An improved method for algebraic analysis of metamorphic mineral assemblages

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Abstract

Singular value decomposition (SVD) provides a simple and straightforward way of detecting univariant reactions in multicomponent mineral assemblages. As originally developed by Fisher (1989), however, the method had the disadvantage that it created model mineral compositions that were not strictly stoichiometric. Model assemblages of stoichiometric minerals can be produced by rewriting the mineral composition matrix in terms of additive and exchange components and then weighting the additive components more heavily than exchange components during SVD analysis.

Prior to SVD analysis, it is generally necessary to use least-squares methods to fit mineral analyses to stoichiometric models based on exchange and additive components; least-squares fitting of this sort may be useful for evaluating mineral analyses even when SVD analysis is not contemplated.

Introduction

Mapping in metamorphic terrain depends upon our ability to identify equilibrium mineral assemblages and map isograds between metamorphic zones. Both procedures require that we determine whether or not mineral assemblages are related by univariant reactions. The most common method of detecting reactions is to search for intersections of mineral tie lines in assemblage diagrams (e.g., Thompson, 1957). Although simple to use, graphical methods cannot deal rigorously with complex multicomponent assemblages. Algebraic methods (e.g., Greenwood, 1967) can handle assemblages with any number of components but have been little used because of the complexity of the regression techniques initially developed. Fisher (1989) proposed a simpler method of algebraic analysis based on singular value composition (SVD), and that technique is now beginning to be more widely used (e.g., Powell, 1990; Gordon et al., 1991; Lang, 1991).

The usefulness of the SVD method can be illustrated by an example from metamorphosed pelitic rocks in northern Idaho. Lang and Rice (1985) mapped a garnet isograd separating chlorite + biotite + muscovite rocks (locally containing Mn-rich garnet) from garnet + chlorite + biotite + muscovite rocks. If the isograd actually separates rocks of different metamorphic grade, at least some of the assemblages on opposite sides of the isograd should contain mineral assemblages that are related by univariant reactions and therefore contain tie lines that intersect in composition space. However, Lang and Rice were unable to find reactions with acceptably low error ratios using the regression techniques available at that time, and so they could not eliminate the possibility that the garnet isograd actually represents a change in bulk rock composition rather than a change in metamorphic grade. Using SVD methods, Fisher (1989) showed that

Lang and Rice's samples TS29 and TS2 were in fact related by univariant reactions like

$$1.00\,bi + 30.95\,ms + 1.94\,pl$$
$$= 0.04\,gt + 1.20\,bi + 0.30\,ch + 30.97\,ms$$
$$+ 0.11\,pl \tag{1}$$
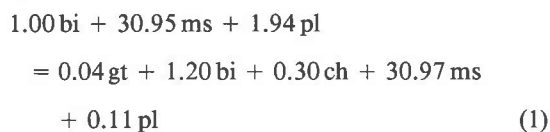
with TS29 (biotite zone) minerals on the left and TS2 (garnet zone) minerals on the right. Consequently their garnet isograd does indeed separate rocks of different metamorphic grade. Furthermore, the large size of the muscovite coefficients in the model reactions shows that the tie-line intersections represented by these reactions are close to muscovite in composition space, suggesting that the reactions responsible for the formation of garnet in these rocks may depend critically upon a small change in muscovite composition with metamorphic grade.

The ease with which these reactions were found illustrates one of the major advantages of SVD techniques over regression methods. Regression techniques require (1) that the user select one mineral as the dependent variable while treating all others as independent variables, and (2) that the number of components exceed the number of minerals. Consequently, complex assemblages cannot generally be analyzed in a single operation; rather, successive subsets of the full assemblages must be analyzed sequentially. These restrictions make regression analysis a complex and time-consuming process and prevent examination of the effects of simultaneous variation in all components of all minerals. Because the SVD technique can model assemblages with any number of minerals in a single operation and can accommodate simultaneous variations in all components of all minerals, it is much more likely to discover subtle, unsuspected reactions like those between TS29 and TS2.

TABLE 1. Hypothetical quartz + orthopyroxene + olivine compositions in conventional and BT components

		Mineral compositions				Residuals		
		Quartz	Opx	Olivine		Quartz	Opx	Olivine
1. Hypothetical analytical data, in conventional oxide components								
	SiO_2	0.990	1.010	1.005				
C	MgO		0.251	0.498				
	FeO		0.748	1.502				
2. Rank 2 model assemblage, in conventional oxide components*					**2. (Rank 2 model) − (analytical data), in oxide components***			
	SiO_2	0.9900	1.0100	1.0050		0.0000	0.0000	0.0000
	MgO	0.0009	0.2492	0.4989		0.0009	−0.0018	0.0009
	FeO	−0.0003	0.7486	1.5017		−0.0003	0.0006	−0.0003
3. Hypothetical analytical data, in BT components								
	SiO_2'	0.990	1.010	1.005				
B	MgO'		0.999	2.000				
	$FeMg_{-1}$		0.748	1.502				
4. Stoichiometric model of analytical data, in BT components					**4. (Stoichiometric model) − (analytical data) in BT components**			
	SiO_2'	1.0000	1.0000	1.0000		0.0100	−0.0100	−0.0050
B_{ls}	MgO'		1.0000	2.0000	$B_{ls} - B$	0.0000	0.0010	0.0000
	$FeMg_{-1}$		0.7485	1.5020		0.0000	0.0005	0.0000
5. Rank 2 model assemblage, in BT components					**5. (Rank 2 BT model) − (stoichiometric model) in BT components**			
	SiO_2'	1.0000	1.0000	1.0000		0.0000	0.0000	0.0000
B_m	MgO'	0.0000	1.0000	2.0000	$B_m - B_{ls}$	0.0000	0.0000	0.0000
	$FeMg_{-1}$	−0.0008	0.7502	1.5012		−0.0008	0.0017	−0.0008
6. Rank 2 BT model assemblage, converted to oxide components					**6. (Rank 2 BT model) − (analytical data) in oxide components**			
	SiO_2'	1.0000	1.0000	1.0000		0.0100	−0.0100	−0.0050
$A' \cdot B_m$	MgO'	0.0008	0.2498	0.4988	$A' \cdot B_m - C$	0.0008	−0.0012	0.0008
	FeO	−0.0008	0.7502	1.5012		−0.0008	0.0022	−0.0008

* From Fisher (1989, p. 72).

But, useful as it is, the SVD approach has one nagging problem: it tends to produce model reactions involving minerals that are not strictly stoichiometric. For example, when Fisher (1989, p. 71–72) analyzed a hypothetical quartz + orthopyroxene + olivine assemblage in the system MgO-FeO-SiO_2 (Table 1, line 1), he found that it was analytically indistinguishable from a model assemblage in which the orthopyroxene lay precisely on the quartz-olivine tie line (Table 1, line 2); consequently the assemblage could represent a frozen univariant reaction rather than a divariant equilibrium assemblage. However, that conclusion can be questioned because none of the minerals in the univariant model assemblage is truly stoichiometric. For example, the ratio (Mg + Fe)/Si in the model pyroxene is 0.988, rather than 1.000. The real question is whether we can find stoichiometric olivine, orthopyroxene, and quartz compositions that are related by a univariant reaction and are also analytically indistinguishable from the original mineral compositions.

To answer that question, we must constrain the SVD analysis so that all mineral compositions obey conventional stoichiometric rules. We can easily do so by using additive and exchange components, a concept first suggested by Bragg (1937) and subsequently embellished by J. B. Thompson and his colleagues (e.g., Thompson, 1982); to reflect their legacy, I will refer to such components as Bragg-Thompson (or BT) components.

To constrain the SVD analysis, we first define end-member compositions for each phase (e.g., $MgSiO_3$ for orthopyroxene or Mg_2SiO_4 for olivine) and then express deviations from those end-member compositions in terms of exchange components describing known substitution schemes (e.g., replacement of Mg by Fe, represented by $FeMg_{-1}$, or replacement of Mg + Si by 2Al, represented by $Al_2Mg_{-1}Si_{-1}$). The mineral compositions are then weighted during SVD analysis so that deviations from the analyzed mineral compositions are expressed solely in terms of variations in the exchange components, and the amounts of the additive components are held fixed. Provided that the exchange components chosen are realistic, this procedure will automatically produce stoichiometric model mineral compositions; each will be specified by the addition of one or more exchange components to a stoichiometric end-member composition. In the example considered here, deviations from the analyzed compositions would be limited to changes in Fe/Mg, and the model orthopyroxene and olivine would have (Mg + Fe)/Si ratios of 1.000 and 2.000, respectively.

This paper first illustrates this procedure by applying it to Fisher's (1989) quartz + orthopyroxene + olivine assemblage, then outlines general procedures for applying the procedure to any assemblage, and then lists algorithms for performing the necessary calculations using the MATLAB software package. MATLAB is a trademark of the MathWorks, Inc., 24 Prime Park Way, Natick, Massachusetts 01760, U.S.A.

Example: Analysis of quartz + orthopyroxene + olivine

Conversion of mineral compositions to BT components

Compositions expressed in terms of conventional oxide components can be converted to BT components using the procedures described by Thompson (1982). The first step is to write a matrix, $\mathbf{A}$, which expresses the composition of the BT components in terms of the original oxide components. In the present example,

$$\mathbf{A} = \begin{matrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & -1 & 1 \end{matrix} \qquad (2)$$

where the rows give the compositions of the BT components SiO_2', MgO', and $FeMg_{-1}$ in terms of the oxide components SiO_2, MgO, and FeO, represented by the columns.

The matrix $\mathbf{A}^t$ relates the matrix of phase compositions expressed in BT components ($\mathbf{B}$) to the matrix of phase compositions in oxide components ($\mathbf{C}$) given in Table 1, line 1:

$$\mathbf{A}^t \cdot \mathbf{B} = \mathbf{C}. \qquad (3)$$

Solving for $\mathbf{B}$,

$$\mathbf{B} = (\mathbf{A}^t)^{-1} \cdot \mathbf{C} \qquad (4)$$

we obtain the mineral compositions in BT components (Table 1, line 3).

To generate a model assemblage of stoichiometric minerals, we must begin with stoichiometric mineral compositions; unfortunately, most mineral analyses are not strictly stoichiometric, owing to small analytical errors. For example, none of the mineral compositions in $\mathbf{B}$ (Table 1, line 3) is strictly stoichiometric; SiO_2' should equal 1.000 for all phases shown, and MgO' should equal 1.000 for orthopyroxene and 2.000 for olivine.

We can avoid this difficulty by using least-squares methods to fit mineral analyses to stoichiometric models expressed in terms of BT components prior to conducting SVD analysis. To do so, we simply add to $\mathbf{A}^t$ and $\mathbf{C}$ additional rows that specify the stoichiometry of the phases involved and then solve Equation 4 while weighting the rows representing the constraints so as to preserve exact stoichiometry. For the present example, the composite matrix $\mathbf{A}^t$ becomes

$$\mathbf{A}^t = \begin{matrix} 1 & 0 & 0 \\ 0 & 1 & -1 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{matrix} \qquad (5)$$

The first three rows represent the original $\mathbf{A}^t$ matrix, whereas the last two flag the columns (SiO_2' and MgO') whose values we wish to constrain. The composite matrix $\mathbf{C}$ becomes

$$\mathbf{C} = \begin{matrix} 0.990 & 1.010 & 1.005 \\ 0 & 0.251 & 0.498 \\ 0 & 0.748 & 1.502 \\ 1.000 & 1.000 & 1.000 \\ 0.000 & 1.000 & 2.000. \end{matrix} \qquad (6)$$

The first three rows represent the original $\mathbf{C}$ matrix, and the last two represent the values of SiO_2' and MgO' that we wish to impose on the compositions of the phases in each column (here quartz, orthopyroxene, and olivine).

Because $\mathbf{A}^t$ so augmented contains more rows than columns, we have an overdetermined set of equations, which must be solved by least-squares methods. To ensure that the stoichiometric constraints are imposed rigorously, we pre-multiply both $\mathbf{A}^t$ and $\mathbf{C}$ by a diagonal weighting matrix, in which the rows corresponding to the stoichiometric constraints are on the order of 100 times the weights for the oxide components (which may be adjusted to reflect variations in analytical uncertainty). In the present case, we assume that Si, Mg, and Fe are all equally well known and use the weighting matrix

$$\mathbf{D} = \begin{matrix} 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 100 & 0 \\ 0 & 0 & 0 & 0 & 100. \end{matrix} \qquad (7)$$

Our weighted equation relating the matrix $\mathbf{B}$ to $\mathbf{C}$ (comparable with the unweighted Eq. 3) now becomes

$$(\mathbf{D} \cdot \mathbf{A}^t) \cdot \mathbf{B} = \mathbf{D} \cdot \mathbf{C}. \qquad (8)$$

The matrix products $\mathbf{D} \cdot \mathbf{A}^t$ and $\mathbf{D} \cdot \mathbf{C}$ are both 5×3 matrices, and $\mathbf{B}$ is a 3×3 matrix, which defines the amount of the three BT components SiO_2', MgO', and $FeMg_{-1}$ in each of the three phases. The least-squares solution $\mathbf{B}_{ls}$ is given by

$$\mathbf{B}_{ls} = [(\mathbf{D} \cdot \mathbf{A}^t) \cdot (\mathbf{D} \cdot \mathbf{A}^t)]^{-1} \cdot (\mathbf{D} \cdot \mathbf{A}^t) \cdot (\mathbf{D} \cdot \mathbf{C}) \qquad (9)$$

(see Van Huffel and Vandewalle, 1991, p. 29) and is listed in Table 1, line 4; stoichiometric constraints are indeed achieved, albeit at the expense of small perturbations in $FeMg_{-1}$.

SVD analysis of assemblages in BT components

Our next task is to determine whether or not the set of stoichiometric mineral compositions ($\mathbf{B}_{ls}$, in Table 1, line 4), contains a univariant reaction. To ensure that stoichiometry is retained, we first weight the matrix by pre-multiplying $\mathbf{B}_{ls}$ with a diagonal matrix $\mathbf{E}$, designed to weight the rows containing the additive components 100 times or so more heavily than that containing the exchange component:

$$\mathbf{E} = \begin{matrix} 100 & 0 & 0 \\ 0 & 100 & 0 \\ 0 & 0 & 1. \end{matrix} \qquad (10)$$

Taking the SVD of the product $\mathbf{E} \cdot \mathbf{B}_{ls}$ gives three matrices defined by the relation

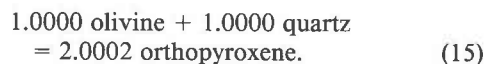$$\mathbf{E} \cdot \mathbf{B}_{ls} = \mathbf{U} \cdot \mathbf{W} \cdot \mathbf{V}^t \tag{11}$$

$$\mathbf{U} = \begin{matrix} 0.5847 & -0.8113 & 0.0000 \\ 0.8112 & 0.5847 & -0.0075 \\ 0.0061 & 0.0044 & 1.0000 \end{matrix} \tag{12}$$

$$\mathbf{W} = \begin{matrix} 267.6239 & 0 & 0 \\ 0 & 91.5280 & 0 \\ 0 & 0 & 0.0020 \end{matrix} \tag{13}$$

$$\mathbf{V} = \begin{matrix} 0.2185 & -0.8863 & 0.4082 \\ 0.5126 & -0.2475 & -0.8165 \\ 0.8247 & 0.3913 & 0.4082. \end{matrix} \tag{14}$$

A fundamental theorem of matrix algebra states that the diagonal elements of $\mathbf{W}$ give the singular values of $\mathbf{E} \cdot \mathbf{B}_{ls}$, the columns of $\mathbf{U}$ corresponding to nonzero singular values give an orthonormal basis for the composition space of $\mathbf{B}_{ls}$, and the columns of $\mathbf{V}$ corresponding to zero singular values give the coefficients of any linear dependencies contained in $\mathbf{B}_{ls}$ (Fisher, 1989, p. 71).

In this case, $\mathbf{W}$ contains three nonzero singular values, indicating that $\mathbf{E} \cdot \mathbf{B}_{ls}$ (and hence $\mathbf{B}_{ls}$) has a rank of 3. But the third singular value is nearly zero, showing that $\mathbf{E} \cdot \mathbf{B}_{ls}$ (and hence $\mathbf{B}_{ls}$) is close to some matrix of rank 2, which we will call $\mathbf{E} \cdot \mathbf{B}_m$. Being of rank 2, $\mathbf{E} \cdot \mathbf{B}_m$ must contain a linear dependency, given by the third column of $\mathbf{V}$, which defines the reaction

$$\begin{aligned} 1.0000 \text{ olivine} + 1.0000 \text{ quartz} \\ = 2.0002 \text{ orthopyroxene.} \end{aligned} \tag{15}$$

To find $\mathbf{E} \cdot \mathbf{B}_m$, we need only define a new diagonal matrix $\mathbf{W}_m$ in which the third singular value is exactly zero, and use Equation 11 to form the matrix product

$$\mathbf{E} \cdot \mathbf{B}_m = \mathbf{U} \cdot \mathbf{W}_m \cdot \mathbf{V}^t. \tag{16}$$

To recover the matrix of unweighted compositions $\mathbf{B}_m$, comparable with the original mineral compositions, we simply pre-multiply $\mathbf{E} \cdot \mathbf{B}_m$ by the inverse of $\mathbf{E}$; the result, $\mathbf{B}_m$, is the model matrix that we seek (Table 1, line 5).

One disadvantage of BT components is that judging the effects of analytical uncertainty can be tricky; it may be easier to convert $\mathbf{B}_m$ back into conventional oxide components by pre-multiplying it by $\mathbf{A}^t$ for comparison with original mineral compositions; the result is given in Table 1, line 6. Although generally larger than those associated with the unconstrained model (Table 1, line 2), the residuals are smaller than the analytical uncertainties of the original compositions. This confirms that the original assemblage is analytically indistinguishable from a stoichiometric univariant assemblage and cannot be inferred to represent a divariant equilibrium state.

GENERALIZED ROUTINES FOR SVD ANALYSIS

Converting mineral compositions to stoichiometric BT components

Begin by selecting an appropriate set of BT components for all minerals in an assemblage (or composite assemblage) containing the oxides needed to form one additive end-member composition for each phase present, along with all necessary exchange components; assume that there are a additive oxide components, c conventional oxide components, e exchange components, and p phases in the assemblage. Write out the $(a + e)$ by $(a + e)$ matrix, $\mathbf{M}$, relating the BT components to conventional oxide components, and take its transpose, $\mathbf{M}^t$. Now form the composite matrix $\mathbf{A}^t$, analogous to $\mathbf{A}^t$ in Equation 5, partitioned as

$$\mathbf{A}^t = \left| \begin{array}{c} \mathbf{M}^t \\ \hline \mathbf{I} \mid \mathbf{Z} \end{array} \right| \tag{17}$$

where $\mathbf{I}$ is an a by a identity matrix, $\mathbf{Z}$ is an a by e zero matrix, and $\mathbf{M}^t$ is defined as above.

Next form the composite matrix $\mathbf{C}$, comparable with $\mathbf{C}$ in Equation 6, partitioned as

$$\mathbf{C} = \left| \begin{array}{c} \mathbf{C}_o \\ \hline \mathbf{C}_a \end{array} \right| \tag{18}$$

where $\mathbf{C}_o$ is the c by p matrix containing the compositions of the minerals in the assemblage expressed in conventional oxide components (components in rows, phases in columns), and $\mathbf{C}_a$ is the a by p matrix giving the amount of each additive oxide in the end-member chosen to represent the phase described by the columns of $\mathbf{C}_o$.

Now pre-multiply $\mathbf{A}^t$ and $\mathbf{C}$ by a diagonal $(c + a)$ by $(c + a)$ weighting matrix, $\mathbf{D}$, analogous to that in Equation 7; the first c terms can be used to weight the conventional components for differing analytical uncertainty, whereas the last a terms should be larger by a factor of approximately 100, to constrain the stoichiometry.

The matrix $\mathbf{B}_{ls}$ of stoichiometric approximations to the original mineral analyses is the least-squares solution to the system of equations

$$(\mathbf{D} \cdot \mathbf{A}) \cdot (\mathbf{D} \cdot \mathbf{B}) = \mathbf{C}. \tag{19}$$

In MATLAB this can all be done in a single operation using the notation

$$\mathbf{B}_{ls} = (\mathbf{D} * \mathbf{A}) / (\mathbf{D} \cdot \mathbf{C}) \tag{20}$$

once the matrices $\mathbf{A}$, $\mathbf{C}$, and $\mathbf{D}$ have been defined.

Analysis of assemblages in BT components

Once the $(a + e)$ by p matrix, $\mathbf{B}_{ls}$ of stoichiometric mineral compositions is available, we first weight it by pre-multiplying $\mathbf{B}_{ls}$ by the diagonal matrix $\mathbf{E}$ with $(a + e)$ terms; the last e terms can be used to weight the exchange components for varying analytical uncertainty, whereas the first a terms should be on the order of 100 times

larger, to constrain the additive oxide components to their stoichiometric values.

We then take the SVD of the product $E \cdot B_{ls}$, obtaining the matrices U, W, and V, which satisfy the relation

$$E \cdot B_{ls} = U \cdot W \cdot V^t. \qquad (21)$$

In MATLAB this is accomplished by simply using the expression $[U, W, V] = \text{svd}(E * B_{ls})$. As before, the diagonal elements of W are the singular values of the weighted matrix B_{ls}, and the number of nonzero singular values gives the rank of B_{ls} (Van Huffel and Vandewalle, 1991, p. 22). Any univariant reactions contained in B_{ls} will be given by the columns of V corresponding to zero singular values.

To determine whether or not B_{ls} is close to a model matrix B_m of some lower rank, say r, form a new matrix W_m by setting to zero all but the largest r singular values in W and find B_m from the relation

$$B_m = U \cdot W_m \cdot V^t \qquad (22)$$

which is equivalent to the MATLAB expression

$$B_m = U * W_m * V'. \qquad (23)$$

In its raw form, B_m is a weighted model matrix of rank r, expressed in terms of BT coefficients. To recover the matrix of mineral compositions in unweighted form, B_u, pre-multiply B_m by the inverse of the weight matrix,

$$B_u = E^{-1} \cdot B_m \qquad (24)$$

or

$$B_u = \text{inv}(E) * B_m \qquad (25)$$

in MATLAB notation.

In order to compare B_u directly with mineral analyses, it is convenient to use Equation 1 to convert the model back to conventional oxide components,

$$C_m = M^t \cdot B_u \qquad (26)$$

which is equivalent to the MATLAB expression

$$C_m = M^t * B_u. \qquad (27)$$

The matrix of residuals

$$R = C - C_m \qquad (28)$$

can then be compared directly with analytical uncertainties to determine whether or not B_u provides an adequate fit to the observed assemblage.

CONCLUSIONS

This paper has shown that by expressing the compositions of minerals in metamorphic assemblages in BT components and weighting the additive components of each mineral 100 or so times as heavily as the exchange components, SVD methods of analysis can be forced to yield stoichiometric mineral assemblages and reactions. In most cases, it will be necessary to fit mineral analyses to stoichiometric model mineral compositions prior to SVD analysis, in order to avoid deviations from strict stoichiometry resulting from analytical error. Least-squares techniques for doing this fitting may be useful even when SVD analysis is not contemplated, inasmuch as they offer a sensitive way of detecting faulty mineral analyses.

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