

## TOWARDS A GENERALIZED SINGULAR VALUE DECOMPOSITION\*

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**Abstract.** We suggest a form for, and give a constructive derivation of, the generalized singular value decomposition of any two matrices having the same number of columns. We outline its desirable characteristics and compare it to an earlier suggestion by Van Loan [SIAM J. Numer. Anal., 13 (1976), pp. 76–83]. The present form largely follows from the work of Van Loan, but is slightly more general and computationally more amenable than that in the paper cited. We also prove a useful extension of a theorem of Stewart [SIAM Rev. 19 (1977), pp. 634–662] on unitary decompositions of submatrices of a unitary matrix.

**1. Introduction and notation.** The singular value decomposition (SVD) of a given  $m \times n$  matrix  $C$  of rank  $k$  is

$$(1.1) \quad U^H C V = S = \text{diag}(\sigma_1, \sigma_2, \dots) \geq 0,$$

where  $U(m \times m)$  and  $V(n \times n)$  are unitary matrices, the superscript  $H$  denotes complex conjugate transpose, and the above notation indicates that  $S(m \times n)$  is zero, except for real nonnegative elements on the leading diagonal. We may order these elements, the singular values of  $C$ , so that  $\sigma_1 \geq \sigma_2 \geq \dots \geq \sigma_k > \sigma_{k+1} = \dots = \sigma_q = 0$ ,  $q = \min\{m, n\}$ . If we know  $m = n$  we write  $S = \text{diag}(\sigma_1, \dots, \sigma_m)$ . A proof of the existence of the SVD can be found, for example, in the book by Lawson and Hanson [6] together with a description of the standard algorithm for computing it. The algorithm is due to Golub and others [3], [4], and a reliable FORTRAN program is available in [2].

We are concerned with generalizing the SVD to any two matrices  $A(m \times n)$  and  $B(p \times n)$  with the same number of columns. This is motivated by the awareness that if  $p = n$  and  $B$  is nonsingular, there are theoretical and numerical problems which require the SVD of  $C \triangleq AB^{-1} = USV^H$  as in (1.1). However forming  $AB^{-1}$  and finding its SVD can lead to unnecessary and large numerical errors when  $B$  is ill conditioned for solution of equations. To avoid this inverse we can state the result in the form  $U^H A = SV^H B$ , and if  $S_B$  is an arbitrary  $m \times m$  positive definite diagonal matrix and  $S_A \triangleq S_B S$  then

$$(1.2) \quad S_B U^H A = S_A V^H B, \quad S_A = \text{diag}(\alpha_1, \alpha_2, \dots), \quad S_B = \text{diag}(\beta_1, \dots, \beta_m),$$

$$\alpha_i = \beta_i \sigma_i, \quad i = 1, 2, \dots, \min\{m, n\}.$$

We will be interested in a decomposition of this form and call it a generalized singular value decomposition (GSVD) of  $A$  and nonsingular  $B$ . We will say  $(\alpha_i, \beta_i)$  is a singular value pair for  $A$  and  $B$ , the arbitrary nature of  $\beta_i$  allowing us a useful flexibility.

In the case of a general  $p \times n$  matrix  $B$ , Van Loan [9] showed if  $m \geq n$  there exist unitary  $U$  and  $V$ , and nonsingular  $X$  so that

$$(1.3) \quad U^H A X = \Sigma_A = \text{diag}(\alpha_1, \alpha_2, \dots), \quad V^H B X = \Sigma_B = \text{diag}(\beta_1, \beta_2, \dots),$$

where  $\Sigma_A$  is  $m \times n$  and  $\Sigma_B$  is  $p \times n$ . Van Loan called this the  $B$ -singular value decomposition of  $A$  (BSVD) and gave examples of its theoretical and practical use. Note that if  $B$  is nonsingular, so is  $\Sigma_B$ , and then  $U^H A = \Sigma_A \Sigma_B^{-1} V^H B$ , which is equivalent to (1.2), so (1.3) gives a generalization of (1.2) for nonsquare  $B$  when  $m \geq n$ .

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Van Loan [9] pointed out that there are difficulties in computing (1.3). We can understand this if we choose unitary  $Q$  so that  $X^{-1}Q = R$  is upper triangular and combine this with (1.3) to give

$$(1.4) \quad U^H A Q = \Sigma_A R, \quad V^H B Q = \Sigma_B R.$$

Here the unitary transformations do not alter the 2-norms of the matrices ( $\|C\|_2 \triangleq \sigma_1$  in (1.1)), and we could hope to find the transformations of  $A$  and  $B$  in (1.4) in a numerically stable computation. However,  $R$  and  $X = QR^{-1}$  can be ill conditioned no matter how we choose the diagonal matrices; e.g.,  $R = \begin{pmatrix} \varepsilon & 1 \\ 0 & 1 \end{pmatrix}$  for very small  $\varepsilon$ . Thus the transforming matrix  $X$  in (1.3) can be ill conditioned, and in general we cannot expect to compute the transformations of  $A$  and  $B$  in (1.3) in a numerically stable way. This argument also points to (1.4) as a more desirable form for the GSVD with a general  $p \times n$  matrix  $B$  than (1.3).

In § 2 we derive a possible form of the GSVD for general  $A$  and  $B$  having the same number of columns. The theoretical development of this in some ways parallels that in [9], but the result is essentially of the form (1.4) rather than the form (1.3), and is likely to be more amenable to reliable computation than the form (1.3). There are also no restrictions on  $m$ ,  $n$ , or  $p$ . Section 3 relates the suggested GSVD to the BSVD of [9], and considers some properties of this GSVD. In § 4, a result of § 2 is used to generalize a known result on unitary matrices. Section 5 summarizes the paper and briefly considers some computational aspects.

**2. A generalized singular value decomposition.** Here we give a constructive development of a GSVD of  $A(m \times n)$  and  $B(p \times n)$  with no restrictions on  $m$ ,  $n$ , or  $p$ . We make extensive use of unitary transformations. In particular, we can find unitary matrices  $P$  and  $Q$  to transform a given matrix  $C$  to the form

$$(2.1) \quad P^H C Q = \begin{pmatrix} R & 0 \\ 0 & 0 \end{pmatrix},$$

where  $R$  is nonsingular with the rank of  $C$ . This can be computed directly in a numerically stable way resulting in upper triangular  $R$  (see for example, [6]) but the rank determination may not be trivial. We can avoid such difficulties by computing the SVD of  $C$ , as in (1.1), but this is an iterative process and is computationally more expensive. Note that in either case, the singular values of  $R$  are the nonzero singular values of  $C$ .

We will now indicate how to derive a GSVD of  $A$  and  $B$  by taking  $C^H = (A^H, B^H)$  and examining the SVDs of submatrices of  $P$  in (2.1).

**THEOREM.** For given  $A(m \times n)$  and  $B(p \times n)$  with  $C^H = (A^H, B^H)$  and  $k = \text{rank}(C)$ , there exist unitary matrices  $U(m \times m)$ ,  $V(p \times p)$ ,  $W(k \times k)$ , and  $Q(n \times n)$  giving

$$(2.2) \quad U^H A Q = \Sigma_A \begin{pmatrix} W^H R, & 0 \\ k & n-k \end{pmatrix}, \quad V^H B Q = \Sigma_B \begin{pmatrix} W^H R, & 0 \\ k & n-k \end{pmatrix},$$

$$(2.3) \quad \Sigma_A \triangleq \begin{pmatrix} I_A & & \\ & S_A & \\ & & O_A \end{pmatrix}_{m \times k}, \quad \Sigma_B \triangleq \begin{pmatrix} O_B & & \\ & S_B & \\ & & I_B \end{pmatrix}_{p \times k},$$

$\begin{matrix} & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \end{matrix} \begin{matrix} r & s & k-r-s \end{matrix}$

where  $R(k \times k)$  is nonsingular with singular values equal to the nonzero singular values of

*C.*  $I_A(r \times r)$  and  $I_B(k - r - s \times k - r - s)$  are unit matrices,  $O_A(m - r - s \times k - r - s)$  and  $O_B(p - k + r \times r)$  are zero matrices with possibly no rows or no columns, and  $S_A \triangleq \text{diag}(\alpha_{r+1}, \dots, \alpha_{r+s})$ ,  $S_B \triangleq \text{diag}(\beta_{r+1}, \dots, \beta_{r+s})$  are real  $s \times s$  matrices. We have

$$(2.4) \quad 1 > \alpha_{r+1} \geq \dots \geq \alpha_{r+s} > 0, \quad 0 < \beta_{r+1} \leq \dots \leq \beta_{r+s} < 1,$$

$$(2.5) \quad \alpha_i^2 + \beta_i^2 = 1, \quad i = r+1, \dots, r+s.$$

*Proof.* In (2.1) let

$$(2.6) \quad C = \begin{pmatrix} A \\ B \end{pmatrix} \begin{matrix} m \\ p \end{matrix}, \quad Q = \begin{pmatrix} Q_1 & Q_2 \end{pmatrix} \begin{matrix} k & n-k \end{matrix}, \quad P = \begin{pmatrix} P_1 & P_2 \end{pmatrix} \begin{matrix} k & k \end{matrix} = \begin{pmatrix} P_{11} & P_{12} \\ P_{21} & P_{22} \end{pmatrix} \begin{matrix} m \\ p \end{matrix}.$$

We have  $\|P_{11}\|_2 \leq \|P_1\|_2 = 1$ , so no singular value of  $P_{11}$  is greater than unity, and we may write the SVD of  $P_{11}$  as

$$(2.7) \quad U^H P_{11} W = \Sigma_A,$$

with  $\Sigma_A$  as in (2.3) and (2.4). Now consider the decomposition

$$(2.8) \quad V^H (P_{21} W) = L = (\lambda_{ij}),$$

where unitary  $V$  is chosen so that  $L(p \times k)$  is lower triangular with real nonnegative diagonal finishing in the bottom right hand corner, i.e.,  $\lambda_{ij} = 0$  if  $p - i > k - j$ , and  $\lambda_{ij} \geq 0$  if  $p - i = k - j$ . The details of this type of triangularization can be found in [5] and [6]. The matrix

$$(2.9) \quad \begin{pmatrix} U^H \\ V^H \end{pmatrix} P_1 W = \begin{pmatrix} \Sigma_A \\ L \end{pmatrix}$$

clearly has orthonormal columns, and from the form of  $\Sigma_A$  in (2.3)

$$(2.10) \quad L = \Sigma_B,$$

where  $\Sigma_B$  is as in (2.3), (2.4), and (2.5). Combining (2.1) with (2.6), (2.9), and (2.10) gives

$$\begin{pmatrix} A \\ B \end{pmatrix} Q = \begin{pmatrix} P_1 R & 0 \end{pmatrix} = \begin{pmatrix} U \Sigma_A W^H R & 0 \\ V \Sigma_B W^H R & 0 \end{pmatrix},$$

from which (2.2) follows, completing the proof.

*Comments.* If  $p = n$  and  $B$  is nonsingular, then  $k = n$ , and (2.2) becomes

$$(2.11) \quad U^H A Q = \begin{pmatrix} S_A & \\ & O_A \end{pmatrix} W^H R, \quad V^H B Q = \begin{pmatrix} S_B & \\ & I_B \end{pmatrix} W^H R,$$

giving the form of (1.2)

$$(2.12) \quad \begin{pmatrix} S_B & \\ & I_B \end{pmatrix} U^H A = \begin{pmatrix} S_A & \\ & O_A \end{pmatrix} V^H B,$$

so the theorem gives a generalization of (1.2) to general nonsquare  $B$ . We see we have only unitary transformations of  $A$  and  $B$  in (2.2), and the comment following (1.4) will apply here.

We note that  $A$  and  $B$  have been treated identically here, apart perhaps from the ordering of elements in (2.3). But the diagonal blocks of  $\Sigma_A$  can be exchanged if those of  $\Sigma_B$  are exchanged in the same way, and similarly for the diagonal elements of  $S_A$  and  $S_B$ . Because of this equal treatment we can refer to (2.2) as a GSVD of  $A$  and  $B$ , rather than

a BSVD as in [9]. There is an easy to remember symmetry in (2.3), the significant elements of  $\Sigma_A$  are on the diagonal starting in the top left corner, and are nonincreasing moving farther from this corner, while the significant elements of  $\Sigma_B$  are on the diagonal finishing in the bottom right corner, and are nonincreasing going away from this corner.

Finally, we note that if  $R$  is the diagonal matrix of singular values of  $C$  in (2.1), then (2.2) involves these and the singular value pairs of  $A$  and  $B$  in a simple way which may be quite useful for theoretical pursuits such as perturbation analyses.

**3. Some properties of this GSVD.** We can relate the decompositions in (2.2) to the work of Van Loan [9] as follows. We have

$$(3.1) \quad U^H A X = (\Sigma_A, \quad 0), \quad V^H B X = (\Sigma_B, \quad 0), \quad X \triangleq Q \begin{pmatrix} R^{-1} W & 0 \\ 0 & I \end{pmatrix},$$

and if  $p \geq k$  in (2.3), we can move the first  $p - k$  rows of  $V^H$  to be the last  $p - k$  rows, so that  $\Sigma_B$  is now zero except for its leading diagonal. The result is equivalent to that in [9], and we certainly have  $p \geq k$  here if  $p \geq n$ , which is equivalent to the restriction in [9] (exchanging  $A$  and  $B$ ).

We can ascribe  $n$  singular value pairs  $(\alpha_i, \beta_i)$ ,  $i = 1, \dots, n$  to  $A$  and  $B$ , one corresponding to each column of  $U^H A X$  and  $V^H B X$  in (3.1). Following (2.3) we take for the first  $k$  of these

$$(3.2) \quad \alpha_i = 1, \quad \beta_i = 0 \quad i = 1, \dots, r,$$

$$(3.3) \quad \alpha_i, \beta_i \text{ as in } S_A \text{ and } S_B, \quad i = r + 1, \dots, r + s,$$

$$(3.4) \quad \alpha_i = 0, \quad \beta_i = 1, \quad i = r + s + 1, \dots, k,$$

and call these nontrivial pairs. Since the remainder correspond to the zero columns in (3.1) and have no particular numerical values attached to them, we will call them the  $n - k$  trivial singular value pairs of  $A$  and  $B$ .

When  $B$  is nonsingular the singular values of  $AB^{-1}$  are  $\alpha_i/\beta_i$ , so in analogy we could talk of generalized singular values and refer to those in (3.2) as infinite, those in (3.3) as ordinary, those in (3.4) as zero, and the remainder as arbitrary or undefined generalized singular values of  $A$  with respect to  $B$ . The use of pairs avoids this distinction between  $A$  and  $B$ .

An interesting example mentioned in [9] is

$$(3.5) \quad A = (1, \quad 0), \quad B = (0, \quad 1).$$

This corresponds to  $O_A$  and  $O_B$  in (2.3) having no rows, but one column each. There is one singular value pair as in (3.2) and one as in (3.4).

In [9] Van Loan showed that these singular value pairs correspond to the following generalization of the singular value concept from the one matrix  $C$  to two matrices  $A(m \times n)$  and  $B(p \times n)$ :

$$(3.6) \quad \text{Find the singular value pairs } (\alpha, \beta), \alpha^2 + \beta^2 \neq 0, \alpha \geq 0, \beta \geq 0, \\ \text{so that } \det(\beta^2 A^H A - \alpha^2 B^H B) = 0.$$

In [9]  $\alpha = 1$ , but here  $A$  and  $B$  have equal rights. We exhibit this correspondence in

terms of our GSVD (2.2), as the result is marginally more complete than in [9]. Note that

$$(3.7) \quad \det(\beta^2 A^H A - \alpha^2 B^H B) = \det \left( \begin{pmatrix} R^H W \\ 0 \end{pmatrix} \begin{pmatrix} \beta^2 I_A & & \\ & \beta^2 S_A^2 - \alpha^2 S_B^2 & \\ & & -\alpha^2 I_B \end{pmatrix} (W^H R, 0) \right).$$

Since the  $n \times n$  matrix whose determinant we are considering has rank at most  $k$ , we can say there are  $n - k$  arbitrary pairs  $(\alpha, \beta)$ ; these are the trivial pairs. We see the remaining pairs are just the nontrivial pairs given in (3.2), (3.3), and (3.4).

**4. Decomposition of unitary matrices.** Stewart [7] proves that if  $P$  is unitary of dimension  $m + p$  with  $m \leq p$ , then there exist unitary matrices  $U$  and  $W$  of dimension  $m$ , and  $V$  and  $Z$  of dimension  $p$ , so that

$$(4.1) \quad \begin{pmatrix} U^H & 0 \\ 0 & V^H \end{pmatrix} P \begin{pmatrix} W & 0 \\ 0 & Z \end{pmatrix} = \begin{pmatrix} C & -S & 0 \\ S & C & 0 \\ 0 & 0 & I_{p-m} \end{pmatrix} \begin{matrix} m \\ m \\ m \end{matrix},$$

with real  $S$  and  $C$ , such that

$$(4.2) \quad C = \text{diag}(\alpha_1, \dots, \alpha_m), \quad 1 \geq \alpha_1 \geq \dots \geq \alpha_m \geq 0,$$

$$(4.3) \quad S = \text{diag}(\beta_1, \dots, \beta_m), \quad 0 \leq \beta_1 \leq \dots \leq \beta_m \leq 1,$$

$$(4.4) \quad C^2 + S^2 = I.$$

The matrix on the right side of (4.1) is a generalization of an orthogonal rotation matrix, and its transpose is its inverse.

Stewart [7] notes that this result is implicit in the work of Davis and Kahan [1], and points out that it “often enables one to obtain routine computational proofs of geometric theorems that would otherwise require considerable ingenuity to establish”. Van Loan [10] emphasizes this and shows how it can be used to analyze some important problems involving orthogonal matrices. Unfortunately, this result could not be used directly here, as  $P$  in (2.6) had no square submatrices of interest in the general case. However, we have effectively used a generalization of (4.1) to prove the GSVD theorem in § 2. This shows a need for this generalization and so we will present it in full here.

**THEOREM.** *Let  $P$  be a unitary matrix of dimension  $m + p = k + q$ , then there exist unitary matrices  $U, V, W, Z$  of dimensions  $m, p, k, q$  respectively, so that*

$$(4.5) \quad \begin{pmatrix} U^H & 0 \\ 0 & V^H \end{pmatrix} P \begin{pmatrix} W & 0 \\ 0 & Z \end{pmatrix} = \begin{pmatrix} I & & & O_S^H & & & \\ & C & & & S & & \\ & & O_C & & & I & \\ \text{---} & O_S & \text{---} & & I & \text{---} & \\ & & S & & & -C & \\ & & & I & & & O_C^H \end{pmatrix} \begin{matrix} r \\ s \\ m-r-s \\ p-k+r \\ s \\ k-r-s \end{matrix}$$

$$(4.6) \quad C = \text{diag}(\alpha_{r+1}, \dots, \alpha_{r+s}), \quad 1 > \alpha_{r+1} \geq \dots \geq \alpha_{r+s} > 0,$$

$$(4.7) \quad S = \text{diag}(\beta_{r+1}, \dots, \beta_{r+s}), \quad 0 < \beta_{r+1} \leq \dots \leq \beta_{r+s} < 1,$$

$$(4.8) \quad C^2 + S^2 = I.$$

*Proof.* We have the same partitioning of  $P$  as in (2.6), so (2.9) and (2.10) with (2.3) show that there exist  $U$ ,  $V$  and  $W$  giving the first  $k$  columns in (4.5). Next, choosing  $Z$  to be unitary so that  $U^H P_{12} Z$  has the form of  $L^H$  in (2.8), and using an argument like (2.9) and (2.10), gives the first  $m$  rows of (4.5). Since each side of (4.5) is a unitary matrix we have

$$V^H P_{22} Z = \begin{pmatrix} F & G & 0 \\ H & N & 0 \\ 0 & 0 & 0 \end{pmatrix} \begin{matrix} p-k+r \\ s \\ p-k+r \end{matrix} \begin{matrix} s \\ s \\ s \end{matrix},$$

and  $SC + NS = 0$ , so  $N = -C$ , and then  $G = H^H = 0$  and  $F$  is unitary. We then obtain (4.5) by making the obvious unitary transformation of either  $V$  or  $Z$ .

*Comments.*  $O_C$  and  $O_S$  may be nonsquare here, and (4.5) is not so easy to remember as (4.1). However, this difficulty is lessened when we note that the leading  $m \times k$  diagonal block, and trailing  $p \times q$  diagonal block, is zero, except for the diagonal starting in the top left corner, with nonincreasing elements moving away from this corner. The remaining off diagonal blocks are zero, except for diagonals starting in the bottom right corners, with nonincreasing elements moving away from these corners.

We can obtain a more familiar form, given a particular  $2 \times 2$  block partition of a unitary matrix by possibly exchanging blocks of rows, blocks of columns, and transposing to give for  $P$

$$(4.9) \quad \begin{matrix} m \\ p \end{matrix} \begin{pmatrix} P_{11} & P_{12} \\ P_{21} & P_{22} \end{pmatrix}, \quad \begin{matrix} p \geq m \geq k, \\ q \geq k. \end{matrix}$$

With this ordering of dimensions it can be shown that there exists a transformation of the form in (4.5), giving for the transformed  $P$

$$(4.10) \quad \begin{pmatrix} C & & & -S \\ & I & & \\ S & & C & \\ & & & I \end{pmatrix} \begin{matrix} k \\ m-k \\ k \\ p-k \end{matrix}.$$

Here  $C^2 + S^2 = I$ , but the nonnegative diagonal matrices  $C$  and  $S$  may have diagonal elements of unity or zero. This is now seen to be a simple, but necessary and nontrivial, generalization of (4.1).

The form (4.10) is dependent on the ordering of the dimensions; whereas the decomposition (4.5) is quite general. Thus, although the parallel with rotation matrices is not so obvious, the form (4.5) will probably be marginally easier to use in the general case than (4.10).

**5. Remarks.** Although good computational practice has been kept in mind, this remains an essentially theoretical paper. We have presented a possible form for the generalized singular value decomposition of two matrices  $A$  and  $B$  having the same number of columns. This decomposition holds for all such pairs, and treats  $A$  and  $B$  equally. In essence, we have shown there exist unitary matrices  $U$ ,  $V$ ,  $W$ , and  $Q$ , so that

$$(5.1) \quad U^H A Q = \Sigma_A (W^H S, \quad 0), \quad V^H B Q = \Sigma_B (W^H S, \quad 0),$$

where  $S$  is the diagonal matrix of the nonzero singular values of  $(A^H, B^H)$ , while  $\Sigma_A$  and  $\Sigma_B$  are zero, except for real nonnegative leading and trailing diagonals respectively. These are related by

$$(5.2) \quad \Sigma_A^H \Sigma_A + \Sigma_B^H \Sigma_B = I_k,$$

and it is these diagonal elements which give the singular value pairs for  $A$  and  $B$ . The right hand sides in (5.1) involve the singular value pairs, a unitary matrix, and the singular values of  $(A^H, B^H)$ . Such forms may prove useful for perturbation analyses, but we have not studied this.

We have also presented the full generalization of a theorem by Stewart [7]. In fact, our generalized singular value decomposition could have been proven directly by making use of this extended result on the decomposition of a unitary matrix.

The proof of existence of our GSVD was constructive, being based on familiar decompositions for which there are generally available numerically stable algorithms, see [2]. In fact, with  $C$  as in (2.6) we could use the SVD to give (2.1), and again to give (2.7). We could also find  $V$  and  $\Sigma_B$  from the SVD of  $P_{21}$  in (2.6). However, we are not saying that combining these individual numerically stable computations will always lead to the desired results.

It has been found in practice that for certain types of problems, the  $W$  obtained by computing the SVD of  $P_{21}$  is distinctly different from the  $W$  obtained by computing the SVD of  $P_{11}$ . On the other hand, computing (2.8) can lead to distinctly nondiagonal  $L$ .

If only the singular value pairs are needed, then computing the SVD of both  $P_{11}$  and  $P_{21}$  appears to be satisfactory. Van Loan [8] used his VZ algorithm to compute the generalized singular values. This algorithm is based on unitary transformations and would most likely give accuracy comparable to that of the present SVD approach. Although both approaches are inefficient, the SVD approach has the advantage of being based on widely available and reliable computational algorithms, [2]. It is not advisable to base computations on the constructive proof of the BSVD in [9] as this involves the inverse of  $S$  in (5.1) early in the computation, and if the largest diagonal element of  $S$  is significantly greater than the smallest, this could introduce unnecessary numerical errors.

In conclusion, even if it is decided that (5.1) is a satisfactory form for the GSVD, we still require a perturbation analysis for the singular value pairs and vectors, and some formidable numerical problems remain to be solved.

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