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APPLICATIONS OF THE FACTORIAL CALCULUS TO GENERAL UNEQUAL NUMBERS ANALYSES

W. T. Federer and M. Zelen

MRC Technical Summary Report #393
April 1963

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ABSTRACT

The necessary elements of the calculus for factorials as developed by Kurkjian and Zelen are described, modified where necessary, and applied to the analysis of unbalanced n-way classifications with fixed effects. Estimators for all main effect and interaction effects parameters are obtained along with the associated variances. The sums of squares for each effect eliminating all other effects is presented in a form suitable for direct computation. This form results in considerable computational saving over the method of fitting constants used in general regression theory. The results are applied to the particular case of proportional frequencies in the subclasses.

APPLICATIONS OF THE FACTORIAL CALCULUS TO GENERAL UNEQUAL NUMBERS ANALYSES[1]

W. T. Federer[2,3] and M. Zelen[3]

1. Introduction

This paper is the second in a series of papers which applies the calculus for factorial arrangements developed by Kurkjian and Zelen [1962] to various problems in the analysis of experiment designs. The first paper dealing with applications [1963] was devoted to the analysis of block and direct product designs. The main object of this paper is to apply this special calculus to an alternate way of treating the analysis of variance with unequal numbers. The usual way this is done is by the method of fitting constants; cf Federer [1957], Yates [1934]. The use of the special methods developed here leads to substantial computational savings over the method of fitting constants.

Section two of this paper contains the necessary parts of the factorial calculus which is the starting point of our investigation. Section three develops the general theory for unequal numbers and section four shows the resulting simplification when the frequencies are proportional.

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[2] On sabbatic leave from Cornell University.

[3] Mathematics Research Center, U. S. Army.

2. Elements of the Factorial Calculus

The notation and special operations used in this paper will be a modified version of the calculus for factorial arrangements introduced in Kurkjian and Zelen [1962]. The modifications are straightforward generalizations which are useful in treating the case of unequal numbers.

Consider a factorial experiment with the n factors $\{A_s\}$ such that factor A_s has m_s levels for $s = 1, 2, \ldots, n$. The i^{th} treatment combination consists of the n-tuple $i = (i_1, i_2, \ldots, i_n)$ where i_s denotes a particular level from factor A_s. The number of treatment combinations is $v = \prod_{s=1}^{n} m_s$. Let Y denote a $v \times 1$ random vector following a multivariate normal distribution with

$$E(Y) = \mathbf{1}\mu + t \tag{2.1}$$

$$V(Y) = \sigma^2 N^{-1} . \tag{2.2}$$

The quantity $\mathbf{1}$ is a $v \times 1$ vector having unity elements, μ is a scalar, t is a $v \times 1$ vector of (fixed) treatment effect; and the matrix N is a $v \times v$ diagonal matrix having only non-zero diagonal elements n_i which denote the number of observations on the i^{th} treatment. The elements of t are not linearly independent, but satisfy a single linear restraint which will be described later.

Also define $\{a_s\}$, $s = 1, 2, \ldots, n$, to denote vectors, termed primitive elements, such that

$$a_s' = [a_s(1), a_s(2), \ldots, a_s(m_s)] .$$

New elements can be formed with the operation of the symbolic direct product (SDP) which is denoted by $\otimes$. The SDP between a_p and a_q is defined to be

$$[a_p \otimes a_q]' = [a_{pq}(1,1),\ a_{pq}(1,2),\ \ldots,\ a_{pq}(1,m_q)\ ,$$

(2.3)

$$a_{pq}(2,1),\ \ldots,\ a_{pq}(2,m_q),\ \ldots,\ a_{pq}(m_p,1),\ \ldots,\ a_{pq}(m_p,m_q)] \quad .$$

Note that the subscript refers to the primitive elements involved and the argument is a vector of two elements which are ordered lexographically. The lexographical order is to hold the first element of the argument fixed at 1 and run through the levels $1, 2, \ldots, m_q$ of A_q; then change the first argument to level 2 of A_p and run through the levels of A_q; etc. The SDP is also defined for more than two primitive elements in the same way; i.e., $a_p \otimes a_q \otimes a_r$, etc. The elements of $a_p \otimes a_q$ denote the vector whose elements are the parameters associated with the two factor interaction between factors A_p and A_q; the elements of $a_p \otimes a_q \otimes a_r$ denote the vector associated with the three factor interactions among factors A_p, A_q, and A_r, etc.

Let x_s be a variable which takes on the values 0 or 1. We define

$$a_s^{x_s} = \begin{cases} a_s & \text{for } x_s = 1 \\ 1 & \text{for } x_s = 0 \end{cases}$$

and use the convention that $a_s \otimes 1 = a_s$. Then, if $x = (x_1, x_2, \ldots, x_n)$, a generalized interaction may be denoted by

$$a^x = a_1^{x_1} \otimes a_2^{x_2} \otimes \dots \otimes a_n^{x_n}$$

and will have $m^x = \prod_{i=1}^{n} m_i^{x_i}$ components.

The model relating the treatment effects to the interaction parameters can be written by defining

$$I_s^{x_s} = \begin{cases} I_s & \text{for } x_s = 1 \\ 1_s & \text{for } x_s = 0 \ ; \end{cases}$$

$$I^x = I_1^{x_1} \times I_2^{x_2} \times \dots \times I_n^{x_n} \quad ,$$

where I_s is $m_s \times m_s$ identity matrix and $\mathbf{1}_s$ is an $m_s \times 1$ column vector having all elements equal to unity. Then we can write

$$t = \sum_x{}' I^x a^x \ , \tag{2.4}$$

where $x = (x_1, x_2, \dots, x_n)$ and the summation $\sum_x{}'$ refers to all the $2^n - 1$ n-digit binary numbers x excluding $x = (0, 0, \dots, 0)$. The components of t are taken in the same lexographical ordering as the n-factor interaction.

The interaction parameters a^x are not linearly independent. Let u_s be a $1 \times n$ vector with all elements equal to zero except for the s^{th} element which is equal to unity and define r by

$$vr = (1_1' \times 1_2' \times \ldots \times 1_n')\, N\, (1_1 \times 1_2 \times \ldots \times 1_n) \;.$$

We then define the $m_s \times m_s$ diagonal matrix

$$W_s = \frac{m_s}{rv}(I^{u_s})'\, N(I^{u_s}) \qquad s = 1, 2, \ldots, n \quad . \tag{2.5}$$

The elements of W_s are proportional to the number of times the various levels of factor A_s appear.

Then a convenient set of restraints among the parameters may be taken to be

$$\left\{\begin{array}{l} 1_p' W_p a_p = 0 \qquad p = 1, 2, \ldots, n; \\[2ex] \begin{bmatrix} 1_p' \times I_q \\ \\ I_p \times 1_q' \end{bmatrix} [W_p \times W_q][a_p \otimes a_q] = 0, \quad p \neq q = 1, 2, \ldots, n \;; \\[4ex] \begin{bmatrix} 1_1' \times I_2 \times \ldots \times I_n \\ I_1 \times 1_2' \times \ldots \times I_n \\ \vdots \\ I_1 \times I_2 \times \ldots \times 1_n' \end{bmatrix} [W_1 \times W_2 \times \ldots \times W_q][a_1 \otimes a_2 \otimes \ldots \otimes a_n] = 0. \end{array}\right. \tag{2.6}$$

With these restraints, it can easily be shown that

$$[1_1' \times 1_2' \times \ldots \times 1_n'][W_1 \times W_2 \times \ldots \times W_n]t = 0 \quad . \tag{2.7}$$

We shall find it convenient to use the following notational convention. Let Z_s $(s = 1, 2, \ldots, n)$ be matrices and $x = (x_1, x_2, \ldots, x_n)$ be an n-digit binary number. Then, we shall always write Z^x and $Z(x)$ to denote

$$(2.8)\qquad \begin{cases} Z^x = Z_1^{x_1} \times Z_2^{x_2} \times \ldots \times Z_n^{x_n} \\ \\ Z(x) = Z_{s_1} \times Z_{s_2} \times \ldots \times Z_{s_p} \text{ for those } x_{s_1} = x_{s_2} = \ldots = x_{s_p} = 1 \,. \end{cases}$$

When the Z_s are scalar quantities (say) $Z_s = z_s$, then

$$(2.9)\qquad z^x = z(x) \,.$$

3. The General Theory of Unequal Numbers

In this section we shall develop the general theory for unequal numbers. Our procedure will be to first find estimates for the various interaction parameters and their variances and then derive the associated sum of squares for use in the analysis of variance. The estimation of the various interactions constitutes no real problem; the difficult problem is to determine the appropriate sums of squares.

Let $W = W_1 \times W_2 \times \ldots \times W_n$; then it can easily be shown that the estimable functions for t_i may be estimated from

$$(3.1)\qquad \hat{t} = [I - \frac{JW}{1'W1}]Y = [I - \frac{JW}{v}]Y$$

where 1 is a $v \times 1$ column vector having all elements unity, $J = 1\,1'$; and I is the $v \times v$ identity matrix.

Consequently we have

$$\text{(3.2)} \qquad \operatorname{var} \hat{t} = \sigma^2 [I - \frac{JW}{v}] N^{-1} [I - \frac{JW}{v}]' \quad .$$

Define the $m_s \times m_s$ matrix M_s by

$$\text{(3.3)} \qquad M_s = [m_s I_s - J_s W_s] W_s^{-1} \quad .$$

Also let

$$\text{(3.4)} \qquad \begin{cases} M_s^{x_s} = \begin{cases} M_s & \text{for } x_s = 1 \\ \mathbf{1}_s' & \text{for } x_s = 0 \end{cases} , \\ \\ M^x = M_1^{x_1} \times M_2^{x_2} \times \ldots \times M_n^{x_n} \end{cases}$$

We note that M^x may also be written as

$$M^x = M(x)(I^x)'$$

where $M(x) = M_{s_1} \times M_{s_2} \times \ldots \times M_{s_p}$ and $x_{s_1} = x_{s_2} = \ldots x_{s_p} = 1$

with the remaining $x_s = 0$; i.e. $M(x)$ is the direct product of those M_s for which $x_s = 1$. We also record for reference

$$\text{(3.5)} \qquad \begin{cases} M_s W_s = m_s I_s - J_s W_s \\ M_s W_s a_s = m_s a_s \\ M_s W_s \mathbf{1}_s = O \end{cases} \quad .$$

After some algebra one can show that

(3.6) $$\hat{a}^x = M^x W \hat{t}/v$$

and

(3.7) $$\operatorname{var} \hat{a}^x = [M^x W N^{-1} W (M^x)'] \, \sigma^2/v^2 \;.$$

Note that the var $\hat{a}^x$ may be written as

$$\operatorname{var} \hat{a}^x = M(x) [(I^x)' W N^{-1} W I^x] M(x) \, \sigma^2/v^2 \;.$$

The variance can be further simplified. For this purpose define

$$W_s^{x_s} = \begin{cases} W_s & \text{if } x_s = 1 \\ I_s & \text{if } x_s = 0 \end{cases}$$

$$W^x = \prod_{s=1}^{n} \times W_s^{x_s} \;.$$

Then the quantity $[(I^x)' W]$ may be written

$$(I^x)' W = \prod_{s=1}^{n} \times (I^{x_s})' W_s = W(x) \prod_{s=1}^{n} \times (I^{x_s})' W_s^{1-x_s} = W(x) (I^x)' W^{1-x} \;.$$

The diagonal matrix $[(I^x)' W N^{-1} W I^x]$ can also be written

$$(I^x)' W N^{-1} W I^x = W(x) \, R(x) \, W(x)$$

where

(3.8) $$R(x) = (I^x)' W^{1-x} N^{-1} W^{1-x} I^x \;.$$

Hence the variance of $\hat{a}^x$ is

$$\text{var } \hat{a}^x = [M(x)\, W(x)\, R(x)\, W(x)\, M(x)]\, \sigma^2/v^2 \quad . \tag{3.9}$$

Note that $R(x)$ and $W(x)$ are diagonal matrices.

It remains to find the sum of squares associated with $\hat{a}^x$. We shall find this making use of a result on quadratic forms recently given by Rao [1962]

<u>Lemma</u>. Let $X = (X_1, X_2, \ldots, X_n)$ have a singular multivariate normal distribution with $E(X) = 0$ and $\text{var } X = \sigma^2 \sum$ where the rank of $\sum$ is f $(f < n)$. Then a necessary and sufficient condition for the quadratic form $X' S X/\sigma^2$ to have a chi-square distribution with f degrees of freedom is that S be a real symmetric $n \times n$ matrix having the properties that

$$\text{(i)} \quad S = S \textstyle\sum S$$
$$\text{(ii)} \quad \textstyle\sum = \sum S \sum \quad .$$

We now turn our attention to finding the matrix S of the above lemma when $\sum = M(x)\ W(x)\ R(x)\ W(x)\ M(x)$. We point out that the degrees of freedom associated with $\hat{a}^x$ is $f(x) = \prod_{s=1}^{n} (m_i - 1)^{x_s}$ (rank of $\text{var } \hat{a}^x$) . Hence there will exist at least $r(x) = m(x) - f(x)$ linearly independent non-estimable functions of a^x . These non-estimable functions will be denoted by

$$K'(x)\, W(x)\, a^x \tag{3.10}$$

where $K'(x)$ is $r(x) \times m(x)$, has rank $r(x)$, and $W(x)$ denotes the direct product of those W_s for which $x_s = 1$.

Define the $m(x) \times m(x)$ matrix $V(x)$ by

$$(3.11) \qquad \begin{bmatrix} W(x)\,M(x) & R^{-1}(x)\,K(x) \\ \\ K'(x)\,R^{-1}(x) & O \end{bmatrix}^{-1} = \begin{bmatrix} V(x) & K(x)\,U(x) \\ \\ U(x)\,K'(x) & O \end{bmatrix}$$

where

$$(3.12) \qquad U(x) = [K'(x)\,R^{-1}(x)\,K(x)]^{-1} \quad .$$

It can be verified that the matrix S of the lemma is

$$(3.13) \qquad S = v^2\,V(x)\,R^{-1}(x)\,V(x) \quad .$$

Therefore, the required sum of squares is

$$(3.14) \qquad v^2(\hat{a}^x)'\,\{V(x)\,R^{-1}(x)\,V(x)\}(\hat{a}^x) \quad .$$

The above sum of squares still requires knowledge of the matrix $V(x)$ which is not known explicitely. Using (3.5), we can write

$$m_s\,a_s = M_s\,\ddot{W}_s\,a_s$$

and therefore

$$(3.15) \qquad m(x)\;\hat{a}^x = M(x)\;W(x)\;\hat{a}^x \quad .$$

Substituting (3.15) in (3.14) results in

$$\left(\frac{v}{m(x)}\right)^2(\hat{a}^x)'\left\{W(x)\,M(x)\,V(x)\,R^{-1}(x)\,V(x)\,M(x)\,W(x)\right\}(\hat{a}^x) \quad .$$

Using the relations of a matrix to its inverse gives

$$W(x)\,M(x)\,V(x) + R^{-1}(x)\,K(x)\,U(x)\,K'(x) = I \quad ,$$

$$K'(x)\,R^{-1}(x)\,V(x) = O \quad .$$

Consequently,

$$W(x)\,M(x)\,V(x)\,R^{-1}(x)\,V(x)\,M(x)\,W(x) = R^{-1}(x)\,[I - K(x)\,U(x)\,K'(x)\,R^{-1}(x)] \quad ,$$

which follows from the fact that the matrix in square brackets in idempotent.

Therefore the sum of squares can be written as

$$(3.16) \qquad \left(\frac{v}{m(x)}\right)^2 (\hat{a}^x)' \left\{ R^{-1}(x)\,[I - K(x)\,U(x)\,K'(x)\,R^{-1}(x)] \right\} (\hat{a}^x) \quad .$$

Since $R(x)$ is a diagonal matrix, the main computational labor is in computing the $r(x) \times r(x)$ inverse matrix

$$U(x) = [K'(x)\,R^{-1}(x)\,K(x)]^{-1} \quad .$$

The sums of squares for main effects may be written explicitely as $r(x) = 1$. In this case for (say) $\hat{a}_s$

$$K'(x) = 1_s' \quad , \qquad W(x) = W_s$$

$R_s = R(x)$

$$= (1' W_1 \times 1_2' W_2 \times \ldots \times I_s \times \ldots \times 1_n' W_n)\, N^{-1} (W_1 1_1 \times W_2 1_2 \times \ldots \times I_s \times \ldots \times W_n 1_n)$$

$$U_s = (1_s' R_s^{-1} 1_s)^{-1} \quad .$$

The sum of squares for the main effect associated with A_s is thus

$$(3.17) \qquad \left(\frac{v}{m_s}\right)^2 \hat{a}_s' \left\{R_s^{-1}\left[I_s - \frac{J_s R_s^{-1}}{U_s}\right]\right\} \hat{a}_s$$

4. Proportional Frequencies

As is well known, the case of proportional frequencies turns out to be particularly simple. The case of proportional frequencies arises when

$$N = N_1 \times N_2 \times \dots \times N_n = \prod_{s=1}^{n} \times N_s$$

where the N_s are such N is the direct product of all N_s .

Define $\bar{n}_s = \mathbf{1}_s' N_s \mathbf{1}_s$; then the W_s quantities are

$$W_s = \frac{m_s}{\bar{n}_s} N_s$$

and

$$W = \prod_{s=1}^{n} \times W_s = \frac{N}{r} \quad .$$

Consequently we have

$$W(x)R(x)W(x) = (I^x)' W N^{-1} W I^x = \frac{(I^x)' N I^x}{r^2} = \frac{v}{r\bar{n}(x)} N(x)$$

and

$$\text{var}\, \hat{a}^x = \frac{\sigma^2}{r^2 v^2}\left[M_1^{x_1} N_1 (M_1^{x_1})' \times M_2^{x_2} N_2 (M_2^{x_2})' \times \dots \times M_n^{x_n} N_n (M_n^{x_n})'\right]$$

Note that

$$M_s^{x_s} N_s (M_s^{x_s})' = \begin{cases} \bar{n}_s M_s & \text{for } x_s = 1 \\ \bar{n}_s & \text{for } x_s = 0 \end{cases} .$$

Therefore the variance can be written as

$$\text{(4.1)} \qquad \operatorname{var} \hat{a}^x = \frac{\sigma^2}{rv} M(x)$$

as $\bar{n}^x = rv$.

The sum of squares associated with $\hat{a}^x$ can easily be written by noting that the second term in (3.16) is a null matrix. This can be demonstrated by writing

$$\text{(4.2)} \qquad R^{-1}(x) = \frac{r\, m(x)^2}{v\, \bar{n}(x)} N(x)$$

and thus

$$K'(x)\, R^{-1}(x)\, \hat{a}^x = \frac{r\, m(x)^2}{v\, \bar{n}(x)} K'(x)\, N(x)\, \hat{a}^x = O \quad .$$

The sum of squares associated with $\hat{a}^x$ is then

$$\text{(4.3)} \qquad \left(\frac{v}{m(x)}\right)^2 (\hat{a}^x)'\, R^{-1}(x) (\hat{a}^x) = \frac{rv}{\bar{n}(x)} (\hat{a}^x)'\, N(x)\, (\hat{a}^x) \quad .$$

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