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# QUARTIC ROTATION CRITERIA AND ALGORITHMS

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Most of the currently used analytic rotation criteria for simple structure in factor analysis are summarized and identified as members of a general symmetric family of quartic criteria. A unified development of algorithms for orthogonal and direct oblique rotation using arbitrary criteria from this family is given. These algorithms represent fairly straightforward extensions of present methodology, and appear to be the best methods currently available.

Key words: factor analysis, simple structure, factor loadings, planar rotations.

## 1. Introduction

Analytic rotation for simple structure in factor analysis proceeds by minimizing or maximizing a criterion which is usually a quartic function of the factor loadings over a family of rotationally equivalent loading matrices. Early work in this area was carried out independently by Carroll (1953), Ferguson (1954), Newhaus and Wrigley (1954), and Saunders (1953). (Harman, 1976, gives a nice account of the history and motivation behind the development of analytic rotation.) Carroll's work dealt primarily with oblique rotation while that of Ferguson, Newhaus and Wrigley, and Saunders was devoted to orthogonal rotation. We will discuss the orthogonal case first. In this case the criteria proposed by the authors named, while expressed in various forms, were all equivalent under orthogonal rotation to the *quartimax* criterion:

$$\text{QMAX} = \sum_{i=1}^{p} \sum_{r=1}^{m} \lambda_{ir}^4, \tag{1}$$

where the $\lambda_{ir}$ denote the components of a $p$ by $m$ matrix $\Lambda = (\lambda_{ir})$ of factor loadings. The algorithms employed by the various authors were also equivalent; all were based on planar rotations. The algorithms proceeded by stepping uniformly through pairs of factors. Each pair was orthogonally rotated in the plane it defined to a position that optimized the relevant criterion over all possible orthogonal rotations of the factor pair. This process was continued until it converged to a loading matrix $\Lambda$ that hopefully optimized the criterion over all loading matrices orthogonally equivalent to an initial loading matrix $A$.

Kaiser (1958) proposed an alternative criterion for orthogonal rotation called the *varimax* criterion:

$$\text{VMAX} = \sum_{i=1}^{p} \sum_{r=1}^{m} \lambda_{ir}^4 - \frac{1}{p} \sum_{r=1}^{m} \left( \sum_{i=1}^{p} \lambda_{ir}^2 \right)^2, \tag{2}$$

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which is again a quartic function of the loadings $\lambda_{ir}$. The algorithm used by Kaiser (1959) to maximize the varimax criterion was, as before, based on planar rotations.

A natural generalization of the quartimax and varimax criteria are the *orthomax* criteria:

$$\text{ORMAX} = \sum_{i=1}^{p} \sum_{r=1}^{m} \lambda_{ir}^4 - \frac{\gamma}{p} \sum_{r=1}^{m} \left( \sum_{i=1}^{p} \lambda_{ir}^2 \right)^2. \tag{3}$$

This family of criteria includes quartimax and varimax by choosing $\gamma$ equal to 0 and 1 respectively. It was apparently suggested by Carroll and appeared in Harman (1960, p. 334). Planar rotation algorithms for the orthomax criteria were implemented and incorporated into the BMDP, SAS, and SPSS factor analysis programs. Jennrich (1970) discussed planar rotation algorithms for orthogonal rotation in a general context which included orthomax rotation and gave several examples.

Independently, Crawford and Ferguson (1970) proposed a family of criteria for orthogonal rotation:

$$\text{CF} = K_1 \sum_{r \neq s} \sum_{i=1}^{p} \lambda_{ir}^2 \lambda_{is}^2 + K_2 \sum_{i \neq j} \sum_{r=1}^{m} \lambda_{ir}^2 \lambda_{jr}^2 \tag{4}$$

that is equivalent to the orthomax family and discussed the application of this family. They apparently also used planar rotations to optimize their criteria.

The algorithms for orthomax rotation used by BMDP and SPSS are discussed in section 3. The algorithm used by SAS is apparently similar if not identical to those used by BMDP and SPSS.

The initial development of analytic rotation in the oblique case was done by Carroll (1953) who introduced the *quartimin* criterion:

$$\text{QMIN} = \sum_{r \neq s} \sum_{i} \lambda_{ir}^2 \lambda_{is}^2. \tag{5}$$

In Carroll (1953), and in other early work on oblique rotation, the $\lambda_{ir}$ represent covariances between the observed variables and what are called *reference factors* (see, e.g., Harman, 1976, p. 270). The quartimin criterion is a natural generalization of the quartimax criterion to the oblique case. As an oblique generalization to the varimax criterion Kaiser (1958) proposed:

$$\text{CMIN} = \sum_{r \neq s} \left( \sum_{i} \lambda_{ir}^2 \lambda_{is}^2 - \frac{1}{p} \sum_{i} \lambda_{ir}^2 \sum_{i} \lambda_{is}^2 \right) \tag{6}$$

which Carroll (1957) called the *covarimin* criterion. Generalizing both these criteria, Carroll (1957, 1960) introduced the *oblimin* family:

$$\text{OBMIN} = \sum_{r \neq s} \left( \sum_{i} \lambda_{ir}^2 \lambda_{is}^2 - \frac{\gamma}{p} \sum_{i} \lambda_{ir}^2 \sum_{i} \lambda_{is}^2 \right). \tag{7}$$

The choices $\gamma = 0$ and $\gamma = 1$ give the quartimin and covarimin criteria.

Carroll (1960) gave an elegant algorithm for optimizing the oblimin criterion applied to a reference structure matrix. This algorithm did not use planar rotations.

Jennrich and Sampson (1966) gave an algorithm for minimizing the quartimin criterion applied directly to the factor loadings. This algorithm was based on planar rotations similar to those used in the orthogonal case. It was later generalized to handle the oblimin family and has been incorporated into the BMDP and SPSS factor analysis programs. It and further generalizations are given in section 4.

Harman (1976) has called the application of oblique rotation criteria to factor loading matrices, rather than to reference structure matrices, *direct* methods. They are conceptually simpler than those using reference factors and for this reason we will restrict our attention here to them. Thus in both the orthogonal and oblique cases the criteria to be optimized will be applied directly to the factor loadings.

There are analytic rotation methods which are not based on quartic criteria. These include, for example, *oblimax* (Saunders, 1961) and *promax* (Hendrickson & White, 1964). Our discussion here, however, is restricted to methods based on quartic criteria.

## 2. Quartic Rotation Criteria

As noted, most analytic rotation criteria for simple loadings are quartic functions of the loadings. If these functions are homogeneous quadratic functions of the squares of the loadings and are row and column symmetric; that is, are invariant under permutations of the rows and columns of the loading matrix, then, as shown in the Appendix, they must have the form:

$$F = \kappa_1 F_1 + \kappa_2 F_2 + \kappa_3 F_3 + \kappa_4 F_4 \tag{8}$$

for some constants $\kappa_1$, $\kappa_2$, $\kappa_3$ and $\kappa_4$ where

$$F_1 = \left(\sum_{i=1}^{p} \sum_{r=1}^{m} \lambda_{ir}^2\right)^2, \quad F_2 = \sum_{i=1}^{n} \left(\sum_{r=1}^{m} \lambda_{ir}^2\right)^2$$
$$F_3 = \sum_{r=1}^{m} \left(\sum_{i=1}^{p} \lambda_{ir}^2\right)^2, \quad F_4 = \sum_{i=1}^{p} \sum_{r=1}^{m} \lambda_{ir}^4. \tag{9}$$

We will call this the *general symmetric family* of quartic criteria. Table 1 gives the choices of $\kappa_1$, $\kappa_2$, $\kappa_3$ and $\kappa_4$ that lead to the criteria discussed in section 1.

TABLE 1.

Specific Criteria in the General Symmetric Family

| | Criterion | $\kappa_1$ | $\kappa_2$ | $\kappa_3$ | $\kappa_4$ | min/max |
|---|---|---|---|---|---|---|
| Orthogonal | Quartimax | 0 | 0 | 0 | 1 | max |
| | Varimax | 0 | 0 | $-1/p$ | 1 | max |
| | Crawford-Ferguson | 0 | $K_1$ | $K_2$ | $-K_1 - K_2$ | min |
| | Orthomax | 0 | 0 | $-\gamma/p$ | 1 | max |
| Oblique | Quartimin | 0 | 1 | 0 | $-1$ | min |
| | Covarimin | $-1/p$ | 1 | $-1/p$ | 1 | min |
| | Oblimin | $-\gamma/p$ | 1 | $\gamma/p$ | $-1$ | min |
| | Crawford-Ferguson | 0 | $K_1$ | $K_2$ | $-K_1-K_2$ | min |

In the orthogonal case the terms in (8) involving $\kappa_1$ and $\kappa_2$ are invariant under rotation, so these may be dropped without loss of generality. Also since the Criteria (8) are equivalent under (positive) scalar multiplication, what remains in the orthogonal case after removing terms involving $\kappa_1$ and $\kappa_2$ is a one dimensional family which is equivalent to both the orthomax and the Crawford-Ferguson families. In the oblique case the general symmetric family is three dimensional and hence generalizes the oblimin and the oblique Crawford-Ferguson families which are one dimensional. Note, however, that specific members of the oblimin family, covarimin for example, involve all four terms in the general symmetric family (8).

A number of other facts are clear from Table 1. Under orthogonal rotation the quartimax and quartimin criteria are equivalent, as are the varimax and covarimin criteria, and the orthomax and oblimin families. While the Crawford-Ferguson and oblimin families are equivalent under orthogonal rotation, they differ under oblique rotation.

Algorithms for the general symmetric family for orthogonal rotation are given in section 3. Those for oblique rotation are given in section 4.

## 3. Orthogonal Rotation Algorithms

As indicated, all of our algorithms will be planar rotation algorithms. In the orthogonal case this means selecting pairs of columns $\lambda_r$ and $\lambda_s$ of the loading matrix $\Lambda$ and transforming them by a rotation of the form

$$\begin{aligned} \tilde{\lambda}_{ir} &= \lambda_{ir} \cos \theta + \lambda_{is} \sin \theta, \qquad \text{and} \\ \tilde{\lambda}_{is} &= -\lambda_{ir} \sin \theta + \lambda_{is} \cos \theta \end{aligned} \tag{10}$$

that maximizes the criterion $F$ over all such transformations. The algorithms step uniformly through all possible pairs until they converge. We have, without loss of generality, assumed here that the maximum, rather than the minimum, of $F$ is required.

Let $F(\theta)$ be the value of $F$ corresponding to the Rotation (10). Jennrich (1970) has shown that $F(\theta)$ must have the form

$$F(\theta) = c + a \cos (4\theta) + b \sin (4\theta). \tag{11}$$

As can be seen from Figure 1, $F(\theta)$ is maximized if and only if the vector ($\cos 4\theta$, $\sin 4\theta$) has the same direction as the vector $(a, b)$. It is sufficient to choose

$$\theta = \tfrac{1}{4} \text{ATAN2} (b, a), \tag{12}$$

where ATAN2 $(b, a)$ is the angle from the vector (0, 1) to the vector $(a, b)$. The slightly strange notation "ATAN2" is used because it happens to be a FORTRAN 77 function.

Since the optimizing values of $\sin 4\theta$ and $\cos 4\theta$ are easily expressed in terms of $a$ and $b$, one can, as observed by Nevels (1986), compute optimizing values for $\sin \theta$ and $\cos \theta$ by using half angle formulas. This replaces the use of trigonometric functions by the use of square root functions and introduces some increase in complexity. The required formulas are given by Nevels.

The problem of finding an optimal rotation is thus reduced to that of finding expressions for $a$ and $b$ in (11). Clearly these take the form

$$\begin{aligned} a &= \kappa_3 a_3 + \kappa_4 a_4, \qquad \text{and} \\ b &= \kappa_3 b_3 + \kappa_4 b_4, \end{aligned} \tag{13}$$

where the $a_i$ and $b_i$ are the "$a$" and "$b$" coefficients for $F_i$ in (9). Since we are considering orthogonal rotation we have assumed without loss of generality, that $\kappa_1 = \kappa_2 = 0$. Substi-

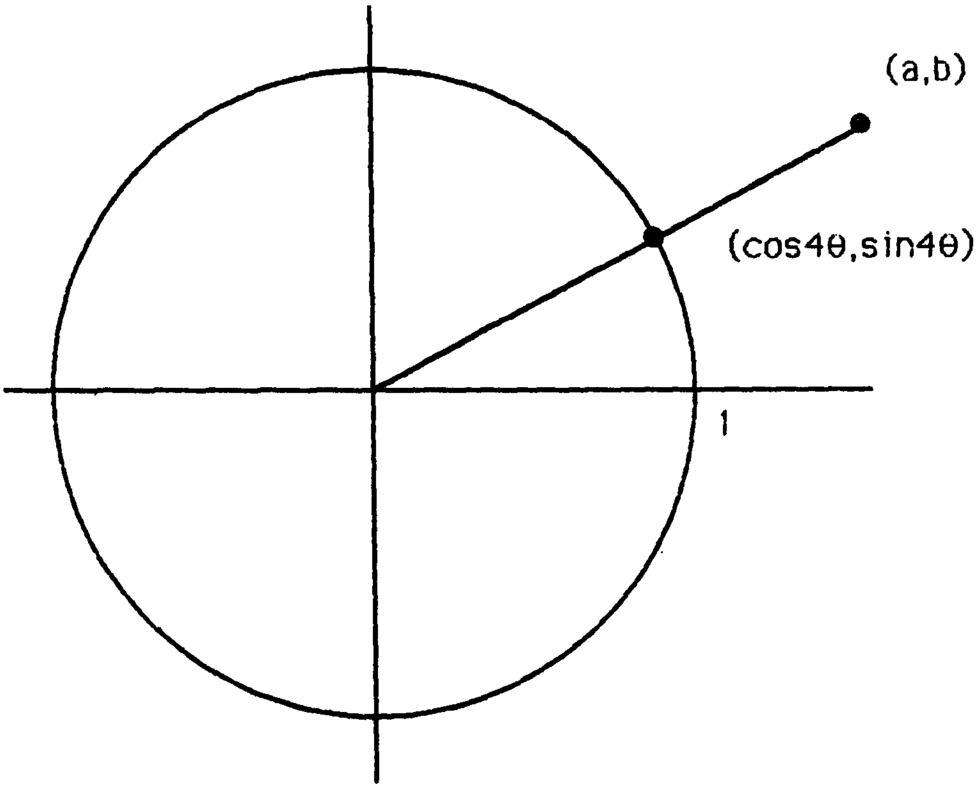


FIGURE 1
Display showing values of 4θ which maximize (11).

tuting $\theta = 0, \pm\pi/8$ in (11), it is easy to show (see Jennrich, 1970, Equation 4) that

$$a_i = F_i(0) - \frac{1}{2}\left[F_i\left(\frac{\pi}{8}\right) + F_i\left(-\frac{\pi}{8}\right)\right], \quad \text{and}$$
$$b_i = \frac{1}{2}\left[F_i\left(\frac{\pi}{8}\right) - F_i\left(-\frac{\pi}{8}\right)\right]. \tag{14}$$

These may be used together with some work to express the required $a_i$ and $b_i$ as

$$a_3 = \tfrac{1}{4}[(\lambda_r, \lambda_r) - (\lambda_s, \lambda_s)]^2 - (\lambda_r, \lambda_s)^2,$$
$$b_3 = (\lambda_r, \lambda_s)[(\lambda_r, \lambda_r) - (\lambda_s, \lambda_s)],$$
$$a_4 = \tfrac{1}{4}(\lambda_r^2, \lambda_r^2) + \tfrac{1}{4}(\lambda_s^2, \lambda_s^2) - \tfrac{3}{2}(\lambda_r^2, \lambda_s^2), \quad \text{and}$$
$$b_4 = (\lambda_r^3, \lambda_s) - (\lambda_r, \lambda_s^3). \tag{15}$$

Here $(\mathbf{x}, \mathbf{y}) = \Sigma\, x_i y_i$, and $\mathbf{x}^2$ and $\mathbf{x}^3$ denote the elementwise square and cube of the vector $\mathbf{x} = (x_i)$ so, for example, $(\lambda_r, \lambda_s^3) = \sum_i \lambda_{ir} \lambda_{is}^3$.

The optimal rotation (10) is defined by (12), (13), and (15). One could avoid using (15), and hence the need to derive it, by using (14) directly as was done by Jennrich (1970). This leads to an algorithm with roughly the same complexity as one based on (15), but one which is a little, roughly a factor of two, slower. Of greater importance to us is the fact that the algorithms based on (15) are very similar to the oblique algorithms in section 4. This makes an implementaton using (15) very simple given one intends to implement the oblique algorithms as well. It is, moreover, easy to verify that (15) leads to the standard quartimax and varimax algorithms as given, for example, by Harman (1976).

Ten Berge (1984) has observed that maximizing the varimax criterion may be formulated as a problem in simultaneously diagonalizing a set of symmetric matrices, and that a planar rotation algorithm for the latter problem is equivalent to the planar rotation algorithm used by Kaiser and used here. Ten Berge's observation may be extended to essentially the entire orthomax family (any orthomax criterion with $\gamma \leq 1$). This represents a reformulation of the orthogonal rotation problem considered here. It does not extend in a natural way to the oblique problem, however, and no direct use of this formulation will be made.

## 4. Oblique Rotation Algorithms

Current planar algorithms for oblique rotation are based on ordered pairs of factors. Following Jennrich and Sampson (1966) the first factor in each pair is rotated in the plane defined by the pair. In terms of the loading matrix $\Lambda$ this means selecting a pair of columns $\lambda_r$ and $\lambda_s$ and applying a transformation of the form

$$\begin{aligned} \tilde{\lambda}_{ir} &= \gamma\lambda_{ir}, \\ \tilde{\lambda}_{is} &= -\delta\lambda_{ir} + \lambda_{is}, \end{aligned} \tag{16}$$

where

$$\gamma^2 = 1 + 2\phi_{rs}\delta + \delta^2, \tag{17}$$

and $\phi_{rs}$ is the $rs$-element in the factor correlation matrix $\Phi$. One finds a value of $\delta$ that minimizes the resulting value of the criterion $F$. Then $\Lambda$ is updated using (16), and the $r$-th row and column of $\Phi$ are updated using

$$\tilde{\phi}_{tr} = \tilde{\phi}_{rt} = \frac{1}{\gamma}\,\phi_{rt} + \frac{\delta}{\gamma}\,\phi_{st}, \qquad t \neq r, \tag{18}$$

Beginning with initial values for $\Lambda$ and $\Phi$ one proceeds by stepping uniformly through all ordered pairs $\lambda_r$ and $\lambda_s$ until the algorithm converges. We have, without loss of generality, assumed here that it is the minimum, rather than the maximum, of $F$ that is required.

Let $F(\delta)$ be the value of $F$ resulting from the transformation (16). Following Jennrich and Sampson (1966) it is easy to show that $F(\delta)$ has the form

$$F(\delta) = a + b\delta + c\delta^2 + d\delta^3 + e\delta^4. \tag{19}$$

This reduces the problem of finding an optimal "rotation" (16) to the relatively simple and routine problem of minimizing a quartic in one variable. The main problem is expressing $a$ through $e$ in (19) in terms of the components of $\Lambda$ and $\Phi$. From (8)

$$\begin{aligned} a &= \kappa_1 a_1 + \kappa_2 a_2 + \kappa_3 a_3 + \kappa_4 a_4 \\ &\;\vdots \qquad\quad \vdots \\ e &= \kappa_1 e_1 + \kappa_2 e_2 + \kappa_3 e_3 + \kappa_4 e_4, \end{aligned} \tag{20}$$

where $a_i$ through $e_i$ are the "$a$" through "$e$" coefficients for the quartic functions $F_i$ in (9). Since the optimal $\delta$ in (19) does not depend on $a$, all that is really required are expressions for $b_i$ through $e_i$ for $i = 1, \cdots, 4$. Let $\lambda_+^2$ denote a vector of row sums of squared loadings so $(\lambda_+^2)_i = \sum_r \lambda_{ir}^2$. Using (9), (16), and (17) one finds after some labor that

$$\begin{aligned} b_1 &= 4\phi_{rs}(1, \lambda_+^2)(\lambda_r, \lambda_r) - 4(1, \lambda_+^2)(\lambda_r, \lambda_s), \\ c_1 &= 4(1, \lambda_+^2)(\lambda_r, \lambda_r) + 4\phi_{rs}^2(\lambda_r, \lambda_r)^2 - 8\phi_{rs}(\lambda_r, \lambda_r)(\lambda_r, \lambda_s) + 4(\lambda_r, \lambda_s)^2, \\ d_1 &= 8\phi_{rs}(\lambda_r, \lambda_r)^2 - 8(\lambda_r, \lambda_r)(\lambda_r, \lambda_s), \\ e_1 &= 4(\lambda_r, \lambda_r)^2, \end{aligned} \tag{21}$$

that

$$\begin{aligned} b_2 &= 4\phi_{rs}(\lambda_+^2, \lambda_r^2) - 4(\lambda_+^2, \lambda_r \lambda_s) \\ c_2 &= 4(\lambda_+^2, \lambda_r^2) + 4\phi_{rs}^2(\lambda_r^2, \lambda_r^2) - 8\phi_{rs}(\lambda_r^3, \lambda_s) + 4(\lambda_r^2, \lambda_s^2), \\ d_2 &= 8\phi_{rs}(\lambda_r^2, \lambda_r^2) - 8(\lambda_r^3, \lambda_s), \\ e_2 &= 4(\lambda_r^2, \lambda_r^2), \end{aligned} \tag{22}$$

that

$$\begin{aligned} b_3 &= 4\phi_{rs}(\lambda_r, \lambda_r)^2 - 4(\lambda_r, \lambda_s)(\lambda_s, \lambda_s), \\ c_3 &= (2 + 4\phi_{rs}^2)(\lambda_r, \lambda_r)^2 + 2(\lambda_r, \lambda_r)(\lambda_s, \lambda_s) + 4(\lambda_r, \lambda_s)^2, \\ d_3 &= 4\phi_{rs}(\lambda_r, \lambda_r)^2 - 4(\lambda_r, \lambda_s)(\lambda_r, \lambda_r), \\ e_3 &= 2(\lambda_r, \lambda_r)^2, \end{aligned} \tag{23}$$

and that

$$\begin{aligned} b_4 &= 4\phi_{rs}(\lambda_r^2, \lambda_r^2) - 4(\lambda_r, \lambda_s^3), \\ c_4 &= (2 + 4\phi_{rs}^2)(\lambda_r^2, \lambda_r^2) + 6(\lambda_r^2, \lambda_s^2), \\ d_4 &= 4\phi_{rs}(\lambda_r^2, \lambda_r^2) - 4(\lambda_r^3, \lambda_s), \\ e_4 &= 2(\lambda_r^2, \lambda_r^2). \end{aligned} \tag{24}$$

Equations (20) through (24) are used to obtain values for $b$, $c$, $d$, and $e$ in (19). The optimal $\delta$ is then found by minimizing the quartic $F(\delta)$ and the corresponding $\gamma$ is given by (17) up to a choice of sign. Either choice will give an optimal rotation which is then defined by (16) and (18).

In implementing the algorithms, it is more efficient to update, rather than recompute, quantities such as $\Lambda$, $\Phi$, and $\lambda_+^2$.

## 5. Summary and Comments

Rotation is basically an expensive computation. Its cost in a factor analysis program often exceeds that of factor extraction and can exceed that of all other computations required in an analysis. Motivated by this, our initial efforts were devoted to finding a better algorithm. Planar rotations are one dimensional optimizations and represent essentially the first algorithms that come to mind. Surely we felt, one can do better. Since error bounds for quadratic functions suggest that a single steepest descent step can be as effective as a complete set of coordinate optimizations (see, e.g., Luenberger, 1973, p. 160) we tried a variety of steepest descent and quasi-Newton algorithms. To oversimplify things only slightly, the planar rotation algorithms uniformly beat our best efforts, usually by a factor of two or more.

After a reasonable amount of effort we decided to switch rather than fight and devote our efforts to tidying up things with regard to the planar rotation algorithms since these, at present at least, seem to represent the state of the art. This involved mostly straightforward extensions of existing algorithms, some of which have already been implemented in factor analysis programs, and putting all the algorithms together in one place. Thus the extension to the general symmetric family is motivated more by a desire to put things in a natural framework than fulfilling an unmet need. IMSL Inc. is currently implementing the planar algorithms discussed here for the general symmetric family for both the orthogonal and oblique cases. These are to be included in the IMSL Library.

## Appendix

We will outline a proof for the assertion at the beginning of section 2. All that needs to be shown is that any homogeneous quadratic function of a two-way table $(x_{ij})$ which is row and column symmetric is a linear combination of the functions

$$\sum_i \sum_j x_{ij}^2, \quad \sum_i \left(\sum_j x_{ij}\right)^2, \quad \sum_j \left(\sum_i x_{ij}\right)^2, \quad \left(\sum_i \sum_j x_{ij}\right)^2. \tag{A1}$$

These are clearly homogeneous quadratic functions (i.e., quadratic functions with no linear or constant terms) which are row and column symmetric. Moreover, by considering tables $(x_{ij})$ which are zero except for the following upper left hand corners

$$\begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}, \quad \begin{pmatrix} 1 & -1 \\ 0 & 0 \end{pmatrix}, \quad \begin{pmatrix} 1 & 0 \\ -1 & 0 \end{pmatrix}, \quad \begin{pmatrix} 1 & -1 \\ -1 & 1 \end{pmatrix}$$

it is easy to see the Functions (A1) are linearly independent.

Any homogeneous quadratic function of $(x_{ij})$ can be written in the form

$$\sum_i \sum_j a_{ij} x_{ij}^2 + \sum_i \sum_{j \neq l} b_{ijl} x_{ij} x_{il} + \sum_{i \neq k} \sum_j c_{ijk} x_{ij} x_{kj} + \sum_{i \neq k} \sum_{j \neq l} d_{ijkl} x_{ij} x_{kl}. \tag{A2}$$

Assume now that (A2) is also row and column symmetric. By considering tables which are zero except for the following upper left hand corners

$$\begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}, \quad \begin{pmatrix} 1 & 1 \\ 0 & 0 \end{pmatrix}, \quad \begin{pmatrix} 1 & 0 \\ 1 & 0 \end{pmatrix}, \quad \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix},$$

and permutations of such tables, it is easy to see that the $a_{ij}$, $b_{ijl}$, $c_{ijk}$, and $d_{ijkl}$ in (A2) can not depend on $i, j, k$, and $l$ and hence that (A2) is a linear combination of 4 homogeneous quadratic functions of $(x_{ij})$ which are row and column symmetric. Thus the space of all such functions has dimension 4 and the functions in (A1) are a basis.

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