PSYCHOMETRIKA—VOL. 56, NO. 4, 631–636
DECEMBER 1991

KRUSKAL'S POLYNOMIAL FOR 2 × 2 × 2 ARRAYS AND A GENERALIZATION TO 2 × n × n ARRAYS

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A remarkable difference between the concept of rank for matrices and that for three-way arrays has to do with the occurrence of non-maximal rank. The set of $n \times n$ matrices that have a rank less than n has zero volume. Kruskal pointed out that a 2 × 2 × 2 array has rank three or less, and that the subsets of those 2 × 2 × 2 arrays for which the rank is two or three both have positive volume. These subsets can be distinguished by the roots of a certain polynomial. The present paper generalizes Kruskal's results to 2 × n × n arrays. Incidentally, it is shown that two $n \times n$ matrices can be diagonalized simultaneously with positive probability.

Key words: rank, three-way arrays, PARAFAC, CANDECOMP, simultaneous diagonalization.

Kruskal (1989, p. 10) has drawn attention to the remarkable fact that the subset of those 2 × 2 × 2 arrays for which the rank is less than the maximum possible rank, has positive volume. Specifically, a 2 × 2 × 2 array cannot have a rank greater than three, but it has either rank three or rank two with positive probability, when its elements are drawn randomly from any reasonable distribution. Kruskal also noted that a certain polynomial, defined only for 2 × 2 × 2 arrays, is crucial in determining the rank of such arrays. It is the purpose of the present paper to show that 2 × n × n arrays ($n \geq 2$) in general have rank n with positive probability and that the occurrence of such a (low) rank can be detected from certain eigenvalues, which are closely related to Kruskal's polynomial in the case $n = 2$. To set the stage for generalizing Kruskal's results, it is convenient to review the determination of the rank of a 2 × 2 × 2 array.

Determining the Rank of a 2 × 2 × 2 Array

Kruskal (1977) has defined the rank of a three-way array in terms of triads. A triad is an outer product three-way array, of the form $\mathbf{a} \times \mathbf{b} \times \mathbf{c}$. For instance, if

$$\mathbf{a} = \begin{pmatrix} 2 \\ 1 \end{pmatrix}, \quad \mathbf{b} = \begin{pmatrix} 5 \\ -1 \end{pmatrix}, \quad \text{and} \quad \mathbf{c} = \begin{pmatrix} 3 \\ 1 \\ 4 \end{pmatrix},$$

then the triad $\mathbf{a} \times \mathbf{b} \times \mathbf{c}$ is the array consisting of two lateral slices $5\mathbf{ac}'$ and $-\mathbf{ac}'$. Equivalently, the triad has the frontal slices $3\mathbf{ab}'$, $\mathbf{ab}'$, and $4\mathbf{ab}'$, and the horizontal slices $2\mathbf{bc}'$ and $\mathbf{bc}'$. The rank of a three-way array is defined as the smallest number of triads needed to decompose it (Kruskal, 1977, 1989). If an array X can be written as $X = \Sigma_{i=1}^{r} \mathbf{a}_i \times \mathbf{b}_i \times \mathbf{c}_i$, then the j-th frontal slice X_j can be written as $\Sigma\, \mathbf{a}_i \times \mathbf{b}_i \times c_{ij} = AC_jB'$, where A contains $\mathbf{a}_1, \ldots, \mathbf{a}_r$ as columns, B contains $\mathbf{b}_1, \ldots, \mathbf{b}_r$ as

The author is obliged to Joe Kruskal and Henk Kiers for commenting on an earlier draft, and to Tom Wansbeek for raising stimulating questions.

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0033-3123/91/1200-90245$00.75/0

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columns, and C_j is the diagonal matrix containing the j-th element of $\mathbf{c}_1, \mathbf{c}_2, \ldots, \mathbf{c}_r$ on the diagonal. Conversely, if each frontal slice X_j of a three-way array can be written as AC_jB' for some diagonal $r \times r$ matrix C_j, then the array can be written as $\Sigma_{i=1}^{r} \mathbf{a}_i \times b_i \times c_i$. It follows that the rank of a $2 \times n \times n$ array, sliced up in two frontal slices X_1 and X_2 of order $n \times n$, equals the smallest value of r for which X_1 and X_2 can be decomposed as

$$X_1 = ADB'; \qquad X_2 = AEB', \tag{1}$$

for certain $n \times r$ matrices A and B, and diagonal $r \times r$ matrices D and E. For a $2 \times 2 \times 2$ array, one may equivalently consider the rank of X in terms of lateral or horizontal 2×2 slices, but we shall stick to X_1 and X_2 as frontal slices unless specified otherwise. The rank of X is zero if and only if X is an array of zeroes. From now on, it is assumed that X is a nonzero array.

A $2 \times 2 \times 2$ array, containing a nonsingular 2×2 slice, cannot have a rank less than two, because we may turn the array over so that this slice becomes one of the frontal slices, to which (1) can be applied. Conversely, every nonzero $2 \times 2 \times 2$ array that doesn't have a nonsingular slice in any direction has either rank one, or it is superdiagonal, for instance, like

$$X_1 = \begin{pmatrix} \alpha & 0 \\ 0 & 0 \end{pmatrix}; \qquad X_2 = \begin{pmatrix} 0 & 0 \\ 0 & \beta \end{pmatrix},$$

for $\alpha \neq 0$ and $\beta \neq 0$. To verify this, consider first the case where some slice is zero. Then the assumed singularity of the "other" slice implies that the array has rank one. So we ignore this case, and assume that $X_1 = (\mathbf{x}|\lambda\mathbf{x})$, where $\mathbf{x}$ is a nonzero vector and λ a scalar. If $\lambda \neq 0$, then the singularity of the lateral slices yields $X_2 = (\delta\mathbf{x}|\varepsilon\mathbf{x})$, for certain scalars δ and ε. If $\lambda = 0$, then either this expression is still valid, for a $\delta \neq 0$, or we have $X_2 = (0|\mathbf{y})$, for arbitrary $\mathbf{y}$, a special case to be treated later. The singularity of the horizontal slices implies that $(1\ \lambda)' = \mu(\delta\ \varepsilon)'$ for some $\mu \neq 0$. So $X_1 = \mathbf{x}(1\ \lambda) = \mathbf{x}(\mu\delta\ \mu\varepsilon)$ and $X_2 = \mathbf{x}(\delta\ \varepsilon)$, and a rank one solution has been constructed. Suppose, however, that $X_1 = (\mathbf{x}|0)$ and $X_2 = (0|\mathbf{y})$ for arbitrary $\mathbf{x}$ and $\mathbf{y}$. Because the horizontal slices are of rank one, X has the superdiagonal form, defined by having precisely 2 nonzero elements that never occur in the same slice. This array has rank two.

From the foregoing, it is easy to detect $2 \times 2 \times 2$ arrays of rank 0 or 1: the rank is 0 if and only if the array has zero entries only, and the rank is 1 if and only if each of the six slices is singular, the superdiagonal matrix excepted, which has rank two. It remains to deal with $2 \times 2 \times 2$ arrays for which at least one slice is nonsingular, and which, therefore, have rank 2 or higher. Without loss of generality, it may be assumed that X_1 is nonsingular.

Kruskal (1983) has shown that the rank of a $2 \times 2 \times 2$ array is at most three, using a rather complicated mathematical argument. A straightforward constructive proof can also be given.

Proof. Let X_1 and X_2 be arbitrary 2×2 matrices, with X_1 nonsingular. For a fixed value of r, a solution (1) exists if and only if a parallel solution exists for

$$X_1X_1^{-1} = ADB'X_1^{-1} \quad \text{and} \quad X_2X_1^{-1} = AEB'X_1^{-1}. \tag{2}$$

Therefore, we may consider a solution (1) for $Y_1 = I$ and $Y_2 = X_2X_1^{-1}$, instead of X_1 and X_2, respectively. Defining for $n = 2$,

$$Y_2 = \begin{pmatrix} y_{11} & y_{12} \\ y_{21} & y_{22} \end{pmatrix},$$

and taking

$$A = \begin{pmatrix} 1 & 0 & y_{12} \\ 0 & 1 & y_{21} \end{pmatrix}; \qquad (X_1')^{-1}B = \begin{pmatrix} 1 & 0 & 1 \\ 0 & 1 & 1 \end{pmatrix};$$

$$D = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \quad \text{and} \quad E = \begin{pmatrix} (y_{11} - y_{12}) & 0 & 0 \\ 0 & (y_{22} - y_{21}) & 0 \\ 0 & 0 & 1 \end{pmatrix}, \tag{3}$$

we obtain an explicit solution for (2) or, equivalently, for (1) if B is obtained from $(X'_1)^{-1}B$. It follows that a $2 \times 2 \times 2$ array cannot have a rank greater than 3. □

The question that remains is to decide whether the rank is two or three, still assuming nonsingularity of X_1. If X_2 is proportional to X_1, that is, if $X_2 = \lambda X_1$ for some scalar λ, then of course a rank two solution does exist. Consider, therefore, the case where X_2 is not proportional to X_1 (nonsingular), and suppose that the array has rank two. Then it follows from (1) that there exist vectors $\mathbf{a}_1$ and $\mathbf{a}_2$ (columns of A) and vectors $\mathbf{b}_1$ and $\mathbf{b}_2$ (columns of B) and scalars d_1, d_2, e_1, and e_2 such that

$$X_1 = d_1\mathbf{a}_1\mathbf{b}_1' + d_2\mathbf{a}_2\mathbf{b}_2', \tag{4}$$

and

$$X_2 = e_1\mathbf{a}_1\mathbf{b}_1' + e_2\mathbf{a}_2\mathbf{b}_2', \tag{5}$$

with d_1 and d_2, the diagonal elements of D, nonzero, and E not proportional to D, which means that $e_1d_1^{-1} \neq e_2d_2^{-1}$. Clearly, both $(X_2 - d_1^{-1}e_1X_1)$ and $(X_2 - d_2^{-1}e_2X_1)$ are singular; hence the equation,

$$|X_2 - \lambda X_1| = 0, \tag{6}$$

must have two distinct real roots. Equation (6) can be expanded as

$$\lambda^2|X_1| + \lambda(x_{21}^{(1)}x_{12}^{(2)} + x_{12}^{(1)}x_{21}^{(2)} - x_{11}^{(1)}x_{22}^{(2)} - x_{22}^{(1)}x_{11}^{(2)}) + |X_2| = 0, \tag{7}$$

with $x_{ij}^{(k)}$ the ij-th element of X_k. This equation has two distinct real roots if and only if the discriminant is positive. This discriminant is Kruskal's polynomial. It can be simplified considerably by working with $Y_1 = X_1X_1^{-1} = I_2$ and $Y_2 = X_2X_1^{-1}$ instead of X_1 and X_2. Then (6) reduces to the characteristic equation of $(X_2X_1^{-1})$ and (7) simplifies to

$$\lambda^2 - \lambda(\text{tr } Y_2) + |Y_2| = 0, \tag{8}$$

which has a positive discriminant if and only if

$$(\text{tr } Y_2)^2 > 4|Y_2|. \tag{9}$$

It follows that (9) is necessary for a rank two solution. Conversely, (9) is also sufficient for a rank two solution, in the case under consideration. That is, if (9) is satisfied, then there exist two real and distinct roots λ_1 and λ_2 for (6). This allows us to define the rank one matrices

$$\mathbf{u}_1\mathbf{v}_1' = (\lambda_1 - \lambda_2)^{-1}(X_2 - \lambda_2 X_1), \tag{10}$$

and

$$\mathbf{u}_2\mathbf{v}_2' = -(\lambda_1 - \lambda_2)^{-1}(X_2 - \lambda_1 X_1). \tag{11}$$

Their sum $\mathbf{u}_1\mathbf{v}_1' + \mathbf{u}_2\mathbf{v}_2'$ equals X_1 and their weighted sum $\lambda_1\mathbf{u}_1\mathbf{v}_1' + \lambda_2\mathbf{u}_2\mathbf{v}_2'$ equals X_2, which shows that a rank two solution has been constructed, where $\mathbf{u}_1$ and $\mathbf{u}_2$ are the columns of A, $\mathbf{v}_1$ and $\mathbf{v}_2$ are the columns of B, $D = I_2$ and $E = \begin{pmatrix}\lambda_1 & 0\\ 0 & \lambda_2\end{pmatrix}$. This shows that (9) is a necessary and sufficient condition for a $2 \times 2 \times 2$ array to have rank 2, given that X_1 is nonsingular, and given that X_2 is not proportional to X_1. Of course, if X_1 is singular, but some other 2×2 slice of the array is not, then the entire reasoning given here remains valid. If both X_1 and X_2 are nonsingular, then we have two characteristic equations: one for $X_2X_1^{-1}$ and one for $X_1X_2^{-1}$. The associated eigenvalues are inversely related. For this reason, it would be ambiguous to speak of "the eigenvalues" of a $2 \times 2 \times 2$ array.

Kruskal (1989, p. 10) pointed out that if his polynomial is zero, the rank may be either 0, 1, 2, or 3, whereas above it was claimed that (9) is necessary and sufficient for rank 2. There is no contradiction, because we first ruled out the case where all slices are singular, and in addition assumed that X_2 is not proportional to X_1. Only after discarding such cases, we arrived at a necessary and sufficient condition for rank 2.

A Generalization to $2 \times n \times n$ Arrays

Kruskal (1989, p.10) pointed out that the polynomial derived from (6) as the discriminant in (7) is only defined for $2 \times 2 \times 2$ arrays. True as this may be, a similar albeit more complicated polynomial exists for $2 \times 3 \times 3$ arrays. The rank of such arrays is at most four. This is evident from Kruskal (1989, p. 10) who pointed out that a $2 \times n \times n$ array has a maximal rank $3n/2$ for n even, and $(3n - 1)/2$ for n odd. Again, as was done above for $2 \times 2 \times 2$ arrays, we ignore exceptional cases and concentrate on the case where X_1 is a nonsingular 3×3 matrix. Then X has either rank three or rank four. Suppose that a rank three solution exists, and that it satisfies the condition that all diagonal elements of ED^{-1} are distinct. Then it follows from (1) that there must be three distinct real roots for the determinantal equation

$$|X_2 - \lambda X_1| = 0, \tag{12}$$

by the same arguments as used above to obtain (6). Again, a discriminant criterion does exist, which means that a generalization of Kruskal's polynomial for $2 \times 2 \times 2$ arrays is feasible. However, evaluating the generalized polynomial for $n = 3$ is already quite complicated and for larger n the complications soon become overwhelming. Fortunately, we need not evaluate polynomials to see whether or not certain roots are distinct and real, if these roots can be obtained directly. Noting that (12) has, for arbitrary n, the same roots as the characteristic equation

$$|X_2X_1^{-1} - \lambda I| = 0, \tag{13}$$

we may obtain the eigenvalues of $X_2X_1^{-1}$ at once and verify whether or not they are real and distinct. If they are, then $X_2X_1^{-1}$ has n linearly independent real eigenvectors, and the eigendecomposition

$$X_2X_1^{-1} = K\Lambda K^{-1}, \tag{14}$$

where Λ is a diagonal $n \times n$ matrix of eigenvalues and K contains the n associated eigenvectors as columns. From (14) an explicit rank n solution for (1) can be constructed by taking $A = K$, $B' = K^{-1}X_1$, $D = I_n$, and $E = \Lambda$, as is readily verified. It can be concluded that a $2 \times n \times n$ array with at least one $n \times n$ nonsingular slice X_1 has rank n if $X_2X_1^{-1}$ has n distinct real eigenvalues. This "eigenvalue criterion" is easy to use because eigenvalues of asymmetric matrices can be evaluated by standard numerical routines. It should be understood that, contrary to the $n = 2$ case treated in the previous section, we now have a *sufficient* condition for rank n, that is not necessary. To see this, construct an arbitrary nonsingular $n \times n$ matrix K and an arbitrary diagonal matrix Λ with nonzero diagonal elements. Upon defining $X_1 = I$ and $X_2 = K\Lambda K^{-1}$, it is seen that the $2 \times n \times n$ array containing X_1 and X_2 has rank n, regardless of distinctness of the diagonal elements in Λ. So it is not necessary for rank n to have all eigenvalues distinct. This does not imply, however, that the eigenvalue criterion can be relaxed: Having merely n real eigenvalues does not guarantee that a rank n solution can be obtained. For instance, if $X_1 = I_3$, and

$$X_2 = \begin{pmatrix} 1 & -1 & 0 \\ 1 & 3 & 0 \\ 0 & 0 & 1 \end{pmatrix},$$

then the eigenvalues of $X_2X_1^{-1}$ are 2, 2, and 1, yet there is no real matrix K such that $X_2X_1^{-1} = K\Lambda K^{-1}$. This array has rank 4.

The eigenvalue criterion suggests that the set of $2 \times n \times n$ arrays of rank n has positive volume, which is a generalization of Kruskal's "surprising" result for $n = 2$. An empirical demonstration was obtained by constructing 100 pairs X_1, X_2 of order $n \times n$, for $n = 2, 3, \ldots, 8$, respectively, with elements sampled form the normal (0, 1) distribution. The number of cases (out of 100) was counted in which n distinct and real eigenvalues of $X_2X_1^{-1}$ were found. For $n = 2, 3, \ldots, 8$, respectively, these numbers were 76, 55, 22, 16, 2, 1, and zero. Clearly, the relative volume of the set of rank-n arrays of order $2 \times n \times n$ rapidly decreases as n increases. The percentage 76 for $2 \times 2 \times 2$ arrays is comparable to the value of 79 reported by Kruskal (1989) and by T. J. Wansbeek (personal communication, June 3, 1989), both of whom used 1000 replications. Although more than 100 replications may be needed to estimate the percentages accurately, this seems hardly interesting. The interesting point is that the phenomenon of $2 \times 2 \times 2$ arrays having nonmaximal rank with positive probability can be generalized to $2 \times n \times n$ arrays. Equivalently, it can be concluded that a pair of asymmetric square matrices can be diagonalized simultaneously with positive probability.

Uniqueness

Harshman (1972) has shown that the PARAFAC decomposition of a $2 \times n \times n$ array, as given in (1), is unique if A and B are of full column rank and all diagonal elements of ED^{-1} are distinct. This condition is satisfied if the eigenvalues of $X_2X_1^{-1}$ are real and distinct, as has been shown above. If the eigenvalues are real but not all distinct, then either a rank n solution does not exist, or it is nonunique. For the $n = 2$ case, non-uniqueness of a rank two solution arises if X_1 and X_2 are proportional nonsingular matrices. Kruskal (1989, p. 12) stated that $2 \times 2 \times 2$ arrays of rank 2 have a unique rank 2 decomposition. This statement is correct, once the case of proportional slices has been excluded.

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Manuscript received 6/12/90
Final version received 11/12/90-