

## ANALYTIC CLASSIFICATION AND QUADRIPLANAR CHARTING OF ANALYSES WITH NINE OR MORE COMPONENTS\*

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## ABSTRACT

Analytic methods are used for the classification of analyses having nine or more components, though under favorable conditions such analyses may also be charted. A square matrix of the third order is formulated with three columns that represent 3-dimensional Cartesian vectors extending outward from the origin. The end points of these vectors are triads of coordinates defined by the percentages of a given analysis. By means of a collineatory transformation, such a matrix is transformed to a new frame of reference wherein these vectors appear as intercepts on new axes of X, Y, and Z. Thus 9 numbers are reduced to 3 unique numerical indices.

The algebraic procedure required for a collineatory transformation consists in the solution of a cubic equation derived from the determinant of a characteristic matrix. The roots of this equation, known as characteristic roots, latent roots, or eigenvalues, are found to be the elements in the principal diagonal of a diagonalized matrix, whose other elements are zeros. The sum of these roots is called the trace or spectrum (T) of the transformed matrix. If the roots are real numbers, their three values together with (100-T) may be taken as quadriplanar coordinates for charting inside or outside a tetrahedron of reference. Thus each analysis may be represented by a single point, which may then be projected either apically or orthogonally onto one or more of the triangular faces of the tetrahedron, for a 2-dimensional representation. Complex roots cannot be charted, but the analyses of most igneous rocks yield real roots.

A refinement of this method by the use of symmetrical matrices eliminates complex roots, and thus renders charting universally feasible. Symmetry with respect to the principal diagonal is produced before diagonalization by post-multiplying an unsymmetrical matrix of the third order by its transpose. A generalization of this operation consists in post-multiplying a rectangular array of the order  $3 \times 4$ ,  $3 \times 5$ ,  $3 \times 6$ , or in general  $3 \times (3+k)$  by its transpose. This constitutes a third method which provides for the classification and charting of 12, 15, 18, or in general  $9+3k$  variables; and if one or two zeros are introduced into the rectangular arrays, any number of variables in excess of 9 may be analyzed. The insertion of one to four zeros in a square matrix of the third order, before it is multiplied by its transpose, makes it possible to handle 8, 7, 6, or 5 variables. These three methods are not interchangeable; instead one is selected and used for the required purpose.

## INTRODUCTION

The classification and charting of a number of variables, especially the components of analyses that sum to 100, is a matter of perennial interest to most scientific workers. In two earlier papers the writer (1948, p. 324-336 and 1949, p. 706-716) presented methods for charting 5, 6, and 7 variables on the triangular and tetrahedral boundaries of hypertetrahedra of 4, 5, and 6 dimensions; but suitable coordinate nets could not be devised for more than 7 variables. These, however, were essentially multiple charts, in that the variables were charted as triads with reference

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to bounding triangles, or at most as tetrads with reference to bounding tetrahedra. Such graphs had the advantage that the variations of 3 or 4 components between consecutive analyses were shown; but the variations of all the components of the analyses could not simultaneously be charted. This is the dilemma in dealing with many variables.

An alternative solution of this problem is a group classification and charting of analyses, whereby the initial variables are so combined as to formulate a smaller number of composite variables. This condensation, however, must be accomplished by algebraic processes such that the new variables are unique, that is, they cannot assume identical values from the components of different analyses. An example of the improper combination of variables would be to add or multiply three components of an analysis. This sum or product would not constitute a unique composite variable, as the same numerical value could be obtained from different analyses. An analogy of the contemplated process, if one were dealing with an equation of 9 variables, would result if this equation was partially differentiated for 3 variables, say

$$\frac{\partial f}{\partial x}, \quad \frac{\partial f}{\partial y} \quad \text{and} \quad \frac{\partial f}{\partial z};$$

and if the new equation was charted with regard to these three partial derivatives after numerical values had been assigned to the other variables. But we are dealing with percentages, or numbers, not with functions, and a process must be devised to combine these into a small number of unique numbers that can be interpreted either as numerical indices of the analyses or as numerical data for empirical charting. It has seemed best to accomplish this objective by the formulation of 3 new variables, each of which is a function of all the components of an analysis. This, however, is group classification and group charting, which will show distinct differences between total analyses, but will not ordinarily show quantitatively the mode of variation of the individual components of analyses. The thinking and perception of the operator must become adjusted to this different objective.

Matrices will be utilized to develop the proposed method. Most geologists are familiar with the elementary properties and uses of determinants, as that topic is treated in courses of college algebra. Matrices, however, are less well understood, for which reason a brief description of the nature of a matrix seems desirable. Perhaps the best way to describe a matrix is to show the differences between it and a determinant. A determinant, as is well known, is a square array of numbers, symbols, or functions in rows and columns, say 3 rows and 3 columns, or in general  $n$

rows and  $n$  columns, enclosed by 2 vertical bars. As the array is square its order may be stated merely by the use of a single digit, calling it a determinant of the  $n$ th order. A matrix is a similar array enclosed by double instead of single vertical bars, but it may be either square or rectangular. If rectangular, its order is stated by 2 digits specifying respectively the number of rows and columns, say the order of  $3 \times 4$ ,  $8 \times 5$ , or in general  $m \times n$ .

A more fundamental difference between a matrix and a determinant is that the matrix is merely an array of elements with assigned meanings, according to the problem under investigation, but with no composite value. A determinant, on the other hand, is a square array of elements, which represents a complex function, that has a determinable numerical or algebraic value. In fact, a determinant may be regarded as a function of some square matrix, such that it may be written as  $|A| = f(\|A\|)$ . Both matrices and determinants may be subjected, not merely to the elementary operations of addition, subtraction, multiplication, division, involution, and evolution, but also to more highly involved algebraic processes, though the manipulative rules are different. A special kind of algebra, called matrix algebra, has been developed for the treatment of matrices.

The operations of ordinary arithmetic and algebra are controlled by five laws, which are as follows:

1. Commutative principle in addition (and subtraction)
2. Commutative principle in multiplication (and division)
3. Associative principle in addition (and subtraction)
4. Associative principle in multiplication (and division)
5. Distributive principle in combined addition and multiplication.

If one or more of these laws is voided, a new type of algebra results, that operates only by the non-voided principles. Thus the commutative principle is voided in the multiplication and division of matrices, wherefore the so-called matrix algebra has been evolved. If both the second and fourth laws are voided, the Cayley algebra results; and other algebras may similarly be developed. In this paper, square and rectangular matrices are multiplied, for which reason the operation of matrix multiplication should be understood; but no further applications of matrix algebra are required.

Matrices originated as tabulations of coefficients in systems of linear equations, providing a shorthand device for the solution of such equations. They are now utilized, however, for many other purposes, according to prior agreement as to the meaning of their elements. They are extensively used in the study of vectors, tensors, and related entities; in variate statistical analysis; in multiple factorial analysis; and in numer-

ous other applications. In this paper, the utilization of matrices is rather empirical, but is related to vectorial and factorial analysis.

#### FORMULATION OF MATRIX

Consider a system of three-dimensional Cartesian coordinates, with a vector that starts at the origin and extends outward into the first octant to a point defined by 3 coordinates. The values of these coordinates will be taken as the percentages of  $\text{SiO}_2$ ,  $\text{Al}_2\text{O}_3$  and  $\text{Fe}_2\text{O}_3$  in a rock analysis recomputed to total 100%. A second vector, likewise starting at the origin, will be connected to a point determined by the percentages of  $\text{FeO}$ ,  $\text{MgO}$ , and  $\text{CaO}$ ; and a third vector will similarly be constructed, using the percentages of  $\text{Na}_2\text{O}$ ,  $\text{K}_2\text{O}$ , and R, where R means the sum of the remaining components of the analysis. These triads are tabulated as three columns to form a square matrix of the third order, though rows instead of columns could equally well be utilized. This matrix may now be operated upon algebraically in such a way that its three component vectors will be transformed to a new system of Cartesian coordinates wherein each vector will become an intercept on one of the new coordinate axes. The terminal of a 3-dimensional intercept has three coordinates, of which two are zeros; and hence for a specified axis it may be identified by a single number. Therefore each of the three original vectors will similarly be represented by a single number, thus reducing nine percentages to three numerical indices.

A change in origin is accomplished in ordinary analytical geometry by stating the coordinates and rotation of the new frame of reference in terms of the old one, and in making the transformation by means of enabling equations. In the present transformation, however, no such data are given but two limiting geometric conditions serve to localize the new frame of reference. One of these is that the coordinates of the three intercepts shall lie on the extension of the three original vectors; the other is that a triangle formed by connecting the ends of the three intercepts shall be parallel to and therefore similar to the triangle formed by joining the terminals of the three original vectors. Owing to these limitations, such a change in the frame of reference is called a collineatory or similarity transformation.

#### DERIVATION AND SOLUTION OF CUBIC EQUATION

A square matrix of the third order, formulated in the manner outlined above, is used to obtain a cubic equation, from which the required numerical indices are derived. Such a matrix, called A, is shown below in generalized form, using the double subscript type of notation for its nine elements. The required transformation is obtained by subtracting from

A the quantity  $\lambda I$ , where  $I$  is the unit or identity matrix, and  $\lambda$  is a general variable.

$$\|A - \lambda I\| = \left\| \begin{vmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{vmatrix} - \lambda \begin{vmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{vmatrix} \right\| = \left\| \begin{vmatrix} a_{11} - \lambda & a_{12} & a_{13} \\ a_{21} & a_{22} - \lambda & a_{23} \\ a_{31} & a_{32} & a_{33} - \lambda \end{vmatrix} \right\|$$

As every square matrix defines a determinant, the matrix  $\|A - \lambda I\|$  may now be interpreted as the determinant  $|A - \lambda I|$ , which is expanded to obtain its algebraic value. This is accomplished, not by the ordinary method of clearing a determinant of the third order, but by means of one of Laplace's expansions, which permits the writing of the coefficients of  $\lambda$  as minor determinants, thus:

$$\begin{aligned} |A - \lambda I| &= -\lambda^3 + (a_{11} + a_{22} + a_{33})\lambda^2 - \left[ \begin{vmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{vmatrix} + \begin{vmatrix} a_{22} & a_{23} \\ a_{32} & a_{33} \end{vmatrix} + \begin{vmatrix} a_{11} & a_{13} \\ a_{31} & a_{33} \end{vmatrix} \right] \lambda \\ &\quad + \begin{vmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{vmatrix} \end{aligned}$$

This reduces to

$$\begin{aligned} f(\lambda) &= -\lambda^3 + (a_{11} + a_{22} + a_{33})\lambda^2 \\ &\quad - [(a_{11}a_{22} + a_{22}a_{33} + a_{11}a_{33}) - (a_{12}a_{21} + a_{23}a_{32} + a_{13}a_{31})]\lambda \\ &\quad + [(a_{11}a_{22}a_{33} + a_{12}a_{23}a_{31} + a_{13}a_{21}a_{32}) - (a_{13}a_{22}a_{31} + a_{23}a_{32}a_{11} + a_{33}a_{12}a_{21})] \end{aligned}$$

Written in generalized form and equated to zero, this equation becomes

$$\lambda^3 + b\lambda^2 + c\lambda + d = 0$$

where  $b$  and  $d$  are negative coefficients, though their numerical values may prove to be either positive or negative. A critical examination of the make-up of coefficients  $b$ ,  $c$ , and  $d$  will convince the most skeptical person that the cubic equation in  $\lambda$  obtained from the percentages of one analysis cannot be duplicated by similar data from any other analysis. The matrix  $\|A - \lambda I\|$  is known as the characteristic matrix of  $A$ ; the cubic equation in  $\lambda$  is called the characteristic equation of  $A$ ; and the roots of this equation are designated as characteristic roots, latent roots, or eigenvalues.

The nature of the roots of a general cubic equation may be predicted from its discriminant, that is,

$$\Delta = 18bcd - 4b^3d + b^2c^2 - 4c^3 - 27d^2$$

If the sign of this discriminant is positive, there are three real roots; if the sign is negative, there are one real and two conjugate complex roots. A third alternative, where  $\Delta = 0$ , will not materialize in dealing with decimal fractions. A trigonometric solution is used if the roots are real; otherwise Cardan's solution is employed. These standard methods of

solving cubic equations will be found in any textbook on the theory of equations, such as that written by Dickson (1939, p. 42-51).

Special mention should be made of a small book by Salzer, Richards, and Arsham (1958), entitled a "Table for the solution of cubic equations." Only 6 of the 161 pages of this book refer to real roots so that these, with the permission of the authors, could be photographed and made available to anyone interested in these methods. For the general cubic, the argument of these tables is a quantity

$$\theta = \frac{q^2}{p^3}, \quad \text{where } p = c - \frac{b^2}{3}, \quad \text{and } q = d - \frac{bc}{3} + \frac{2b^3}{27};$$

but for the cubics solved in this paper, it must be remembered that the coefficients  $b$  and  $d$  are negative. The tables yield the values of  $f_1(\theta)$ ,  $f_2(\theta)$ , and  $f_3(\theta)$ ; and the three roots are

$$\lambda_n = -\frac{q}{p} f_n(\theta) - \frac{b}{3}.$$

It should be noted that the value of  $\lambda_1$ , as used in this manuscript, is derived from  $f_3(\theta)$ ,  $\lambda_2$  from  $f_2(\theta)$ , and  $\lambda_3$  from  $f_1(\theta)$ . On the other hand, the real root of a Cardan solution, which is derived from  $f_1(\theta)$  of the tables, is designated by the writer as  $\lambda_1$ . Even with the preliminary computations required, these tables obviate a large part of the labor of solving cubic equations by standard methods.

#### APPLICATION OF EIGENVALUES

An important theorem of matrix algebra states that any nonsingular ( $|A| \neq 0$ ) matrix with distinct latent roots may be reduced by a colineatory transformation to a diagonal matrix, wherein the elements of the principal diagonal are the latent roots or eigenvalues of the given matrix. All other elements of the diagonal matrix are zeros. This process, called the diagonalization of a matrix, is shown below, first in generalized form where  $\lambda_1$ ,  $\lambda_2$ , and  $\lambda_3$  are the latent roots of the characteristic cubic; and second in specific numerical form, where the 9 elements of the original matrix are the percentages in a mean analysis of 90 biotite granites, and the 3 elements in the diagonal matrix are the derived eigenvalues.

$$\begin{aligned} \left\| \begin{array}{ccc} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{array} \right\| &\rightarrow \left\| \begin{array}{ccc} \lambda_1 & 0 & 0 \\ 0 & \lambda_2 & 0 \\ 0 & 0 & \lambda_3 \end{array} \right\| \\ \left\| \begin{array}{ccc} 71.66 & 1.10 & 3.06 \\ 14.49 & 0.87 & 4.13 \\ 1.46 & 1.97 & 1.26 \end{array} \right\| &\rightarrow \left\| \begin{array}{ccc} 71.967 & 0 & 0 \\ 0 & -1.709 & 0 \\ 0 & 0 & 3.532 \end{array} \right\| \end{aligned}$$

This diagonal matrix is unique except for the order in which the latent roots are enumerated, as the transformation does not assign the intercepts represented by these numbers to particular axes of the new frame of reference. Obviously, therefore, the elements of the principal diagonal, which constitute the numerical indices of this method, could be written in the order  $a_{11}a_{22}a_{33}$ ,  $a_{11}a_{33}a_{22}$ ,  $a_{22}a_{11}a_{33}$ ,  $a_{22}a_{33}a_{11}$ ,  $a_{33}a_{11}a_{22}$ , or  $a_{33}a_{22}a_{11}$ . In reality a geometric study will show that at least 6 frames of reference will satisfy this transformation. This indeterminacy has been overcome in the following way. A cubic equation with real roots is solved by means of several algebraic substitutions, of which the last makes use of the trigonometric function  $\cos X$ . After the first root is obtained from  $\cos X$ , the other roots are obtained respectively from  $\cos (120^\circ + X)$  and  $\cos (240^\circ + X)$ . The roots  $\lambda_1$ ,  $\lambda_2$ , and  $\lambda_3$  in the principal diagonal are enumerated in this order.

Twenty groups of analyses of igneous rocks and 4 of mafic minerals taken from granitic rocks were selected to show the application of this method. These are presented in Table 1.

The eigenvalues derived from these 24 groups of analyses are shown in the first three columns of Table 2. It will be noted that 22 of the derived cubics yield real roots, and that the exceptions are the rock ijolite and the mineral biotite. In general it appears that most igneous rocks can be represented by 3 real numerical indices, though exceptions other than the two cited have also been found.

Certain relationships appear in these eigenvalues. The values of  $\lambda_1$  are near yet invariably greater than the percentages of  $\text{SiO}_2$  in the original analyses, but no linear relationship exists, as most of the differences range from 0.2 unit to 2.8 units, though larger differences result from the two Cardan solutions. Negative values of  $\lambda_2$  are characteristic of the granites, adamellite, tonalite, syenite, monzonite, nepheline syenite, shonkinite, and muscovite. The lamprophyres and monzonite have larger values of  $\lambda_3$  than the more felsic granitic rocks; hornblende and augite show still larger values; and pyroxenite and peridotite are characterized by the highest values of  $\lambda_3$ . Somewhat different relationships exist for eigenvalues derived from symmetrical matrices.

The sum of each set of three real eigenvalues, which in Table 2 ranges from 50 to 82, is known as the trace or spectrum of the diagonal matrix and is designated as T. The eigenvalues corresponding to each trace could empirically be charted as trilinear coordinates referred to an equilateral triangle having one side equal to the specified trace, and T unit divisions along each side of the triangle. This plotting, however, would not be convenient, as many triangles of different sizes would have to be shown.

TABLE 1. ANALYSES OF IGNEOUS ROCKS AND GRANITIC MAFIC MINERALS

| Analyses |     | Petrographic character           | SiO <sub>2</sub> | Al <sub>2</sub> O <sub>3</sub> | Fe <sub>2</sub> O <sub>3</sub> | FeO   | MgO   | CaO   | Na <sub>2</sub> O | K <sub>2</sub> O | R    |
|----------|-----|----------------------------------|------------------|--------------------------------|--------------------------------|-------|-------|-------|-------------------|------------------|------|
| Group    | No. |                                  |                  |                                |                                |       |       |       |                   |                  |      |
| 1        | 7   | High-silica granite (Johannsen)  | 74.88            | 11.66                          | 1.66                           | 1.40  | 0.05  | 0.65  | 3.99              | 4.87             | 0.84 |
| 2        | 2   | Two-mica granite (Johannsen)     | 75.52            | 14.82                          | 1.27                           | 0.73  | 0.20  | 1.72  | 3.47              | 4.58             | 0.69 |
| 3        | 90  | Biotite granite (Tschirwinsky)   | 71.66            | 14.49                          | 1.46                           | 1.10  | 0.87  | 1.97  | 3.06              | 4.13             | 1.26 |
| 4        | 34  | Adamellite (Johannsen)           | 67.76            | 14.97                          | 1.60                           | 2.11  | 1.45  | 2.76  | 3.67              | 4.09             | 1.59 |
| 5        | 19  | Tonalite (Johannsen)             | 66.29            | 15.68                          | 1.22                           | 3.11  | 2.15  | 4.57  | 4.24              | 1.42             | 1.32 |
| 6        | 184 | Gabbro (Johannsen)               | 49.14            | 17.45                          | 3.75                           | 5.95  | 6.60  | 10.59 | 2.58              | 1.00             | 2.94 |
| 7        | 161 | Basalt (Daly)                    | 48.78            | 15.85                          | 5.37                           | 6.34  | 6.03  | 8.91  | 3.18              | 1.63             | 3.91 |
| 8        | 9   | Pyroxenite (Johannsen)           | 51.10            | 2.45                           | 1.92                           | 6.61  | 27.22 | 6.90  | 0.26              | 0.06             | 3.48 |
| 9        | 10  | Peridotite (Johannsen)           | 41.95            | 5.74                           | 4.65                           | 6.82  | 26.97 | 6.04  | 1.11              | 0.63             | 6.09 |
| 10       | 32  | Minette (Johannsen)              | 51.13            | 14.24                          | 3.76                           | 4.39  | 6.09  | 6.37  | 2.40              | 4.95             | 6.67 |
| 11       | 54  | Kersantite (Johannsen)           | 52.96            | 15.66                          | 4.25                           | 4.41  | 5.79  | 6.01  | 3.28              | 3.10             | 4.54 |
| 12       | 15  | Vogesite (Johannsen)             | 50.31            | 15.38                          | 3.71                           | 5.29  | 6.33  | 7.58  | 3.03              | 2.74             | 5.63 |
| 13       | 14  | Spessartite (Johannsen)          | 53.07            | 15.81                          | 3.05                           | 4.83  | 6.27  | 7.61  | 3.60              | 2.40             | 3.36 |
| 14       | 10  | Syenite (Rosenbusch)             | 60.06            | 16.16                          | 2.63                           | 3.37  | 3.29  | 4.26  | 3.08              | 5.21             | 1.94 |
| 15       | 6   | Monzonite (Rosenbusch)           | 53.66            | 15.88                          | 3.73                           | 4.52  | 4.54  | 7.77  | 3.65              | 4.11             | 2.44 |
| 16       | 7   | Normal diorite (Rosenbusch)      | 54.88            | 17.34                          | 2.97                           | 6.23  | 4.64  | 7.46  | 3.48              | 1.52             | 1.48 |
| 17       | 43  | Nepheline syenite (Daly)         | 54.63            | 19.89                          | 3.37                           | 2.20  | 0.87  | 2.51  | 8.26              | 5.46             | 2.81 |
| 18       | 20  | Essexite (Rosenbusch)            | 48.60            | 17.51                          | 4.42                           | 5.72  | 4.00  | 8.88  | 4.30              | 2.28             | 4.29 |
| 19       | 16  | Shonkinitite (Rosenbusch)        | 46.71            | 14.82                          | 5.45                           | 4.41  | 5.66  | 8.36  | 4.87              | 4.90             | 4.82 |
| 20       | 6   | Ijolite (Rosenbusch)             | 44.32            | 18.41                          | 3.78                           | 4.71  | 4.34  | 9.86  | 9.35              | 1.98             | 3.25 |
| 21       | 4   | Muscovite, granitic (Johannsen)  | 45.66            | 31.45                          | 4.21                           | 0.94  | 0.90  | 0.63  | 0.82              | 10.50            | 4.89 |
| 22       | 34  | Biotite, granitic (Tschirwinsky) | 36.52            | 17.00                          | 7.61                           | 14.67 | 9.32  | 0.88  | 1.13              | 8.19             | 4.68 |
| 23       | 4   | Hornblende, granitic (Johannsen) | 48.05            | 5.30                           | 2.43                           | 9.95  | 13.97 | 15.94 | 1.44              | 0.90             | 2.02 |
| 24       | 4   | Augite, granitic (Tschirwinsky)  | 50.80            | 4.17                           | 5.44                           | 6.62  | 12.36 | 18.61 | 1.28              | 0.29             | 0.43 |



Such unequal triangles, however, will fit at different altitudes within a tetrahedron with a base of 100 unit divisions of the same magnitude; and it is clear that such parallel triangles will lie at distances of  $(100 - T)$  above the basal triangle of the tetrahedron. Therefore the 3 eigenvalues,  $\lambda_1 = \alpha$ ,  $\lambda_2 = \beta$ , and  $\lambda_3 = \gamma$ , and the corresponding altitude  $(100 - T) = \delta$ , as shown in the first four columns of Table 2, will constitute 4 quadriplanar coordinates suitable for charting each analysis as a single point within, or for one or more negative eigenvalues, outside a tetrahedron of ref-

TABLE 2

| No. | Quadriplanar coordinates |             |              |       | Trilinear coordinates<br>(Apical projection) |         |          | Trilinear coordinates<br>(Orthogonal projection) |         |          |
|-----|--------------------------|-------------|--------------|-------|--|---------|----------|--|---------|----------|
|     | $\lambda_1$              | $\lambda_2$ | $\lambda_3$  | 100-T | $\alpha$                                     | $\beta$ | $\gamma$ | $\alpha$   | $\beta$ | $\gamma$ |
| 1   | 75.194                   | -1.393      | 1.970        | 24.23 | 99.24  | -1.84   | 2.60     | 83.27  | 6.68    | 10.05    |
| 2   | 72.748                   | -2.251      | 2.913        | 26.59 | 99.10  | -3.07   | 3.97     | 81.61  | 6.61    | 11.78    |
| 3   | 71.967                   | -1.709      | 3.532        | 26.21 | 97.53  | -2.32   | 4.79     | 80.70  | 7.03    | 12.27    |
| 4   | 68.361                   | -1.752      | 4.191        | 29.20 | 96.55  | -2.47   | 5.92     | 78.10  | 7.98    | 13.92    |
| 5   | 67.192                   | -0.047      | 2.616        | 30.24 | 96.32  | -0.07   | 3.75     | 77.27  | 10.03   | 12.70    |
| 6   | 51.870                   | 2.545       | 4.265        | 41.32 | 88.39  | 4.34    | 7.27     | 65.64  | 16.32   | 18.04    |
| 7   | 51.595                   | 1.572       | 5.554        | 41.28 | 87.86  | 2.68    | 9.46     | 65.36  | 15.33   | 19.31    |
| 8   | 51.771                   | 3.453       | 26.576       | 18.20 | 63.29  | 4.22    | 32.49    | 57.84  | 9.52    | 32.64    |
| 9   | 44.428                   | 5.830       | 24.751       | 24.99 | 59.23  | 7.77    | 33.00    | 52.76  | 14.16   | 33.08    |
| 10  | 52.827                   | 0.525       | 10.538       | 36.11 | 82.69  | 0.82    | 16.49    | 64.86  | 12.56   | 22.58    |
| 11  | 54.809                   | 0.911       | 7.570        | 36.71 | 86.60  | 1.44    | 11.96    | 67.04  | 13.15   | 19.81    |
| 12  | 52.520                   | 1.433       | 8.317        | 37.73 | 84.34  | 2.30    | 13.36    | 65.10  | 14.01   | 20.89    |
| 13  | 55.048                   | 0.770       | 6.882        | 37.30 | 87.80  | 1.23    | 10.98    | 67.48  | 13.20   | 19.32    |
| 14  | 61.219                   | -2.160      | 6.230        | 34.71 | 93.77  | -3.31   | 9.54     | 72.79  | 9.41    | 17.80    |
| 15  | 55.538                   | -2.093      | 7.195        | 39.36 | 91.59  | -3.45   | 11.86    | 68.66  | 11.03   | 20.31    |
| 16  | 57.289                   | 0.122       | 3.589        | 39.00 | 93.92  | 0.20    | 5.88     | 70.29  | 13.12   | 16.59    |
| 17  | 56.105                   | -1.492      | 3.697        | 41.69 | 96.22  | -2.56   | 6.34     | 70.00  | 12.41   | 17.59    |
| 18  | 51.463                   | 0.266       | 5.161        | 43.11 | 90.46  | 0.47    | 9.07     | 65.83  | 14.64   | 19.53    |
| 19  | 49.234                   | -0.881      | 8.837        | 42.81 | 86.09  | -1.54   | 15.45    | 63.50  | 13.39   | 23.11    |
| 20  | 48.018                   | 1.946       | $\pm 4.270i$ | 48.09 |  |         |          |  |         |          |
| 21  | 46.426                   | -0.716      | 5.741        | 48.55 | 90.23  | -1.39   | 11.16    | 62.61  | 15.47   | 21.92    |
| 22  | 44.525                   | 2.998       | $\pm 3.712i$ | 49.48 |  |         |          |  |         |          |
| 23  | 49.697                   | 0.986       | 13.356       | 35.96 | 77.60  | 1.54    | 20.86    | 61.69  | 12.97   | 25.34    |
| 24  | 51.694                   | 0.0125      | 11.883       | 36.41 | 81.29  | 0.02    | 18.69    | 63.83  | 12.15   | 24.02    |

erence. The charting of negative trilinear and quadriplanar coordinates has been described in an earlier paper by the writer (Mertie, 1949, p. 707-710).

Perspective drawings would be required to show the positions of many points located by quadriplanar coordinates. Obviously one could not take the time and trouble to do this, and it therefore seems best to project these points onto one or more of the triangular faces of the tetrahedron of reference. A perspective drawing of the inside of a lined tetrahedron is shown in Fig. 1 to illustrate two ways of making the required

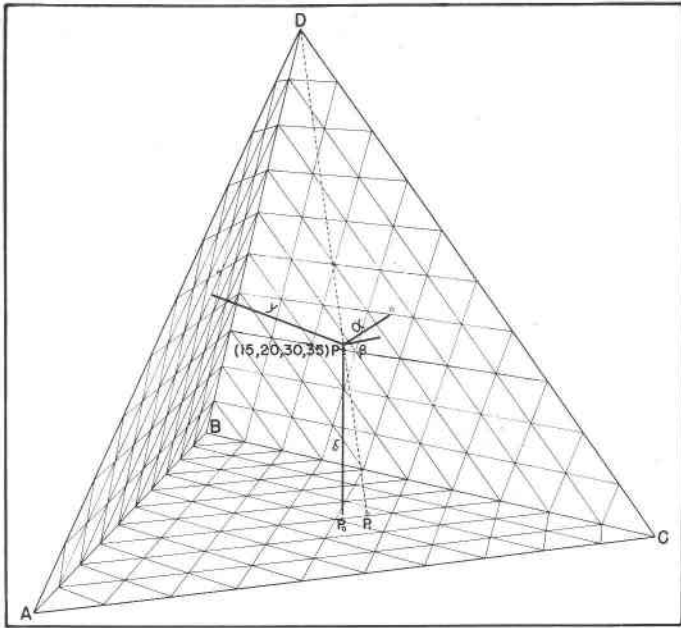


FIG. 1. Perspective drawing of inside of lined tetrahedron, showing apical and orthogonal projections of quadriplanar coordinates.

projection. The point  $P$  may be projected apically by the line  $DP$  to  $P_1$ , in which case the trilinear coordinates of  $P$  on the triangle  $ABC$  will be the quadriplanar coordinates  $\alpha$ ,  $\beta$ , and  $\gamma$ , recomputed to 100%. A second method is to project  $P$  orthogonally onto  $ABC$ , in which case the trilinear coordinates of  $P_0$  will be

$$\left(\alpha + \frac{\delta}{3}\right), \left(\beta + \frac{\delta}{3}\right), \text{ and } \left(\gamma + \frac{\delta}{3}\right).$$

This formula may be generalized for the boundaries of hypertetrahedra. By either method, however, a single projection is inadequate, as two points with different quadriplanar coordinates could by either of the two cited methods occupy identical positions in the projection. Moreover, one point that was projected apically might coincide with another point projected orthogonally; but if the projections were reversed, these two points would no longer be superposed. Therefore a projection into one plane of all points by both methods of projection will assure that at least two of the four projected positions of two original points will be unique.

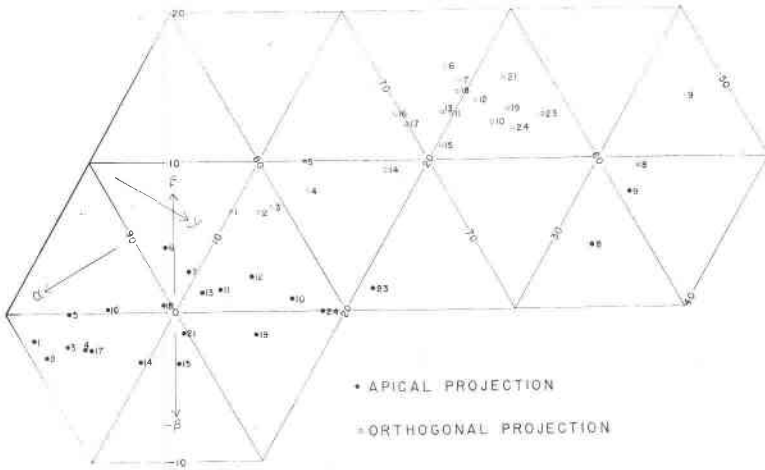


FIG. 2. Projection of quadriplanar coordinates on base of tetrahedron.

The relative positions of the quadriplanar coordinates derived from 19 igneous rocks and 3 granitic minerals are shown in Fig. 2, projected both apically and orthogonally, in order to avoid projections on two triangular faces. The numerical data for these two projections are given respectively in columns 5-7 and 8-10 of table 2. It happens that these values cause no identical superpositions produced from any of the suggested causes, though points 4 and 17, when apically projected, are close together. By orthogonal projection, however, they are far apart. For this particular assemblage of analyses, a somewhat greater dispersion of points is attained by orthogonal projection. In both projections, the granitic rocks lie at one end of the sequence, the ultrabasic rocks at the other end, and the other 15 rocks and minerals at various intermediate positions.

Variations in the charted positions of analyses resulting from differences in the percentages of specified components are not ordinarily apparent. However, some idea of the magnitude and direction of displacement of a particular point could be obtained in the following way. Suppose that an analysis showing 5%  $K_2O$  is so changed that it becomes 2%. This decrement might be added to the percentage of  $Na_2O$ , or proportionately to  $Na_2O$  and  $CaO$ , or it might be distributed throughout the analysis. After the disposition is made, however, a new cubic equation and a new set of eigenvalues may be computed; and for some specific distribution of the 3%  $K_2O$ , the displacement of the projected point will be apparent.

## SYMMETRIC MATRICES

The method of classification and charting so far outlined has the defect that complex numbers may emerge as the latent roots of matrices derived from some analyses; and in applying this method to many kinds of analyses, complex roots might become very prevalent. A refinement of the first method permits the elimination of all complex roots, though the process adds two arithmetical steps. A matrix of real elements that is symmetrical to its principal diagonal is known to have a characteristic equation that yields only real roots. The matrices heretofore used can be rendered symmetrical in the following way. If the rows and columns of a matrix are interchanged, a second matrix is produced that is called the transpose of the first. Either addition or multiplication of a matrix  $A$  and its transpose  $A'$  will yield a new matrix that is symmetrical with regard to its principal diagonal. Addition, however, does not insure uniqueness, so that multiplication, which is a combination of multiplication and addition, is used. But owing to this process, the elements of  $AA'$  become large and unwieldy; and they are therefore reduced to total 100 by dividing each element by  $S/100$ , where  $S$  is their sum. This method of producing a symmetrical matrix, and of obtaining its eigenvalues, is illustrated below for the rock ijolite.

$$\begin{aligned}
 & \text{Ijolite, 9 components, from } 3 \times 3 \text{ matrix} \\
 AA' = & \begin{vmatrix} 44.32 & 4.71 & 9.35 \\ 18.41 & 4.34 & 1.98 \\ 3.78 & 9.86 & 3.25 \end{vmatrix} \times \begin{vmatrix} 44.32 & 18.41 & 3.78 \\ 4.71 & 4.43 & 9.86 \\ 9.35 & 1.98 & 3.25 \end{vmatrix} \\
 = & \begin{vmatrix} 2073.87 & 854.89 & 244.36 \\ 854.89 & 361.68 & 118.82 \\ 255.36 & 118.82 & 240.89 \end{vmatrix}
 \end{aligned}$$

Divided by 51.1256, we get

$$\begin{vmatrix} 40.56 & 16.72 & 4.78 \\ 16.72 & 7.07 & 2.33 \\ 4.78 & 2.33 & 4.71 \end{vmatrix} \rightarrow \begin{vmatrix} 48.13 & 0 & 0 \\ 0 & 0.13 & 0 \\ 0 & 0 & 4.09 \end{vmatrix}$$

This process leads to an important generalization. Given an analysis of 12 components which are written as a  $3 \times 4$  matrix, whose transpose is therefore a  $4 \times 3$  matrix. These two matrices are conformable for multiplication, as expressed in the language of matrix algebra, and their product  $AA'$  becomes a symmetrical matrix of the third order, which is diagonalized as in the original method. An example is given below where ijolite is taken with 12 instead of 9 components, by the separate enumeration of  $MnO$ ,  $H_2O$ ,  $TiO_2$ , and  $P_2O_5$ . The matrix  $AA'$  is nonsingular, and the latent roots are shown to be real numbers.

Ijolite, 12 components, from  $3 \times 4$  matrix

$$AA' = \begin{vmatrix} 44.32 & 4.71 & 9.86 & 0.68 \\ 18.41 & 0.13 & 9.35 & 1.36 \\ 3.78 & 4.34 & 1.98 & 1.08 \end{vmatrix} \times \begin{vmatrix} 44.32 & 18.41 & 3.78 \\ 4.71 & 0.13 & 4.34 \\ 9.86 & 9.35 & 1.98 \\ 0.68 & 1.36 & 1.08 \end{vmatrix}$$

$$= \begin{vmatrix} 2084.13 & 909.66 & 208.23 \\ 909.66 & 428.22 & 90.14 \\ 208.23 & 90.14 & 38.21 \end{vmatrix}$$

Divided by 49.6660, we get

$$\begin{vmatrix} 41.96 & 18.32 & 4.19 \\ 18.32 & 8.62 & 1.81 \\ 4.19 & 1.81 & 0.77 \end{vmatrix} \rightarrow \begin{vmatrix} 50.48 & 0 & 0 \\ 0 & 0.34 & 0 \\ 0 & 0 & 0.53 \end{vmatrix}$$

This method may be extended to  $3 \times 5$ ,  $3 \times 6$ , and in general  $3 \times (3+k)$  rectangular arrays, where  $k$  is positive. This generalization and its extension thus constitute a third method for the classification and charting of analyses having 12, 15, 18, or in general  $9+3k$  components that total 100. But the number of variables need not necessarily be divisible by 3, as one or two zeros may be substituted for absent components in any rectangular array, before post-multiplication by its transpose.

The classification and charting of fewer than 9 variables constitutes another topic. It might be thought that a  $3 \times 2$  matrix, involving 6 variables, could be multiplied by its transpose, thus producing a symmetrical matrix of the third order analogous to those obtained from  $3 \times 5$ ,  $3 \times 6$ , and  $3 \times (3+k)$  matrices. But the symmetrical matrix thus obtained will be found to be singular, and therefore unusable.<sup>1</sup> A  $2 \times 3$  matrix also involves 6 variables, but when multiplied by its transpose yields a square matrix of the second order which will have a quadratic characteristic equation. The eigenvalues derived from such an equation are not unique.

Fewer than 9 variables, however, can be handled by another method. Given a nonsingular square matrix of the third order, such as heretofore shown in generalized form. For the production of 8, 7, 6, or 5 variables, zeros may be substituted as follows:

For 8 variables, let  $a_{12}=0$ ; for 7 variables, let  $a_{12}=a_{21}=0$ ; for 6 variables, let  $a_{12}=a_{21}=a_{23}=0$ ; and for 5 variables, let  $a_{12}=a_{21}=a_{23}=a_{32}=0$ .

Any of these four alternatives will yield a usable cubic characteristic equation. An example is given below of a weighted mean analysis of all

<sup>1</sup> Theorem. If any real matrix of the order  $m \times (m+k)$  and rank  $r=m$  be post-multiplied by its transpose, two alternatives exist: if  $k$  is nonnegative, the resulting symmetrical matrix  $AA'$  of the  $m$ th order is nonsingular; but if  $k$  is negative, the matrix  $AA'$  is singular.

the platinum metals produced by the Goodnews Bay Mining Co., of Alaska, from 1934 to 1959, inclusive. The mean analysis and its matrix are given below:

|           |                |       |      |      |
|-----------|----------------|-------|------|------|
| Platinum  | 84.38 per cent | 84.38 | 0    | 1.35 |
| Iridium   | 11.49          |       |      |      |
| Osmium    | 2.21           | 0     | 2.21 | 0    |
| Ruthenium | 0.18           |       |      |      |
| Rhodium   | 1.35           | 11.49 | 0.18 | 0.39 |
| Palladium | 0.39           |       |      |      |

The characteristic equation of this matrix is

$$\lambda^3 - 86.98\lambda^2 + 204.7384\lambda - 38.4467 = 0,$$

whose discriminant is positive, so that the latent roots are real. It therefore is unnecessary to render the matrix symmetrical before diagonalization. The derived eigenvalues are 84.564, 0.206, and 2.210; and  $100 - T = 13.02$ . This may readily be charted either by the apical or orthogonal projection.

Square matrices of the fourth order contain 16 elements; and therefore  $4 \times 4$ ,  $4 \times 5$ ,  $4 \times 6$ , and in general  $4 \times (4+k)$  matrices could be used for 16, 20, 24, or in general  $16+4k$  variables, where  $k$  is nonnegative. The derived characteristic equations, however, are quartics, which are more laborious to solve than cubics; and the five resulting coordinates must be charted on the boundaries of hypertetrahedra of four dimensions. For these reasons, and because matrices of the third order suffice for 9 or any larger number of variables, the utilization of matrices of the fourth order is not recommended.

#### SUMMARY STATEMENT

Three general methods have been presented for the classification and charting of analyses that are recomputed to total 100 per cent. The first method employs unsymmetrical matrices of the third order, from each of which three eigenvalues and a trace are derived. These are utilized in quadriplanar charting unless the eigenvalues include complex numbers. A second method uses the same original matrices, but they are rendered symmetrical before diagonalization, thus eliminating complex eigenvalues. A third method uses rectangular arrays of the order  $3 \times (3+k)$  that are transformed into symmetrical matrices of the third order, after which they are treated as in the first and second methods. This permits the classification and charting of 12, 15, 18, or in general  $9+3k$  variables. By substituting one or two zeros in the rectangular matrices, the third method allows all analyses with more than 9 components to be utilized.

And by substituting from one to four zeros in square matrices of the third order, before multiplication by their transposes, either the first or the second method permits the use of analyses with 8, 7, 6, or 5 components.

It must be understood that numerical indices and graphs which result from these three methods are not comparable. Even analyses of 12 components, classified and charted by the third method, cannot be tabulated or graphed with similar data obtained by the same method from 15 or more components. A choice of methods that suits the problem in hand is first made; thereafter only one method is used for each group of related analyses.

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Mathematics is like geology and mineralogy in that no single exposition includes a complete discussion of all phases of a subject; and therefore for particular topics numerous books are needed. The appended bibliography of books on matrices and related topics is not intended to be an enumeration of all the principal treatises on these subjects. The dozen cited books on matrices include only treatises of comparatively recent origin that have been consulted by the writer in the preparation of this paper. They range from elementary treatments to others that are too advanced to be readily assimilated by a non-mathematician, such as the writer; but even the more abstruse of these discussions contain items that may not elsewhere be available. An example is the volume by Frazer, Duncan, and Collar (1957), which is an advanced treatise; yet it includes four introductory chapters on matrix algebra that are readily understandable and contain many numerical examples of great value.

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