

MULTIVARIATE ORTHOGONAL POLYNOMIALS

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I. INTRODUCTION

It is well known that the work of fitting a regression function which is a polynomial in one variable can be greatly simplified by the use of orthogonal polynomials. The earliest reference to orthogonal polynomials seems to be in some work by Tchebycheff as far back as 1857. It was not until early in the twentieth century, however, that their use in statistics began to be fully appreciated.

Since 1930 much has been written concerning the application of orthogonal polynomials to statistical data. Some of the more prominent articles are those by Allan (1930), Wishart (1933), Aitken (1933), Fisher (1938) and Van Der Reyden (1943).

In many research problems it is required to fit a regression function which is a polynomial in more than one variate. For example, in a milk-testing problem Morton and Vincent (1949) fitted a function relating the influence of time and temperature of storage on milk quality. A suitable function was found to be a polynomial of degree three in temperature of storage and of degree two in the time of storage as follows:

$$(1.1) \quad y = b_0 + b_1t + b_2t^2 + b_3T + b_4tT + b_5t^2T + b_6T^2 \\ + b_7tT^2 + b_8t^2T^2 + b_9T^3 + b_{10}tT^3 + b_{11}t^2T^3$$

where y is the predicted quality (measured as number of hours

to reduce a given quantity of methylene blue); b_0, b_1, \dots, b_{11} represent the regression constants; t = storage time in hours; and T = storage temperature in degrees centigrade. A graphical presentation of the surface represented by (1.1) is given in Figure 1. We may refer to functions of this kind as multivariate polynomials and express them in the general form

$$(1.2) \quad \hat{y} = \sum_{i_1=0}^{\alpha_1} \sum_{i_2=0}^{\alpha_2} \dots \sum_{i_k=0}^{\alpha_k} b_{i_1, i_2, \dots, i_k} x_1^{i_1} x_2^{i_2} \dots x_k^{i_k}$$

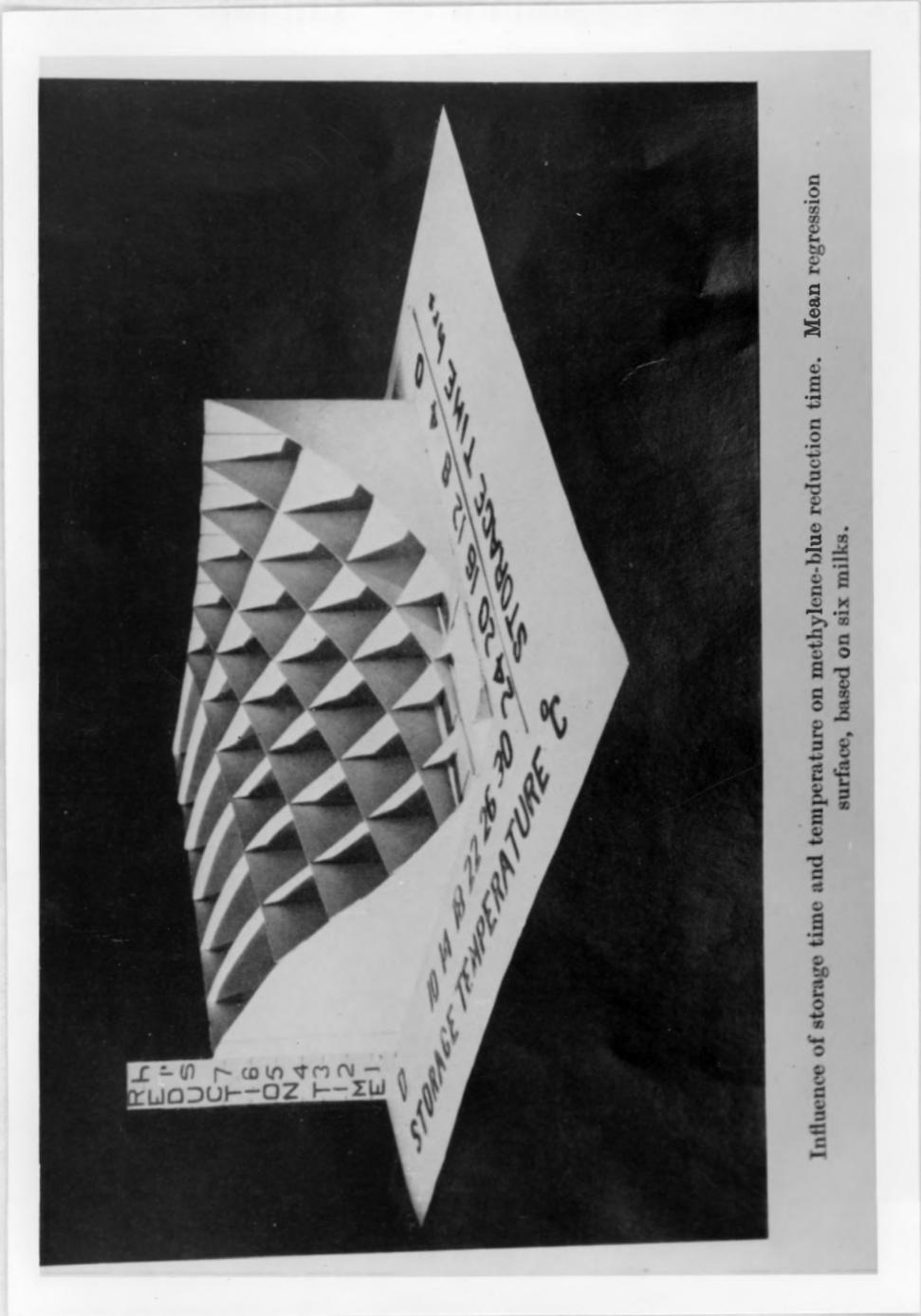
$$i_1 = 0, 1, \dots, \alpha_1$$

$$i_2 = 0, 1, \dots, \alpha_2$$

$$i_k = 0, 1, \dots, \alpha_k$$

The object of this thesis is to define special orthogonal polynomials and develop efficient methods for employing them which have the same advantages with respect to functions of the type (1.2) as do univariate orthogonal polynomials in the simple case $k=1$. These new polynomials may be usefully termed "multivariate orthogonal polynomials."

The idea of using polynomials of this type is implicit in various analyses of factorial designs first given by F. Yates (1937). George W. Tyler (1949) and D. B. DeLury (1950) use them a little more explicitly in evaluating definite integrals for simple one and two dimensional cases



Influence of storage time and temperature on methylene-blue reduction time. Mean regression surface, based on six milks.

($k = 1, 2$). It is proposed here to develop a method whereby multivariate orthogonal polynomials can be used most efficiently as independent variables in a regression analysis for which the Morton and Vincent milk problem is a typical example. Brief reference to the possibility of using them in this way was given by Tyler and DeLury. However, further work is required in developing this method, in (a) explicitly defining the multivariate orthogonal polynomials as separate and distinct regression variables, (b) defining their properties, and (c) developing methods for handling cases with dimensions $k > 2$.

II. GENERAL REGRESSION THEORY

Given a sample of stochastic variables y_1, y_2, \dots, y_n , it is often appropriate to express their respective expected values $\theta_1, \theta_2, \dots, \theta_n$ as a linear function of a set of fixed parameters $\beta_1, \beta_2, \dots, \beta_r$ as follows:

$$(2.1) \quad \theta_\alpha = \beta_1 x_{1\alpha} + \beta_2 x_{2\alpha} + \dots + \beta_r x_{r\alpha}, \quad \alpha = 1, 2, \dots, n,$$

where the x values are known fixed constants generally termed regression variables. The expression (2.1) is generally referred to as the true regression function of y on the variables x_1, x_2, \dots, x_r .

If we now define a set of errors E_1, E_2, \dots, E_n as the deviation of each observation from its expected value, i.e. we may write

$$(2.2) \quad y_\alpha = \theta_\alpha + E_\alpha, \quad \alpha = 1, 2, \dots, n,$$

it often happens that these errors can be assumed to be normally and independently distributed with equal variance, σ^2 . That is, the joint probability density of the errors is given by¹

$$(2.3) \quad f(E_1, E_2, \dots, E_n; \sigma^2) = (2\pi\sigma^2)^{-n/2} e^{-\frac{1}{2} \cdot \frac{SE_\alpha^2}{\sigma^2}}.$$

1. It will be convenient to use S to denote summation over the range $\alpha = 1, 2, \dots, n$ throughout the entire thesis.

The complete probability model for this data can thus be given in the form of the joint density function

$$f(y_1, y_2, \dots, y_n; \beta_1, \beta_2, \dots, \beta_r; \sigma^2) = \frac{1}{(2\pi\sigma^2)^{n/2}} e^{-\frac{1}{2}S(y_\alpha - \sum_{i=1}^r \beta_i x_{i\alpha})^2 / \sigma^2}.$$

This may be described as the multiple linear regression model with normal independent and homogeneous errors.

2.1 Estimation of the Unknown Parameters:

For this model it is readily shown that the methods of maximum likelihood and the method of least squares estimation give the same results. If we let b_1, b_2, \dots, b_r be the least squares estimates of $\beta_1, \beta_2, \dots, \beta_r$ respectively, the function

$$(2.5) \quad \hat{y}_\alpha = b_1 x_{1\alpha} + b_2 x_{2\alpha} + \dots + b_r x_{r\alpha} \quad \alpha = 1, 2, \dots, n$$

is known as the "least squares regression equation" and the errors

$$(2.6) \quad e_\alpha = y_\alpha - \hat{y}_\alpha \quad \alpha = 1, 2, \dots, n,$$

may be termed the "least squares errors".

The method of least squares consists of finding the regression coefficients b_1, b_2, \dots, b_r so that the error sum of squares

$$(2.7) \quad Se_\alpha^2 = S(y_\alpha - b_1 x_{1\alpha} - b_2 x_{2\alpha} - \dots - b_r x_{r\alpha})^2$$

is minimized. These values are obtained by solving the following normal equations.

$$\begin{aligned}
 & b_1 a_{11} + b_2 a_{12} + \dots + b_r a_{1r} = g_1 \\
 & b_1 a_{21} + b_2 a_{22} + \dots + b_r a_{2r} = g_2 \\
 (2.8) \quad & \vdots \\
 & \vdots \\
 & b_1 a_{r1} + b_2 a_{r2} + \dots + b_r a_{rr} = g_r
 \end{aligned}$$

where $a_{ij} = \sum x_{ia} x_{ja}$

and $g_i = \sum x_{ia} y_a$.

A sufficient condition for these equations to have a unique solution is that the determinant $|A|$, where A is the matrix of the coefficients a_{ij} , does not vanish. This solution is given by

$$(2.9) \quad b_j = \sum_{i=1}^r c_{ij} g_i$$

where c_{ij} is the ij^{th} element of the inverse matrix A^{-1} .

2.2 Analysis of Variance:

An unbiased estimate s^2 of σ^2 which has $n-r$ degrees of freedom, being distributed as $\frac{1}{n-r} \sigma^2 \chi_{n-r}^2$ is generally obtained from the following analysis of variance.

Analysis of Variance for Regression

Source of Variation	S.S.	d.f.	M.S.
Regression	$R_r = \sum_{i=1}^r b_i g_i$	r	R_r/r
Error	$SS_e = SS_T - R_r$	n-r	$s^2 = SS_e/n-r$
Total	$SS_T = Sy_a^2$	n	

The equalities $R_r = \sum_{i=1}^r b_i g_i$ and $SS_e = SS_T - R_r$ are readily demonstrated and provide useful short cuts in the methods of calculation.

2.3 Distribution of Regression Coefficients:

Given that the multiple regression model with normal independent and homogeneous errors holds, the following can be proven about the distribution of each of the b's:

- the expected value, $E(b_i)$, is β_i ;
- the variance-covariance matrix is $[c_{ij}] \sigma^2$;
- b_i is normally distributed; and
- if b_i^* be used to denote any other unbiased estimate of β_i then by Markoff's theorem² $\sigma_{b_i}^2 \leq \sigma_{b_i^*}^2$.

2. W. G. Cochran (1945).

2.4 Fundamental Theorem of Multiple Regression:

The most important theorem in connection with significance testing in multiple regression work is one which might well be termed the fundamental theorem of multiple regression and may be stated as follows: Given that the multiple linear regression model with normal independent and homogeneous errors is appropriate for a given set of data, let $x_1, x_2, \dots, x_k, x_{k+1}, x_{k+2}, \dots, x_r$ represent any partition of the regression variates. Define a null hypothesis as

$$H_0: \beta_{k+1} = \beta_{k+2} = \dots = \beta_r.$$

Let R_k and R_r be the regression sums of squares obtained on fitting a regression equation to the first k x 's alone and to the entire r x 's respectively. Let s^2 be the unbiased estimate of the error variance, σ^2 . Define a test ratio as

$$(2.10) \quad T = \frac{(R_r - R_k)/r-k}{s^2}$$

Then,

(a) s^2 is distributed as $\frac{1}{n-r}\sigma^2\chi_{n-r}^2$, and

(b) if H_0 is true, $(R_r - R_k)/r-k$ is distributed as

$\frac{1}{r-k}\sigma^2\chi_{r-k}^2$ and thence T is distributed as

$F_{r-k, n-r}$. Since s^2 and $(R_r - R_k)/r-k$ are distributed independently.

III. UNIVARIATE ORTHOGONAL POLYNOMIALS

3.1 A Useful Transformation:

A valuable theorem in multiple linear regression work is the following³: Let

$$(3.1) \quad z_{i\alpha} = L_{i1}x_{1\alpha} + L_{i2}x_{2\alpha} + \dots + L_{ir}x_{r\alpha} \quad \begin{array}{l} i = 1, 2, \dots, r \\ \alpha = 1, 2, \dots, n \end{array}$$

be a linear non-singular transformation of the x 's. Let

$$(3.2) \quad \hat{y}'_{\alpha} = b'_1 z_{1\alpha} + b'_2 z_{2\alpha} + \dots + b'_r z_{r\alpha}$$

be the least squares regression line fitted to the new variables, z . Put

$$(3.3) \quad \hat{y}'_{\alpha} = b''_1 x_{1\alpha} + b''_2 x_{2\alpha} + \dots + b''_r x_{r\alpha}$$

for the function linear in the x 's obtained by substituting the values (3.1) for the z 's in equation (3.2). Then the theorem states that $\hat{y}'_{\alpha} = \hat{y}_{\alpha}$. That is, the least squares values of \hat{y} are the same whether the regression is fitted directly on the x variables or on the transformed variables, z . From this it follows that the sums of squares for regression and for error are invariant when calculated from (3.3) or from (2.4).

3.2 Orthogonal Regression Variates:

In making the transformation illustrated in the preceding section, one may choose the L 's so that

3. W. G. Cochran (1945)

$$(3.4) \quad S z_{i\alpha}^2 = 1; \text{ and } S z_{i\alpha} z_{j\alpha} = 0$$

This is called an orthogonal transformation. By imposing this condition of orthogonality, the normal equations for the regression on the z 's are

$$(3.5) \quad b_i^z = S(z_{i\alpha} y) / S z_{i\alpha}^2 = S(z_{i\alpha} y), \quad i = 1, 2, \dots, r.$$

Noting the work required in solving these normal equations as compared with the normal regression equations of \hat{y} on the x 's, the advantage of having orthogonal regression variates can be readily seen.

If the transformation of x 's to z 's is chosen, as it can be, so that $L_{ij} = 0$ where $j > i$, (in which case the matrix of the elements L_{ij} is said to be triangular), the additional regression sums of squares, $R_r - R_k$, is given

simply by the sum $\sum_{i=k+1}^r b_i^z z_i$. In many cases this reduces

the amount of work in applying the fundamental theorem by 95 percent or more.

In some cases, however, the work required in finding a triangular transformation so that the z 's will be orthogonal will require just as much effort as the trouble it saves in the fitting of the regression directly to the x 's. In such cases, a linear transformation of this kind is generally not worth while. In other cases, however, as we shall see in the following subsection, such transformations are very useful.

3.3 Orthogonal Polynomials:

In the problem of fitting a polynomial curve to a regression variable, it often happens that the values of the variable are equally spaced. Because of this, it is only necessary to work out one transformation which will suit many different problems. This transformation has been obtained in the form of sets of transformed variate values which are termed orthogonal polynomials and are denoted by ξ_i' . In fitting a polynomial regression of degree h , that is a curve of the form

$$(3.6) \quad y = b_0x^0 + b_1x^1 + b_2x^2 + \dots + b_hx^h,$$

$h+1$ orthogonal polynomials ξ_0' , ξ_1' , ..., ξ_h' may be written as

$$(3.7) \quad \begin{aligned} \xi_0' &= x^0 \\ \xi_1' &= k_{10}x^0 + k_{11}x^1 \\ &\vdots \\ \xi_h' &= k_{h0}x^0 + k_{h1}x^1 + \dots + k_{hh}x^h \end{aligned}$$

where K is a non-singular matrix of arbitrary constants chosen so that the ξ_i' 's are orthogonal and consist of simple integral values.

With only a change in scale and a change in location, these polynomials can be directly applicable to a large group of curve fitting problems. These ξ_i' values along with

their sums of squares are tabled in Fisher and Yates (1949) "Statistical Tables" for $n=1$ to $n=75$ and for $i=1$ to 5 ; $\xi_0^i = 1$ for all observations and does not require tabling. DeLury (1950) has tabled a complete set of orthogonal polynomial values for $i=1, 2, \dots, 25$ and up to $n=26$. This saves a lot of repeated calculations in separate problems.

IV. MULTIVARIATE ORTHOGONAL POLYNOMIALS

4.1 Theoretical Considerations:

Consider the problem of fitting a multivariate polynomial regression function of the general form

$$(4.1) \quad \hat{y} = \sum_{\substack{i_1=0,1,\dots,\alpha_1 \\ i_2=0,1,\dots,\alpha_2 \\ \vdots \\ i_k=0,1,\dots,\alpha_k}} b_{i_1,i_2,\dots,i_k} x_1^{i_1} x_2^{i_2} \dots x_k^{i_k}$$

A set of multivariate orthogonal polynomials can be defined for problems like these which give the same advantages as do the univariate polynomials in the simple one dimensional case ($k=1$).

To facilitate the definition it is desirable to introduce some further notation.

$$\text{Let} \quad \begin{array}{ll} x_{1a_1}, & a_1 = 0, 1, \dots, \alpha_1 \\ x_{2a_2}, & a_2 = 0, 1, \dots, \alpha_2 \\ \vdots & \vdots \\ x_{ka_k}, & a_k = 0, 1, \dots, \alpha_k \end{array}$$

represent each of the values of the respective x 's, and put y_{a_1, a_2, \dots, a_k} for the observed value of y taken at the a_j^{th} value of x_j , $j=1, 2, \dots, k$.

Let the notation y_α , $\alpha=1,2,\dots,n$ be ordered with respect to the new notation y_{a_1,a_2,\dots,a_k} by the correspondence between α and a_1,a_2,\dots,a_k indicated in Table I.

Let ξ_{i_1,i_2,\dots,i_k} denote a multivariate orthogonal polynomial of degrees i_1,i_2,\dots,i_k with respect to each of the k dimensions. The number of these which can be usefully defined in any problem is limited to n , and the degrees, $i_j = 0, 1, \dots, \alpha_j$; $j = 1, 2, \dots, k$.

In the same way as the k dimensional notation y_{a_1,a_2,\dots,a_k} is ordered in the single dimensional form y_α , so the notation ξ_{i_1,i_2,\dots,i_k} can be ordered in the form ξ_i where $i = 1, 2, \dots, n$ bears the same relation to i_1, i_2, \dots, i_k as does α to a_1, a_2, \dots, a_k in Table I.

A multivariate orthogonal polynomial will now be defined as

$$(4.2) \quad \xi_i = \xi_{i_1,i_2,\dots,i_k} = \xi_{i_1}^{i_1} \cdot \xi_{i_2}^{i_2} \cdots \xi_{i_k}^{i_k},$$

where $\xi_{i_j}^{i_j}$ is the i_j^{th} degree univariate orthogonal polynomial for x_j , $j = 1, 2, \dots, k$.

The all important property of these multivariate polynomials is their mutual orthogonality which may be demonstrated as follows:

Table I

Correspondence Between Single and k Dimensional Orders

α	α_1	α_2	$\alpha_3 \dots \alpha_k$	α	α_1	α_2	$\alpha_3 \dots \alpha_k$	α	α_1	α_2	$\alpha_3 \dots \alpha_k$
1	0	0	0...0	m+1	0	0	1...0	n-m+1	0	0	$\alpha_3 \dots \alpha_k$
2	1	0	0...0	m+2	1	0	1...0	n-m+2	1	0	$\alpha_3 \dots \alpha_k$
.
.
α_1+1	α_1	0	0...0	m+ α_1+1	α_1	0	1...0	n-m+ α_1+1	α	0	$\alpha_3 \dots \alpha_k$
α_1+2	0	1	0...0	m+ α_1+2	0	1	1...0	n-m+ α_1+2	0	1	$\alpha_3 \dots \alpha_k$
α_1+3	1	1	0...0	m+ α_1+3	0	1	1...0	n-m+ α_1+3	1	1	$\alpha_3 \dots \alpha_k$
.
.
$2(\alpha_1+1)$	α_1	i	0...0	m+2(α_1+1)	α_1	i	1...0	n-m+2(α_1+1)	α	i	$\alpha_3 \dots \alpha_k$
.
.
.
$\alpha_2(\alpha_1+1)+1$	0	α_2	0...0	m+ $\alpha_2(\alpha_1+1)+1$	0	α_2	1...0	n-m+ $\alpha_2(\alpha_1+1)+1$	0	α_2	$\alpha_3 \dots \alpha_k$
$\alpha_2(\alpha_1+1)+2$	1	α_2	0...0	m+ $\alpha_2(\alpha_1+1)+2$	1	α_2	1...0	n-m+ $\alpha_2(\alpha_1+1)+1$	1	α_2	$\alpha_3 \dots \alpha_k$
.
.
.
m	α_1	α_2	0...0	2m	α_1	α_2	1...0	n	α_1	α_2	$\alpha_3 \dots \alpha_k$

Note: For convenience in tabling, $m = (\alpha_1+1)(\alpha_2+1)$; also, $n = \prod_{i=1}^k (\alpha_i+1)$.

$$(4.3) \quad S(\xi_i, \xi_{i'}) = S_{\xi_{i_1, i_2, \dots, i_k}} \cdot \xi_{i'_1, i'_2, \dots, i'_k} \\ = S_{\xi_{i_1, i_2, \dots, i_k, a_1, a_2, \dots, a_k}} \cdot \xi_{i'_1, i'_2, \dots, i'_k, a_1, a_2, \dots, a_k}$$

Then summing with respect to the various dimensions separately, this can be written as

$$(4.4) \quad \sum_{a_1=1}^{a_1} \sum_{a_2=1}^{a_2} \dots \sum_{a_k=1}^{a_k} \xi_{i_1, a_1} \xi_{i_2, a_2} \dots \xi_{i_k, a_k} \\ \cdot \xi_{i'_1, a_1} \cdot \xi_{i'_2, a_2} \dots \xi_{i'_k, a_k} \\ = \sum_{a_1=1}^{a_1} \xi_{i_1, a_1} \cdot \xi_{i'_1, a_1} \cdot \sum_{a_2=1}^{a_2} \xi_{i_2, a_2} \cdot \xi_{i'_2, a_2} \dots \sum_{a_k=1}^{a_k} \xi_{i_k, a_k} \cdot \xi_{i'_k, a_k} \\ = 0$$

provided the equalities $i_1 = i'_1, i_2 = i'_2, \dots, i_k = i'_k$ do not all hold. This shows that ξ_i and $\xi_{i'}, i \neq i'$ are mutually orthogonal.

In the case $i = i'$ we obtain the sum of squares $S\xi_{i\alpha}^2$ as

$$(4.5) \quad S\xi_{i\alpha}^2 = \sum_{a_1=1}^{a_1} \xi_{i_1, a_1}^2 \cdot \sum_{a_2=1}^{a_2} \xi_{i_2, a_2}^2 \dots \sum_{a_k=1}^{a_k} \xi_{i_k, a_k}^2$$

which is most useful in computing the required sums of squares

for the new multivariate orthogonal polynomials direct from the sum of squares values tabled by Fisher and Yates. Because of the orthogonality property, the regression coefficient for each multivariate orthogonal polynomial is obtained from the simple formula

$$(4.6) \quad b_i = \frac{\sum y \epsilon_i}{\sum \epsilon_i^2} \quad i = 1, 2, \dots, n.$$

The additional regression sum of squares, $R_r - R_k$, due to fitting $r-k$ additional variables, is obtained simply from

the sum $\sum_{i=k+1}^r b_i \sum y \epsilon_i$ where the summation is taken over the

new regression coefficients multiplied by the respective sum of products terms. This means that the work required for the application of the significance test of the fundamental theorem is relatively very small. In practice, this theorem will be applied generally as each term is added.

Ideally it would be desirable to have a measure of the experimental error and to keep on taking out terms until the residual error in the regression analysis is reduced to the order of this figure. In certain cases an experimental error could be decided upon arbitrarily, keeping in mind the the conditions under which the data have been collected, and

this could be used in the same way. If neither of these methods are practicable, it might be desirable to fit a regression coefficient for every degree of freedom and to develop a method for allotting to the residual error term those degrees of freedom which have the smallest mean squares, combining them to give a homogeneous set. This may be referred to as the method of "pooling for error". Care would have to be taken in this method to allow for the a posteriori nature of the selection of the error terms in deciding when to stop the pooling process.

In the following problem it was necessary to adopt a procedure consisting of a compromise between these approaches.

4.2 Shortcuts in Calculation:

Method of folding.

Fisher and Yates (1949) have developed a shortcut method by fitting a univariate polynomial to sums and differences of pairs of the observations instead of to the observations themselves. This technique may be referred to as a "method of folding" the data. It makes use of the symmetry of univariate orthogonal polynomials to halve the number of calculations necessary in determining the sums of products $Sy\xi_i^r$, $i=1,2,\dots,r$.

An extension of this method to multivariate orthogonal polynomials whereby the data may be folded with respect to

each of the k dimensions involved has been developed. This method is straight forward and reduces the number of calculations for obtaining the sums of products by approximately $\frac{2^k-1}{2^k} \cdot 100$ percent. This may be illustrated by the following example.

Consider a two dimensional case in which x_1 and x_2 take on 4 and 5^4 values respectively, and denote by y_{a_1, a_2} the value corresponding to the a_1^{th} x_1 value and the a_2^{th} x_2 value.

The first step is to "fold with respect to the first variable, x_1 ". This constitutes the calculation of the following sums and differences in two separate stages.

Table II

<u>Sums</u> (y_{a_1, a_2}^+)		<u>Differences</u> (y_{a_1, a_2}^-)	
$y_{20}^+ = y_{20} + y_{10}$	$y_{30}^+ = y_{30} + y_{00}$	$y_{20}^- = y_{20} - y_{10}$	$y_{30}^- = y_{30} - y_{00}$
$y_{21}^+ = y_{21} + y_{11}$	$y_{31}^+ = y_{31} + y_{01}$	$y_{21}^- = y_{21} - y_{11}$	$y_{31}^- = y_{31} - y_{01}$
$y_{22}^+ = y_{22} + y_{12}$	$y_{32}^+ = y_{32} + y_{02}$	$y_{22}^- = y_{22} - y_{12}$	$y_{32}^- = y_{32} - y_{02}$
$y_{23}^+ = y_{23} + y_{13}$	$y_{33}^+ = y_{33} + y_{03}$	$y_{23}^- = y_{23} - y_{13}$	$y_{33}^- = y_{33} - y_{03}$
$y_{24}^+ = y_{24} + y_{14}$	$y_{34}^+ = y_{34} + y_{04}$	$y_{24}^- = y_{24} - y_{14}$	$y_{34}^- = y_{34} - y_{04}$

The next step is to "fold with respect to the second variable, x_2 ", obtaining the following sums and differences

4. We thus have the case $\alpha_1=3$ and $\alpha_2=4$.

from the first step.

Table III

<u>Sums of Sums</u> (++)			<u>Sums of Differences</u> (-+)		
$y_{22}^{++} = y_{22}^+$	$; y_{32}^{++} = y_{32}^+$	$;$	$y_{22}^{-+} = y_{22}^-$	$; y_{32}^{-+} = y_{32}^-$	
$y_{23}^{++} = y_{23}^+ + y_{21}^+$	$; y_{33}^{++} = y_{33}^+ + y_{31}^+$	$;$	$y_{23}^{-+} = y_{23}^- + y_{21}^-$	$; y_{33}^{-+} = y_{33}^- + y_{31}^-$	
$y_{24}^{++} = y_{24}^+ + y_{20}^+$	$; y_{34}^{++} = y_{34}^+ + y_{30}^+$	$;$	$y_{24}^{-+} = y_{24}^- + y_{20}^-$	$; y_{34}^{-+} = y_{34}^- + y_{30}^-$	
<u>Differences of Sums</u> (+-)			<u>Differences of Differences</u> (--)		
$y_{22}^{+-} = y_{22}^+ - y_{22}^+$	$; y_{32}^{+-} = y_{32}^+ - y_{32}^+$	$;$	$y_{22}^{--} = y_{22}^- - y_{22}^-$	$; y_{32}^{--} = y_{32}^- - y_{32}^-$	
$y_{23}^{+-} = y_{23}^+ - y_{21}^+$	$; y_{33}^{+-} = y_{33}^+ - y_{31}^+$	$;$	$y_{23}^{--} = y_{23}^- - y_{21}^-$	$; y_{33}^{--} = y_{33}^- - y_{31}^-$	
$y_{24}^{+-} = y_{24}^+ - y_{20}^+$	$; y_{34}^{+-} = y_{34}^+ - y_{30}^+$	$;$	$y_{24}^{--} = y_{24}^- - y_{20}^-$	$; y_{34}^{--} = y_{34}^- - y_{30}^-$	

It may be noted that when the independent variable has an odd number of values (e.g. $n=5$ in this example) the center values are repeated in summing and become "0" in differencing.

The sums of products $Sy \cdot \epsilon_1$ are then calculated from Table III instead of the original y observations. For example, consider the orthogonal polynomial values for a linear effect in x_1 by a quadratic in x_2 , represented by ϵ_{12} (in two dimensional notation) shown as follows:

Table IV: Values of ξ_{12}

-6	-2	2	6
3	1	-1	-3
6	2	-2	-6
3	1	-1	-3
-6	-2	2	6

Note the symmetry of the table. To get $Sy\xi_{12}$ we simply multiply the lower three values of the last two columns in Table IV by the appropriate subsection in Table III, which in this case is the one for sums of differences (-+). The rule for selecting the corresponding set of y values is to match odd subscripts of $\xi_{i_1, i_2, \dots, i_k}$ with values obtained by differencing and even subscripts with values obtained by summing. Thus the y values corresponding to ξ_{12} are found in the y_{a_1, a_2}^{-+} set. The sum of products obtained in this way is seen to be the same as the required sum of products. This is demonstrated by the following:

$$\begin{aligned}
 (4.7) \quad \sum_{a_1, a_2} y_{a_1, a_2}^{-+} \xi_{12} &= -2(y_{22}^{-+}) -1(y_{23}^{-+}) +2(y_{24}^{-+}) -6(y_{32}^{-+}) \\
 &\quad -3(y_{33}^{-+}) +6(y_{34}^{-+}) \\
 &= -2(y_{22}^{-+}) -1(y_{23}^{-+} + y_{21}^{-+}) +2(y_{24}^{-+} + y_{20}^{-+}) -6(y_{32}^{-+}) -3(y_{33}^{-+} + y_{31}^{-+}) \\
 &\quad +6(y_{34}^{-+} + y_{30}^{-+})
 \end{aligned}$$

$$\begin{aligned}
&= -2(y_{22}-y_{12}) -1(y_{23}-y_{13}+y_{21}-y_{11}) +2(y_{24}-y_{14}+y_{20}-y_{10}) \\
&\quad -6(y_{32}-y_{02}) -3(y_{33}-y_{03}+y_{31}-y_{01}) +6(y_{34}-y_{04}+y_{30}-y_{00}) \\
&= -6y_{00} + 3y_{01} + 6y_{02} + 3y_{03} - 6y_{04} - 2y_{10} +y_{11} +2y_{12} \\
&\quad +y_{13} - 2y_{14} + 2y_{20} - y_{21} - 2y_{22} - y_{23} + 2y_{24} +6y_{30} \\
&\quad -3y_{31} - 6y_{32} - 3y_{33} + 6y_{34} \\
&= \sum y_{\alpha} \xi_{i\alpha}
\end{aligned}$$

The main value of this shortcut lies in the fact that once Table III has been completed the same subsections of the table apply to the calculation of many of the required sums of products. Thus subsection (++) applies to the calculation of the sums of products with ξ_{00} , ξ_{20} , ξ_{22} , ξ_{02} , ξ_{04} and ξ_{24} ; subsection (+-) with ξ_{01} , ξ_{21} , ξ_{03} and ξ_{23} ; and so on.

The above folding procedure may be extended in like manner to cases involving more than two dimensions, the savings increasing with the number of dimensions.

Use of I. B. M. punch cards.

In passing it may be noted that these calculations are of such nature that punched card methods could be applied to them to great advantage. Thus "n" cards could be prepared by punching the observed values "y" on each card in the first two or three columns. The univariate orthogonal polynomial

values corresponding to the y 's could then be punched in the succeeding columns. From here the multiplying devices of an I. B. M. "Multiplier" could be used to provide both the additional multivariate orthogonal polynomial values needed and the sum of products $Sy\xi_j$. In this method the folding procedure might also be used to economize in cards, but it is doubtful that the benefits would compensate for the time required to construct the folded tables. Unfortunately, I. B. M. equipment was not available for the problem that follows and a calculating machine was used.

4.3 Application to a Specific Problem:

H. C. Breckon (1950) conducted an experiment with heat transfer in an externally heated fluidized bed of sova beads in which 450 temperature observations (y_α) were made. These readings were taken inside a vertical fluidized chamber, 30 inches in length and 3 inches in diameter. Each observation was the mean of 3, 4, or 5 individual readings. However, most means were based on four observations and for convenience it was assumed that each had the same expected variance, σ^2 .

The purpose of the experiment was to find the relationship of these readings with the following factors: x_1 , distance from center of chamber in inches; x_2 , height in chamber in inches; x_3 , mass superficial air velocity of dry

air forced through the column measured in lbs./hr./sq. ft.; x_4 , temperature maintained at the chamber wall. The levels investigated for each of the factors are shown together with the corresponding univariate orthogonal polynomial values in Table V.

Table V

	Distance from Center of Chamber (in inches)				
x_1	0	5/8	1 1/8	1 3/8	1 1/2
ϵ_2^*	-20	-17	-8	7	28
ϵ_4^*	18	9	-11	-21	14
ϵ_6^*	-20	1	22	-17	4
ϵ_8^*	70	-56	28	-8	1

	Height in Column (in inches)					
x_2	0	6	12	18	24	30
ϵ_1^*	-5	-3	-1	1	3	5
ϵ_2^*	5	-1	-4	-4	-1	5
ϵ_3^*	-5	7	4	-4	-7	5
ϵ_4^*	1	-3	2	2	-3	1
ϵ_5^*	-1	5	-10	10	-5	1

	Mass Superficial Air Velocities (in lbs./hr./sq.ft.)				
x_3	832	1020	1116	1218	1338
ϵ_1^*	-2	-1	0	1	2
ϵ_2^*	2	-1	-2	-1	2
ϵ_3^*	-1	2	0	-2	1
ϵ_4^*	1	-4	6	-4	1

	Temperature at Chamber Wall (°F)		
x_4	200	400	600
ξ_1	-1	0	1
ξ_2	1	-2	1

Readings were taken at each of the $n = 5 \times 6 \times 5 \times 3 = 450$ combinations of these levels, and are given in Appendix A.

Our aim in this problem is to fit a multivariate polynomial function which will explain the variations in the observed values in terms of the above x values. The method of multivariate polynomials first requires the transformation of these x values to univariate polynomials. In the following analysis this was done as shown in Table V.

In this particular example a circumstance, which we shall refer to subsequently as "the symmetry feature," arises which requires special comment. Since the x_1 readings extend from the center of the column to the outside over the length of one radius, it is reasonable to fit a polynomial with respect to x_1 which would give a continuous function when mapped along a complete diameter. With this in mind, only polynomials with even subscripts were defined with respect to x_1 as is shown in Table V. Further, in the fitting process, all readings taken at values of x_1 other than $x_1 = 0$ were assumed to be the sum of pairs of readings taken along a complete diameter, each

one being paired with its image reflected about the center. The reading taken at $x_1 = 0$ was reduced by one-half. The data treated in this way is shown in Appendix A. Following this idea through, it was necessary to assume in the fitting process that the number of original observations was $n' = 810$, and that the data as observed was already folded with respect to x_1 .

In the analysis of variance the error mean square is approximately one-half of what it would have been had each observation been treated as a single value. No attempt has been made to change this, however, since the same factor is present in each term of the analysis. This factor is not exactly one-half due to the separate treatment at $x_1 = 0$. This, further invalidates the assumption of homogeneity of variance but not, it is considered, to a serious extent.

It should also be observed that the x_1 and x_3 values are not quite equally spaced. However, if we let $x_1' = f(x_1)$ such that the values of x_1' are equally spaced, for all practical purposes it is as reasonable to investigate the polynomial relationships in terms of the x_1' 's as the x_1 's.

Upon defining $\epsilon_0' = 1$ for each dimension, the full set of orthogonal polynomials for the problem may now be obtained from Table V using the relationship $\epsilon_{i_1, i_2, i_3, i_4}' = \epsilon_{i_1}' \cdot \epsilon_{i_2}' \cdot \epsilon_{i_3}' \cdot \epsilon_{i_4}'$. For example, ϵ_{2222}' has the values shown

in part in Table VI. The complete table consists of eight sections which are mirror images of the values in Table VI reflected about the center of each of the axes for x_2 , x_3 , and x_4 . It is not necessary to "unfold" with respect to x_1 because of "the symmetry feature" discussed above.

The set of "folded" y values, corresponding to the ξ_{2222} values in Table VI is given in Table VII.

Table VI

		-2			-1			2								
		-20	-17	-8	7	28	-20	-17	-8	7	28	-20	-17	-8	7	28
-2	1	-80	-68	-32	28	112	-40	-34	-16	14	56	80	68	32	-28	-112
	3	-240	-204	-96	84	336	-120	-102	-48	42	168	240	204	96	-84	-336
	5	-400	-340	-160	140	560	-200	-170	-80	70	280	400	340	160	-140	-560
	1	40	34	16	-14	56	20	17	8	-7	-28	-40	-34	-16	14	56
	3	120	102	48	-42	-168	60	51	24	-21	-84	-120	-102	-48	42	168
	5	200	170	80	-70	-280	100	85	40	-35	-140	-200	-170	-80	70	200

Table VII

		Values of y^{++++}														
313	643	656	582	775	512	1063	1140	1039	1443	453	972	1125	1075	1472		
241	491	526	518	715	475	968	1013	966	1320	437	918	1047	1043	1449		
223	447	458	461	557	424	852	872	876	1049	448	906	933	912	1102		
587	1202	1241	1138	1490	1157	2379	2476	2272	2998	868	1819	2103	2103	2991		
547	1113	1125	1072	1380	980	2003	2134	2074	2741	945	1934	2071	2015	2722		
435	874	896	894	1073	900	1828	1878	1817	2180	884	1790	1833	1800	2126		

Then working from these two tables

$$(4.8) \quad \sum_{\alpha=1}^{810} y_{\alpha} \xi_{2222} = \sum \xi_{2222} y^{++++} = (-80)(313) + (-68)(643) + \dots + (280)(2126) = \underline{313,485}.$$

The orthogonal polynomial sum of squares,

$$(4.9) \quad \sum_{\alpha=1}^{810} \xi_{2222}^2 = \sum_{\alpha_1=0}^9 \xi_{2a_1}^2 \cdot \sum_{\alpha_2=0}^6 \xi_{2a_2}^2 \cdot \sum_{\alpha_3=0}^5 \xi_{2a_3}^2 \cdot \sum_{\alpha_4=0}^3 \xi_{2a_4}^2 = (2772)(80)(14)(6) = \underline{16,299,360}.$$

The corresponding regression coefficient,

$$(4.10) \quad b_{2222} = \frac{313,485}{16,299,360} = .01923.$$

All the regression coefficients obtained in this way correct to three decimal places are given in Table VIII. The values in the table have been doubled since due to the methods employed to allow for the symmetric feature, the "working y values" are one-half of the actual observed values.

Table VIII. Regression Coefficients (b_{11234})

		$i_3 = 0$					$i_3 = 1$					$i_3 = 2$					$i_3 = 3$					$i_3 = 4$				
$i_1 = 0$		2	4	6	8	0	2	4	6	8	0	2	4	6	8	0	2	4	6	8	0	2	4	6	8	
$i_4 = 0$	0	268.637	1.641	.825	.633	..038	7.038	-.420	.135	-.054	-.015	-1.041	.173	-.058	**	**	2.059	-.037	**	**	**	.532	**	**	**	**
	1	22.726	-.033	-.015	**	**	-2.618	.040	**	.	.	-.717	.021	**	.	.	.380	**	.	.	.	**	.	.	.	
	2	-6.824	-.131	-.057	-.069	**	-1.690	.051	-.020	.	.	1.060	.045	.012	.	.	-.343	.011	.	.	.	-.074	**	**	.	.
	3	-.631	.022	**	**	**	.534	-.010204	**	.	.	.	-.281087
	4	.504	-.058	**	**	**	.299	-.847	.024	**	.	.	.619	-.195	**	**	.	.
	5	**	**	**	**	**	.107	**094	**
$i_4 = 1$	0	115.585	.623	.484	.314	**	4.983	-.210	**	**	.	-3.536	.157	**	.	.	1.681	-.070	**	.	.	-.625	**	.	.	.
	1	11.064	-.030	**	-.027	**	-3.237	.066	**	**	.	.144	-.009836	**
	2	-5.396	-.051	-.029	-.030	**	-.717	.025	.	.	.	1.384	-.055	.	.	.	-.771	**	**	.	.	.
	3	.246	.010	**	**	.	.760	**	-.426	**
	4	**	**	**	**	.	**	-.936	1.279	-.352
	5	-.128	.007	**	**	.	.302	**
$i_4 = 2$	0	1.319	-.056	**	**	**	.978	.028	.	.	.	-1.174	**	.	.	.	-1.185	**	.	.	.	-.760
	1	-1.252	**	**	**	.	-.214	.008274	.011	.	.	.	**	**
	2	**	**	**	.	.	.289	**	.	.	.	**	.038	**	.	.	.234056
	3	.308	**	-.306	.010	.	.	.	**041
	4	-.276185	**666	-.240
	5	-.090	**	-.110

** investigated but not significant
 * not investigated

The regression sum of squares due to fitting ξ_{2222} ,

$$(4.11) \quad \text{Reg. SS} = \frac{(313,485)^2}{16,299,360} = \underline{6029}.$$

An analysis of variance is given below followed by a break-down of the individual degrees of freedom in the table of mean squares (Table IX).

Analysis of Variance

Source of variation	S.S. ⁵	d.f.	M.S. ⁵
Regression	18,563,698	117	158,644
Error	25,085	333	75
<hr/>			
Total	18,588,783	450	

5. These terms include a common factor of $\frac{1}{2}$ (see page 28).

Table IX

Table of Mean Squares

$\epsilon_{i_1 i_2 i_3 i_4}$	M.S.	$\epsilon_{i_1 i_2 i_3 i_4}$	M.S.	$\epsilon_{i_1 i_2 i_3 i_4}$	M.S.
0000	14,613,586	2200	14,898	0130	484
2000	167,946	4200	2,071	0210	16,190
4000	30,645	6200	2,936	0220	8,923
6000	17,837	2300	928	0230	668
8000	410	2400	976	0240	217
				0310	3,466
0100	1,220,110	2001	16,156	0320	711
0200	132,010	4001	7,042	0330	960
0300	2,419	6001	2,919	0340	648
0400	240	2002	393	0410	170
				0420	1,898
0010	20,063	2010	22,015	0430	725
0020	9,261	4010	1,632	0440	504
0030	1,717	6010	263	0510	194
0040	803	8010	122	0530	152
		2030	166		
0001	1,803,591	2020	5,222	0101	192,803
0002	704	4020	423	0102	7,412
				0201	55,026
2100	809	0110	32,377	0301	245
4100	121	0120	3,403	0302	1,149

$\epsilon_{i_1 i_2 i_3 i_4}$	M.S.	$\epsilon_{i_1 i_2 i_3 i_4}$	M.S.	$\epsilon_{i_1 i_2 i_3 i_4}$	M.S.
0402	144	0441	1,094	2201	1,514
0501	93	0122	997	4201	342
0502	138	0322	3,188	6201	379
		0522	581		
0011	6,705	0342	289	2110	2,326
0012	775	0212	950	2200	4,865
0021	4,725	0412	129	4220	258
0022	1,563	0232	623	2420	470
0031	763	0432	1,679	2310	353
0032	1,138	0231	2,246	2120	865
0041	739	0431	2,060	2210	4,616
0042	3,278	0242	252	4210	513
		0442	1,527	2230	212
0111	33,012				
0211	1,944	2011	3,661	2221	4,946
0311	4,681	2012	189	2222	6,029
0511	1,036	2031	404	2122	480
0121	92	2021	2,883	2322	1,174
0131	2,204			2111	4,265
0331	1,469	2101	424	2211	753
0112	434	2501	86	2121	122
0221	10,138	6101	248	2112	200
0421	1,546	2301	132		

Least squares estimates, \hat{y}_α , have been calculated from the regression coefficients and $\epsilon_{i_1 i_2 i_3 i_4}$ terms corresponding to a portion of the data. These are given in Table X together with the corresponding observed values, y_α , in the order $\begin{matrix} y_\alpha \\ \hat{y}_\alpha \end{matrix}$.

Table X

		$a_3=4$				
		$a_1 = 0$	1	2	3	4
a_2						
0		228	231	217	189	229
		220	220	209	187	244
1		348	352	358	318	425
		341	351	354	321	429
$a_4=2$	2	396	403	408	382	528
		403	416	427	383	510
3		438	443	452	431	554
		435	448	454	417	549
4		428	431	441	426	550
		425	435	442	427	545

This table is not complete but will serve to illustrate the final results of the least squares estimation.

In fitting the least squares estimate it would have been most desirable to use the method of "pooling for error" previously discussed. However, since no I. B. M. equipment

was available it was impracticable to fit all the terms this requires. Instead, it was decided arbitrarily to include in the error all mean squares lower than 75, and the fitting process was continued until the residual mean square was reduced to this figure. In doing this, the regression on polynomials which were products of polynomials already found to give significant regression coefficients were investigated first. The arbitrary choice of a mean square of 75 implies that the standard deviation of the errors about the estimated values is $\sqrt{2 \times 75}$ or a little more than 12 degrees fahrenheit. This was considered a satisfactory compromise relative to the additional work required to reduce it further.

Value of the Method

The value of the method will vary according to the purposes of the experimenter. The following are examples of the many end results which could be obtained.

(a). A given experimenter may be interested primarily in obtaining the least squares estimates themselves from the point of view of giving the best estimate for y at any combination of the independent variables. In this case the table of estimated values would provide the best estimates in the sense of having minimum variance. Thus in the heat transfer example the best estimate of the temperature in the

column at a distance $1 \frac{1}{8}$ inches from the center, 6 inches from the bottom, with mass superficial air velocity of 1338 lbs./hr./sq.ft., and with temperature of outer wall at 600 degrees fahrenheit is 354 degrees fahrenheit. The observed reading in the chamber at this point was 358.

(b). Interest might lie more in the significance of each of the regression coefficients, or in batches of the regressions, e.g. the experimenter may be interested in the over-all regression due to $\xi_{01_2 00}$, or in the individual regression coefficients to evaluate the effects of an independent variable.

(c). In the preceding problem the investigator was primarily interested in the partial effect of each variable on the temperature with the remaining variables held constant. This effect could be graphed by summing over the three fixed variables and plotting the sums with respect to the fourth variable. Further, from the fitted function, $\hat{y}_\alpha = \sum b \xi$ we are able to obtain a function of the form

$$(4.12) \quad \hat{y}_\alpha = \sum b_{i_1 i_2 i_3 i_4} x_1^{i_1} x_2^{i_2} x_3^{i_3} x_4^{i_4},$$

and by taking the partial derivatives of \hat{y}_α with respect to each of the x variables we are able to plot the relationships between y and the independent variables at any point in the

chamber. The latter method gives a more complete picture of the true relationships existing.

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Appendix A.

$\sqrt{a_1 a_2 a_3 a_4}$

		$a_3 = 0$					$a_3 = 1$					$a_3 = 2$					$a_3 = 3$					$a_3 = 4$				
$a_1 = 0$		1	2	3	4	0	1	2	3	4	0	1	2	3	4	0	1	2	3	4	0	1	2	3	4	
a_2	$a_4 = 0$	0	1	2	3	4	0	1	2	3	4	0	1	2	3	4	0	1	2	3	4	0	1	2	3	4
0	0	92	91	94	98	115	94	94	97	100	116	92	92	95	98	116	86	86	89	90	110	92	93	94	93	112
1	1	96	99	111	114	158	100	101	112	120	164	96	100	117	116	171	96	98	110	112	152	112	111	115	113	156
2	2	106	113	153	137	197	110	116	135	136	202	108	114	138	141	200	144	146	149	138	191	148	149	150	147	195
3	3	120	129	154	158	211	122	130	158	158	205	170	170	176	172	217	176	180	185	167	208	176	176	179	173	211
4	4	136	146	175	176	227	144	153	174	178	222	194	196	201	191	232	196	198	201	190	231	182	183	186	182	221
5	5	152	162	188	189	218	190	192	196	192	214	204	205	206	203	224	196	199	201	199	219	180	180	182	181	203
0	0	88	90	101	107	165	94	95	101	108	157	94	95	102	104	157	84	83	89	93	135	128	131	128	119	155
1	1	104	114	156	161	294	104	115	154	152	274	114	119	150	159	273	168	168	169	145	231	230	243	245	213	283
2	2	136	159	230	230	283	136	154	222	217	353	280	284	298	252	365	262	270	276	241	334	282	290	290	259	369
3	3	176	204	284	286	431	320	329	329	292	388	346	359	358	330	410	306	310	313	289	368	312	319	321	300	289
4	4	220	239	318	356	469	358	364	367	349	421	368	372	376	359	442	320	321	323	320	394	320	322	328	313	403
5	5	364	366	381	370	414	358	359	363	361	399	352	352	356	357	400	312	315	319	314	358	316	319	323	316	368
0	0	88	91	107	108	199	100	101	114	125	207	106	107	120	125	209	184	204	221	151	243	228	231	217	189	229
1	1	108	120	177	203	390	120	130	192	205	397	332	345	327	298	400	338	349	357	311	417	348	352	358	318	425
2	2	148	168	262	312	524	388	407	428	361	521	420	432	437	371	511	416	427	433	387	531	396	403	408	382	528
3	3	204	238	363	363	571	496	509	522	468	577	476	486	490	454	562	462	464	466	457	563	438	443	452	431	554
4	4	480	492	508	483	595	512	516	522	509	595	472	472	480	467	577	454	458	466	449	563	428	431	441	426	550
5	5	512	513	517	512	557	498	499	502	505	556	468	470	475	468	524	452	453	458	455	515	424	429	434	430	493