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AN EXTENSION OF KRAWTCHOUK'S POLYNOMIALS TO THE CONSTRUCTION OF ORTHOGONAL POLYNOMIALS FOR UNEQUALLY WEIGHTED MEANS

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ABSTRACT

A simple method is described for the construction of a set of orthogonal polynomials for any case where the proportions of observations follow a binomial distribution. The least squares equation which fits the data is determined using the properties of orthogonal polynomials and the analysis of variance technique. The computations required for determining orthogonal polynomials are described with an example.

KEY WORDS: Krawtchouk's and Orthogonal Polynomials

INTRODUCTION

The method of orthogonal polynomials are used to fit a polynomial model of any order in one variable provided the values of the independent variable are equally spaced and/or equally weighted (Draper and Smith, 1981). These limitations restricts its use in many possible applications because orthogonal coefficients when the independent variable are unequally spaced and/or unequally weighted are not available in statistical tables; they must be calculated (Narula, 1979; Okolo and Bamiduro, 2003).

In the usual applications of orthogonal polynomials for cases of equal numbers of observations at all points on the scale of the independent (trend) variable, a set of linearly independent functions is used (Copper, 1971 and Kuo et al., 1991) whose members satisfy the condition of orthogonality

$$\sum_{i=1}^{n} f_j(x_i) f_k(x_i) = \delta_{jk}, \tag{1}$$

where n is the number of levels on the trend variable x, $f_j(x)$ and $f_k(x)$ are members of the set of orthogonal functions, and $\delta_{jk} = 0$ if j ≠ k. According to Okolo and Bamiduro (2004), this condition is a special case of the more general property of orthogonality, i.e. where $f_j(x)$ and $f_k(x)$ are said to be orthogonal under the weight function w(x) if

$$\sum_{i=1}^{n} w(x_i) f_j(x_i) f_k(x_i) = \delta_{jk}. \tag{2}$$

Several sets of functions which are orthogonal in this sense are known (Askey, 1975), and some may prove useful for the analysis of trend in certain cases of unequal numbers of observations at the different levels of x. In a particular application, this will depend mainly upon whether or not the values of $w(x_i)$ are adequate representations of the proportions of observations at the points x_i, i = 1, 2, ..., n.

Szego (1975) reported that the Krawtchouk's polynomials are orthogonal on a finite or enumerable set of points. He developed their weight function as the binomial probabilities

$$w(x) = \binom{n}{x} P^x q^{n-x} \quad \text{for p, q > 0 and p + q = 1.} \tag{3}$$

For a given weight function w(x), consider the case where the proportions of observations associated with the treatment levels x_i in an experiment follow a consistent structure, that is, some functional relation, such as equation (3). It may be necessary to develop procedures that can be used to generate orthogonal coefficients for such definite relationship.

This paper applies the weight function for the Krawtchouk's polynomials described by Szego (1975) to the construction of orthogonal polynomials where the numbers of observations at the different treatment levels are determined by the corresponding proportions in the population.

DEVELOPMENT

Let C_j denote the coefficient of $f_j(x)$ in the regression equation. If $w(x_i) = N_i$, the number of observations at x_i, then, the least squares curve $\hat{Y}$ which best fits the n observations Y_{x_i} can be expressed as the condition that the

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Error sum of squares (SSE) = $\sum_{i=1}^{n} w(x_i)(Y_{x_i} - \hat{Y})^2$ (4)

be minimal (Farebrother, 1974). Using the orthogonality property given in equation (2), the normal equations resulting from a least squares differentiation of SSE according to Robert et. al. (1975) are:

$$C_0\sum_{i=1}^{n} w(x_i)f_0^2(x_i) + 0 + 0 + --- + 0 = \sum_{i=1}^{n} w(x_i)Y_{x_i}f_0(x_i)$$

$$0 + C_1\sum_{i=1}^{n} w(x_i)f_1^2(x_i) + 0 + 0 + --- + 0 = \sum_{i=1}^{n} w(x_i)Y_{x_i}f_1(x_i)$$

$$0 + 0 + C_2\sum_{i=1}^{n} w(x_i)f_2^2(x_i) + 0 + --- + 0 = \sum_{i=1}^{n} w(x_i)Y_{x_i}f_2(x_i)$$

$$0 + 0 + 0 + C_3\sum_{i=1}^{n} w(x_i)f_3^2(x_i) + 0 + --- + 0 = \sum_{i=1}^{n} w(x_i)Y_{x_i}f_3(x_i)$$

$$0 + 0 + 0 + --- + C_j\sum_{i=1}^{n} w(x_i)f_j^2(x_i) = \sum_{i=1}^{n} w(x_i)Y_{x_i}f_j(x_i) \quad (5)$$

The solution to the system (5) is

$$C_0 = \frac{\sum_{i=1}^{n} w(x_i)Y_{x_i}f_0(x_i)}{\sum_{i=1}^{n} w(x_i)f_0^2(x_i)},$$

$$C_1 = \frac{\sum_{i=1}^{n} w(x_i)Y_{x_i}f_1(x_i)}{\sum_{i=1}^{n} w(x_i)f_1^2(x_i)},$$

$$C_2 = \frac{\sum_{i=1}^{n} w(x_i)Y_{x_i}f_2(x_i)}{\sum_{i=1}^{n} w(x_i)f_2^2(x_i)},$$

$$C_3 = \frac{\sum_{i=1}^{n} w(x_i)Y_{x_i}f_3(x_i)}{\sum_{i=1}^{n} w(x_i)f_3^2(x_i)},$$

$$C_j = \frac{\sum_{i=1}^{n} w(x_i)Y_{x_i}f_j(x_i)}{\sum_{i=1}^{n} w(x_i)f_j^2(x_i)}. \quad (6)$$

It is evident, therefore, that each regression coefficient can be calculated independently of all the others.

The error sum of squares can be written (Kuo et. al., 1991)as

$$
\begin{aligned}
SSE &= \sum_{i=1}^{n} w(x_i)\left[Y_{x_i} - \hat{Y}\right]^2 \\
&= \sum_{i=1}^{n} w(x_i)\left[Y_{x_i} - \bar{Y}\right]^2 - \sum_{i=1}^{n} w(x_i)\left[\hat{Y}_i - \bar{Y}\right]^2 \\
&= \sum_{i=1}^{n} w(x_i)\left[Y_{x_i} - \bar{Y}\right]^2 - C_1^2\sum_{i=1}^{n} w(x_i)f_1^2(x_i) \\
&\quad - C_2^2\sum_{i=1}^{n} w(x_i)f_2^2(x_i) - \dots\dots\dots - C_j^2\sum_{i=1}^{n} w(x_i)f_j^2(x_i) \\
&= SST - SS_{C_1} - SS_{C_2} - \dots\dots\dots - SS_{C_j} \qquad (7)
\end{aligned}
$$

The quantity SST

$$
\begin{aligned}
&= \sum_{i=1}^{n} w(x_i)\left[Y_{x_i} - \bar{Y}\right]^2 \\
&= \sum_{i=1}^{n} w(x_i)Y_{x_i}^2 - C_0^2\sum_{i=1}^{n} w(x_i)f_0^2(x_i) \\
&= \sum_{i=1}^{n} w(x_i)Y_{x_i}^2 - SS_{C_0} \qquad (8)
\end{aligned}
$$

is the total sum of squares and $SS_{C_j} = C_j^2\sum_{i=1}^{n} w(x_i)f_j^2(x_i)$ is the reduction in sums of squares due to fitting the jth degree polynomial. Furthermore, due to the orthogonality of f_j's, the reductions of the error sum of squares due to each successive power of x are independent. Thus, it is possible to immediately assess the importance of each additional power of x and any added term that does not reduce SSE significantly may be considered redundant

The SS_{C_j} is calculated by means of equation (6) to yield the result

$$
\begin{aligned}
SS_{C_j} &= C_j^2\sum_{i=1}^{n} w(x_i)f_j^2(x_i) \\
&= \left[\frac{\sum_{i=1}^{n} w(x_i)Y_{x_i}f_j(x_i)}{\sum_{i=1}^{n} w(x_i)f_j^2(x_i)}\right]^2 \sum_{i=1}^{n} w(x_i)f_j^2(x_i) \\
&= \frac{\left[\sum_{i=1}^{n} w(x_i)Y_{x_i}f_j(x_i)\right]^2}{\sum_{i=1}^{n} w(x_i)f_j^2(x_i)} \qquad (9)
\end{aligned}
$$

with 1 degree of freedom. Equation (9) is used to prepare the analysis of variance table (Elhay et. al., 1991).

Suppose the proportions of observations follow a binomial distribution, the Krawtchouk's polynomials (Szego, 1975) could be applied since the weight function is

$$w(x) = \binom{n}{x} p^x q^{n-x}, \quad \text{for p, q > 0 and p + q = 1.}$$

The symmetric distribution (p = q =1/2) would probably be applied more often than any other, and it is especially convenient, since the values of $k_{n,j}(x)$, the Krawtchouk's polynomial of the jth degree can be generated by the following recursion relations which are adapted from Szego (1975) and are valid for use with $w(x) = \binom{n}{x}$.

$$K_{n,0}(x) = 1, \qquad x = 0, 1, 2, \ldots, n.$$

$$K_{n,j}(0) = \binom{n}{j}, \qquad j = 0, 1, 2, \ldots, n$$

$$K_{n,j}(x) = K_{n,j}(x-1) - K_{n,j-1}(x-1) - K_{n,j-1}(x), \qquad \begin{cases} x = 1, 2, \ldots, n. \\ j = 1, 2, \ldots, n. \end{cases}$$

The construction of a table of $K_{n,j}(x)$ for a given n, according to these recursion relations, is quickly accomplished as exemplified in Table 1.

Table 1 The values of $K_{n,j}(x)$ for n = 5, p = q = ½

		J					
W(x)	x	0	1	2	3	4	5
0	0	1	5	10	10	5	1
5	1	1	3	2	−2	−3	−1
10	2	1	1	−2	−2	1	1
10	3	1	−1	−2	2	1	−1
5	4	1	−3	2	2	−3	1
1	5	1	−5	10	−10	5	-1

The first column is filled in immediately with ones, and the first row is filled in with the binomial coefficients. Then each of the remaining cells is filled in with the value obtained by subtracting the sum of the cells to the upper left and directly to the left, from the cell directly above. In checking for errors, it is valuable to note the symmetrical properties of the table, and that there are j sign changes in row j or column j.

If the regression equation is to be used for interpolation, explicit formulas are needed for $K_{n,j}(x)$ since the recursion relations give values only for x an integer. The following generating formula is valid for p = q = ½ , and the formulas derived from it give the same values as the recursion relations for integral values of x (Szego, 1975):

$$K_{n,j}(x) = \binom{n}{j} \sum_{r=0}^{j} (-2)^r \frac{\binom{x}{r}\binom{j}{r}}{\binom{n}{r}}, \tag{10}$$

and in particular,

$$K_{n,0}(x) = 1$$

$$K_{n,1}(x) = \binom{n}{1}\left[1 - 2\frac{x}{n}\right]$$

$$K_{n,2}(x) = \binom{n}{2}\left[1 - 4\frac{x}{n} + 4\frac{x(x-1)}{n(n-1)}\right]$$

$$K_{n,3}(x) = \binom{n}{3}\left[1 - 6\frac{x}{n} + 12\frac{x(x-1)}{n(n-1)} - 8\frac{x(x-1)(x-2)}{n(n-1)(n-2)}\right], etc.$$

EXAMPLE

The method and its use will be illustrated by means of a hypothetical data.

Suppose it is desired to fit a third order polynomial of crop yield on applied fertilizer. The experiment was planned with ten replications of each fertilizer rate, but, due to an accident during harvest, yield data from a number of replicates were lost. The data is shown in Table 2.

Table 2: Crop yield

Crop yields (cwt/acre)	Fertilizer rate (kg/acre)	No. of replications w(x)
8	0	1
12	1	5
22	2	10
31	3	10
36	4	5
44	5	1

In Table 3, the details of all computations are outlined.

Table 3: Outline of computational procedures

Y	$w(x)$	$k_{5,0}$	$k_{5,1}$	$k_{5,2}$	$k_{5,3}$	$w(x)Yk_{5,0}$	$w(x)Yk_{5,1}$	$w(x)Yk_{5,2}$	$w(x)Yk_{5,3}$	$w(x)k_{5,0}^2$	$w(x)k_{5,1}^2$	$w(x)k_{5,2}^2$	$w(x)k_{5,3}^2$	$w(x)Y^2$
8	1	1	5	10	10	8	40	80	80	1	25	100	100	64
12	5	1	3	2	-2	60	180	120	- 120	5	45	20	20	720
22	10	1	1	-2	-2	220	220	- 440	- 440	10	10	40	40	4840
31	10	1	-1	-2	2	310	- 310	- 620	620	10	10	40	40	9610
36	5	1	-3	2	2	180	- 540	360	360	5	45	20	20	6480
44	1	1	-5	10	-10	44	- 220	440	- 440	1	25	100	100	1936
Sum	32					822	-630	-60	60	32	160	320	320	23,650

The C_i are calculated as follows;

$$C_0 = \frac{\sum_{i=1}^{n} w(x_i)Yk_{5,0}}{\sum_{i=1}^{n} w(x_i)k_{5,0}^2} = \frac{822}{32} = 25.6875$$

$$C_1 = \frac{\sum_{i=1}^{n} w(x_i)Yk_{5,1}}{\sum_{i=1}^{n} w(x_i)k_{5,1}^2} = \frac{-630}{160} = -3.9375$$

$$C_2 = \frac{\sum_{i=1}^{n} w(x_i)Yk_{5,2}}{\sum_{i=1}^{n} w(x_i)k_{5,2}^2} = \frac{-60}{320} = -0.1875$$

$$C_3 = \frac{\sum_{i=1}^{n} w(x_i)Yk_{5,3}}{\sum_{i=1}^{n} w(x_i)k_{5,3}^2} = \frac{60}{320} = 0.1875$$

The sums of squares are then calculated as shown below and are used to prepare the analysis of variance table.

$$SS_T = \sum_{i=1}^{n} w(x_i)Y_{x_i}^2 = 23{,}650$$

$$SS_{C_0} = \frac{\left[\sum_{i=1}^{n} w(x_i)Yk_{5,0}\right]^2}{\sum_{i=1}^{n} w(x_i)k_{5,0}^2} = \frac{(822)^2}{32} = 21{,}115.125$$

$$SS_{C_1} = \frac{\left[\sum_{i=1}^{n} w(x_i)Yk_{5,1}\right]^2}{\sum_{i=1}^{n} w(x_i)k_{5,1}^2} = \frac{(-630)^2}{160} = 2{,}480.625$$

$$SS_{C_2} = \frac{\left[\sum_{i=1}^{n} w(x_i)Yk_{5,2}\right]^2}{\sum_{i=1}^{n} w(x_i)k_{5,2}^2} = \frac{(-60)^2}{320} = 11.25$$

$$SS_{C_3} = \frac{\left[\sum_{i=1}^{n} w(x_i)Yk_{5,3}\right]^2}{\sum_{i=1}^{n} w(x_i)k_{5,3}^2} = \frac{(60)^2}{320} = 11.25$$

The analysis of variance in Table 4 summarizes the sums of squares needed to test the coefficients in the orthogonal model and the corresponding residual sums of squares.

Table 4: Analysis of variance

Source	Df	SS	MS
Total	32	23,650.00	
Constant	1	21,115.125	21,115.125
residual31		2,534.875	81.770
Linear	1	2,480.625	2,480.625
residual30		54.25	1.808
Quadratic	1	11.25	11.25
residual29		43.00	1.48
Cubic	1	11.25	11.25
Residual	28	31.75	1.13

The mean squares for each term are compared to the corresponding residual mean squares by an F-test as shown in Table 5.

Table 5: F – TESTS

Regression term	$F_{(Computed)}$	$F_{(tabular)}$	Comment
Constant	f = 256.23	$F_{1,31;\,0.05}$ = 4.16	Significant
Linear	f = 1372.03	$F_{1,30;0.05}$ = 4.17	Significant
Quadratic	f = 7.60	$F_{1,29;0.05}$ = 4.18	Significant
Cubic	f = 9.96	$F_{1,28;0.05}$ = 4.20	Significant

The fitted orthogonal model is thus

$Y = 25.6875 - 3.9375k_{n,1}(x) - 0.1875k_{n,2}(x) + 0.1875k_{n,3}(x)$

where the $K_{n,j}(x)$ are evaluated in terms of x according to equation (10) with n = 5.

CONCLUSION

Orthogonal polynomials are commonly used in the analysis of variance for the construction of orthogonal contrasts among equally spaced levels of a treatment factor. The existence of statistical tables giving the compounding coefficients for these particular contrasts often influences the experimenter to choose an equal weighting at the different treatment levels. Orthogonal polynomials when treatment levels are unequally spaced and/or unequally weighted are not available in statistical tables. They must be calculated. For cases where the proportions of observations follow a binomial distribution, the simple method described for constructing orthogonal polynomials frees the experimenter from this sometimes undesirable restriction.

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