1, \ldots, \beta_s$ can be evaluated using the results of Section 4.

5.1. *Analogue Designs*

These are designs in which the elements of the paired comparison variance–covariance matrix are proportional to the elements of the classical response surface variance–covariance matrix with the same design points. The advantage of such designs is that they enable certain desirable properties of classical response surface designs (e.g. rotatability, orthogonality, uniform information) to be readily reproduced.

Theorem 5.1. If a classical response surface design has certain properties dependent on the relative sizes of the elements of the variance–covariance matrix then the analogue paired comparison response surface design (*B–T*) has approximately the same properties if

$$r_{ij} = \left[N \left\{ \phi_{ij} \sum_{k<l}\sum \phi_{kl}^{-1} \right\}^{-1} + 0{\cdot}5 \right], \tag{5.1}$$

where $[x]$ indicates the integral part of x and $N = \sum\sum_{i>j} r_{ij}$ (this would be chosen in advance). The properties are exactly obtained if all r_{ij} are integers before the integerization stage.

Proof.

$$\begin{aligned} e_{lr}\{(\lambda'_{lr})\} &= \text{element } (l,r) \text{ of matrix } (\lambda'_{lr}) \\ &= \sum_{i<j}\sum r_{ij}\, \phi_{ij}(x_{rj} - x_{ri})\,(x_{lj} - x_{li}). \end{aligned}$$

Let us allow the r_{ij} to take any positive real values. Then for a given value of N we can select values of r_{ij} such that

$$r_{ij}\,\phi_{ij} = K, \quad \text{for any } i,j,$$

where K is some constant and $N = \sum\sum_{i>j} r_{ij}$.
Hence

$$\begin{aligned} e_{lr}\{(\lambda'_{lr})\} &= K \sum_{i>j}\sum (x_{rj} - x_{ri})\,(x_{lj} - x_{li}) \\ &= 0{\cdot}5Kt \left\{ \sum_i x_{ri}\, x_{li} - t^{-1} \sum_i \sum_j x_{rj}\, x_{li} \right\} \\ &= 0{\cdot}5Kt \left\{ \sum_i (x_{ri} - \bar{x}_r)\,(x_{li} - \bar{x}_l) \right\}. \end{aligned} \tag{5.2}$$

Thus for the selected set of r_{ij}'s, the elements of $(\lambda'_{lr})^{-1}$ are proportional to the elements of the equivalent classical response surface variance–covariance matrix. In order to determine the r_{ij} we note that

$$N = \sum_{k<l}\sum r_{kl} = \sum_{k<l}\sum K\phi_{kl}^{-1}.$$

Therefore

$$K = N \left\{ \sum_{k<l}\sum \phi_{kl}^{-1} \right\}^{-1}$$

and

$$r_{ij} = N\left\{\phi_{ij} \sum\sum_{k<l} \phi_{kl}^{-1}\right\}^{-1}. \tag{5.3}$$

Of course, the r_{ij} must be integral and hence the property is only approximately true. The larger the value of N, the more valid is the approximation.

Lemma. If all the regression coefficients β_i are zero, so $p_i = 1$, then an analogue design is obtained by assessing each pair an equal number of times.

Proof. Since $\beta_i = 0$, for any i, then $p_i = 1$, for any i. Hence

$$\phi_{ij} = 2\theta^2/(\theta+1)^3.$$

Therefore

$$r_{ij} = \left\{0{\cdot}5N\theta^{-2}(\theta+1)^3 \left(0{\cdot}5\theta^{-2} \sum\sum_{k<l} (\theta+1)^3\right)^{-1}\right\}$$

$$= N\bigg/\binom{t}{2}.$$

The analogue design obtained using Theorem 5.1 is one of many and does not necessarily provide the variance–covariance matrix with the smallest elements. An additional complication is that restrictions may have to be placed on the design, e.g. material limitations on certain treatments. A more flexible method of obtaining analogue designs is required therefore and a method will be presented here which uses linear programming techniques. The properties of the designs so obtained, other than those directly connected with the variance–covariance matrix, (e.g. bias, robustness) are beyond the scope of this paper.

5.2. *A Design Formulation*

In the following, only the properties of the β_i $(i = 1, \ldots, s)$ will be considered. The extension to include the parameter θ is obvious.

Using equations (4.3) and (4.4), we may write

$$\begin{bmatrix} \lambda'_{11} \\ \lambda'_{12} \\ \vdots \\ \lambda'_{lr} \\ \vdots \\ \lambda'_{ss} \end{bmatrix} =$$

$$\begin{bmatrix} \phi_{12}(x_{11}-x_{12})^2 & \phi_{13}(x_{11}-x_{13})^2 & \cdots & \phi_{t-1,t}(x_{1,t-1}-x_{1t})^2 \\ \cdots & \cdots & \cdots & \cdots \\ \phi_{12}(x_{r1}-x_{r2})(x_{l1}-x_{l2}) & \cdots & \cdots & \phi_{t-1,t}(x_{r,t-1}-x_{r,t})(x_{l,t-1}-x_{lt}) \\ \cdots & \cdots & \cdots & \cdots \end{bmatrix} \begin{bmatrix} r_{12} \\ r_{13} \\ \vdots \\ r_{t-1,t} \end{bmatrix}$$

or

$$\boldsymbol{\lambda}' = Z\mathbf{r}. \tag{5.4}$$

Let λ^*_{ij} be the elements of the inverse of the variance–covariance matrix in the classical response surface case. Then, using obvious notation, we require a set of r_{ij} such that

$$c\boldsymbol{\lambda}^* = Z\mathbf{r}, \tag{5.5}$$

subject to the restriction that $\sum\sum_{i<j} r_{ij} = N$, where c is an unknown constant of proportionality.

This may be considered as an integer programming problem with $s(s+1)/2$ simultaneous objective functions. Many linear programming computer programs have facility for simultaneous objective functions and, provided N is large, these may be used to obtain a design which is very close to that having the variance–covariance matrix with the smallest elements.

Example

Consider the unidimensional model

$$y = \beta_1 x + \beta_2 x^2$$

The design coordinates chosen (after coding) are

$$x = -2,\ -1,\ 1,\ 2.$$

The elements of the inverse of the variance–covariance in the classical response surface case are proportional to $\lambda^*_{11} = 10$, $\lambda^*_{22} = 9$ and $\lambda^*_{12} = 0$.

If we assume that $\theta = 1$ and $\beta_i = 0$, for any i and set $N = 150$, then equations (5.5) become

$$\begin{bmatrix} 10c \\ 9c \\ 0 \end{bmatrix} = \begin{bmatrix} 1 & 9 & 16 & 4 & 9 & 1 \\ 9 & 9 & 0 & 0 & 9 & 9 \\ -3 & -9 & 0 & 0 & 9 & 3 \end{bmatrix} \begin{bmatrix} r_{12} \\ r_{13} \\ r_{14} \\ r_{23} \\ r_{24} \\ r_{34} \end{bmatrix}, \tag{5.6}$$

subject to the constraint

$$r_{12}+r_{13}+r_{14}+r_{23}+r_{24}+r_{34} = 150. \tag{5.7}$$

By the lemma to Theorem 5.1 an analogue design is given when $r_{ij} = 150/6 = 25$ for all i,j. This can be seen to satisfy (5.6) and (5.7) with $c = 100$.

An alternative analogue design may be obtained by using linear programming with (5.6) as the simultaneous objective functions to be maximized and (5.7) as the constraint. The solution obtained by this method is: $r_{12} = 0$, $r_{13} = 70{\cdot}59$, $r_{14} = 8{\cdot}82$, $r_{23} = 0$, $r_{24} = 70{\cdot}59$ and $r_{34} = 0$ with $c = 141{\cdot}2$. After integerization, we have the following design: $r_{12} = 0$, $r_{13} = 71$, $r_{14} = 9$, $r_{23} = 0$, $r_{24} = 70$ and $r_{34} = 0$. This design has, ignoring the slight modification due to the integerization, the variance–covariance matrix with the smallest elements of any analogue design and hence might be suitable for a particular experiment on this basis alone. However, the equi-replication design obtained using Theorem 5.1 may have other properties (e.g. robustness to the assumption of the magnitude of the β's and θ) which in other circumstances make it a better choice. As stated earlier, such considerations are beyond the scope of this paper.

6. Tests of Hypotheses

6.1. *Test of the Parameters* β_i

The null hypothesis H_0: $\beta_k = 0$ for all k is to be tested against the alternative that at least one of the β_k is non-zero, viz. H_A: $\beta_k \neq 0$ for some k.

Under H_0, equation (3.3) becomes

$$\frac{d\ln\mathscr{L}}{d\theta} = 2\theta n_0/(\theta^2-1) - \sum_{i\neq j}\sum m_{ij}/(\theta+1).$$

Now $\sum\sum_{i\neq j} m_{ij} = N+n_0$, hence $\hat{\theta}' = (N+n_0)/(N-n_0)$, where $\hat{\theta}'$ is the estimate of θ under H_0. Therefore

$$\ln\mathscr{L}_w = n_0 \ln(\hat{\theta}'^2-1) - (N+n_0)\ln(1+\hat{\theta}')$$

If $\mathscr{L}_\Omega$ is the likelihood when (3.1) is maximized with respect to all parameters, then using the generalized likelihood ratio approach, the test statistic

$$T_1 = 2\ln\mathscr{L}_w - 2\ln\mathscr{L}_\Omega$$

has, under H_0 and for large N, an asymptotic χ^2 distribution with s degrees of freedom.

6.2. *Test of Parameter* θ

The null hypothesis H_0: $\theta = \theta_0$ is to be tested against the alternative H_A: $\theta \neq \theta_0$.

Using the generalized likelihood ratio approach, the test statistic

$$T_2 = 2\ln\mathscr{L}_{\theta=\theta_0} - 2\ln\mathscr{L}_{\theta=\hat{\theta}}$$

has, under H_0 and for large N, an asymptotic χ^2 distribution with one degree of freedom, where $\ln\mathscr{L}_{\theta=\theta_0}$ is equation (3.1) maximized with respect to β_i, for all i and $\theta = \theta_0$, and $\ln\mathscr{L}_{\theta=\hat{\theta}}$ is equation (3.1) maximized with respect to all parameters.

6.3. *Test of the Total Model*

We require to test the suitability of the Bradley–Terry model and the chosen regression model in a particular application. The χ^2 goodness-of-fit test is concerned with testing the entire model and in this case the appropriate test statistic is

$$\chi^2 = \sum_{i<j}\sum \left\{\frac{(n_{i.ij} - r_{ij}\hat{p}_{i.ij})^2}{r_{ij}\hat{p}_{i.ij}} + \frac{(n_{j.ij} - r_{ij}\hat{p}_{j.ij})^2}{r_{ij}\hat{p}_{j.ij}} + \frac{(n_{0.ij} - r_{ij}\hat{p}_{0.ij})^2}{r_{ij}\hat{p}_{0.ij}}\right\}$$

where

$$\hat{p}_{i.ij} = \hat{p}_i(\hat{p}_i + \hat{\theta}\hat{p}_j)^{-1}$$

and

$$\hat{p}_{0.ij} = \hat{p}_i\hat{p}_j(\hat{\theta}^2-1)\{(\hat{p}_i+\hat{p}_j\,\hat{\theta})(\hat{\theta}\hat{p}_i+\hat{p}_j)\}^{-1}$$

with obvious notation.

This statistic is approximately distributed as a χ^2 distribution with $\{t(t-1)-s-1\}$ degrees of freedom, for large samples. The closer $r_{ij}\hat{p}_{i.ij}$ is to $n_{i.ij}$ for all (i,j), the more accurate is the χ^2 approximation.

6.4. *Other Tests*

The generalized likelihood ratio approach may be used to obtain tests of other hypotheses, e.g. parallel surfaces, equality of threshold parameters between several experiments and order of assessing. Details will be omitted since the approach should be obvious from Sections 6.1 and 6.2.

7. Example

A 3^2 factorial design is used to determine the effect of varying gel and flavour concentration on the subjective evaluation of flavour strength. Previous results indicated that it would be sufficient to evaluate each pair of treatments an equal number of times. The experimental design coordinates were as given in Table 1.

Table 1

No.	1	2	3	4	5	6	7	8	9
x_1 = Flavour concentration (ml/l·2 l)	0·6	4·8	9·0	0·6	4·8	9·0	0·6	4·8	9·0
x_2 = Gel concentration (g/l)	0·0	0·0	0·0	2·4	2·4	2·4	4·8	4·8	4·8

Assessors were asked to state which sample of each pair had the lesser flavour strength, a decision of "no difference" being allowed. The results obtained are shown in Table 2. The first number in each cell is the number of assessors who said that the row sample had a higher flavour strength than the column sample. The second number in the upper triangle gives the number of ties.

Table 2

	1	2	3	4	5	6	7	8	9
1		2, 7	0, 1	5, 10	2, 7	0, 2	12, 9	13, 5	10, 3
2	16		6, 5	17, 7	9, 8	8, 6	24, 0	16, 5	15, 7
3	21	11		22, 4	14, 5	11, 7	24, 3	22, 3	17, 6
4	10	2	2		3, 9	2, 4	12, 5	10, 6	8, 11
5	15	6	4	14		5, 9	20, 2	15, 5	13, 9
6	22	12	4	18	11		27, 0	19, 5	18, 2
7	3	2	1	6	0	1		2, 8	2, 5
8	9	3	0	6	2	1	13		6, 8
9	12	2	2	9	5	2	21	8	

The fitted quadratic response surface is given by

$$y = -0{\cdot}432x_1 + 0{\cdot}016x_1^2 - 0{\cdot}359x_2 + 0{\cdot}116x_2^2 + 0{\cdot}025x_1 x_2$$

with $\theta = 2{\cdot}00$. Fig. 1 is a plot of this surface.

The test of the quadratic fit gave $T_1 = 431{\cdot}3$ with 5 degrees of freedom, significant at the 0·1 per cent level; and the test of the overall model lack of fit gave $T_2 = 49{\cdot}4$ with 66 degrees of freedom (non-significant).

The variance–covariance matrix of the parameters is given in Table 3, which gives the following 95 per cent confidence interval on each of the fitted parameters:

$$-0{\cdot}660 \leqslant \beta_1 \leqslant -0{\cdot}204,$$
$$-0{\cdot}006 \leqslant \beta_{11} \leqslant 0{\cdot}038,$$
$$-0{\cdot}716 \leqslant \beta_2 \leqslant -0{\cdot}001,$$
$$0{\cdot}047 \leqslant \beta_{22} \leqslant 0{\cdot}186,$$
$$-0{\cdot}004 \leqslant \beta_{12} \leqslant 0{\cdot}053,$$
$$1{\cdot}86 \leqslant \theta \leqslant 2{\cdot}14.$$

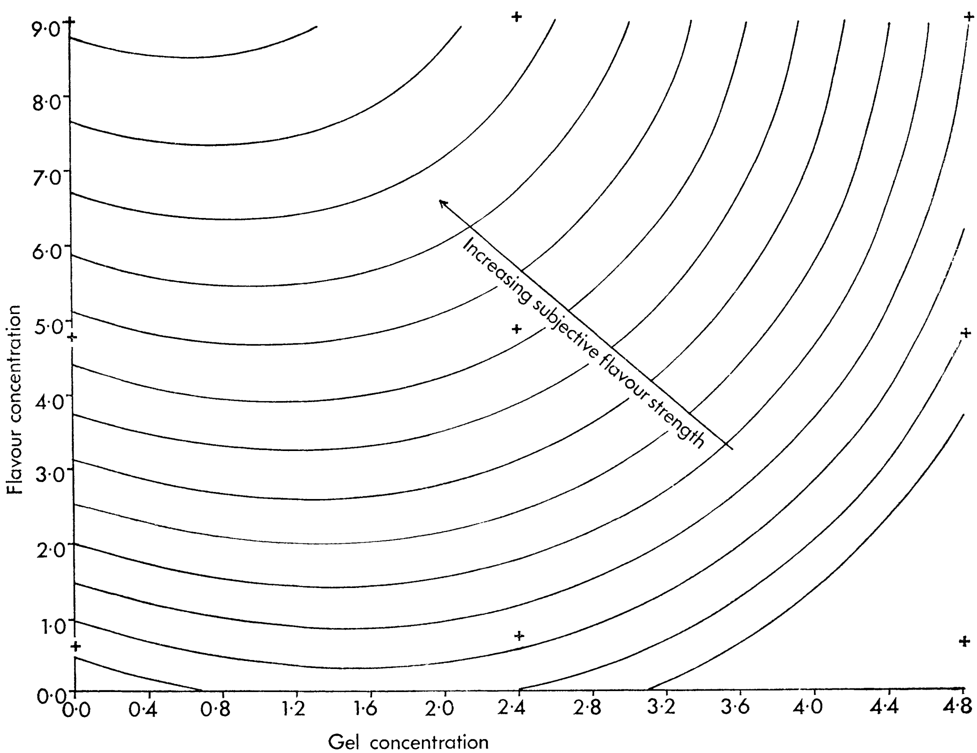

FIG. 1. Gel–flavour paired comparison response surface. Contours join points of equal subjective flavour strength.

The approximate analogue design given by Theorem 5.1 based on the fitted values of the parameters is as shown in Table 4.

The aim of this experiment was to describe the response surface; hence, an analogue design requiring extra comparisons between those design points having the most widely differing responses (e.g. (3, 4)) is reasonable. Where the aim is to find alternative compositions for an existing product, greater precision is required between design points having similar responses. The linear programming approach would be useful here in order to construct a design for this particular purpose.

TABLE 3

	β_1	β_{11}	β_2	β_{22}	β_{12}	θ
β_1	0·01353	−0·00119	0·00252	−0·00023	−0·00042	−0·00096
β_{11}	−0·00119	0·00013	0·00001	0·00002	−0·00001	0·00004
β_2	0·00252	0·00001	0·03330	0·00570	−0·00086	−0·00080
β_{22}	−0·00023	0·00002	−0·00570	0·00125	−0·00003	0·00026
β_{12}	−0·00042	−0·00001	−0·00086	−0·00003	0·00021	0·00005
θ	−0·00096	0·00004	−0·00080	0·00026	0·00005	0·00492

TABLE 4

1	2	3	4	5	6	7	8	9	
	21	35	16	20	28	18	16	16	1
		18	20	16	16	38	22	18	2
			32	18	16	80	37	28	3
				19	26	19	16	16	4
					17	36	21	18	5
						60	29	23	6
							18	20	7
								16	8
									9

8. DISCUSSION

The method presented here, besides being subject to the usual limitations of paired comparison methods, requires rough estimates of the parameters in order to obtain the desired variance–covariance matrix. Provided the surface is fairly flat, a reasonable variance–covariance matrix will be obtained if all pairs are replicated the same number of times. However, in surfaces with steep gradients, ill-conditioned variance–covariance matrices could be obtained by using an equally replicated design. A solution to this problem would be to run a small experiment to obtain rough parameter estimates before carrying out the full-scale trial.

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