On the Asymptotic Behavior of Scaled Singular Value and QR Decompositions

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Abstract. Asymptotic expressions are derived for the singular value decomposition of a matrix some of whose columns approach zero. Expressions are also derived for the QR factorization of a matrix some of whose rows approach zero. The expressions give insight into the method of weights for approximating the solutions of constrained least squares problems.

1. Introduction. It is well known that certain widely used matrix decompositions change in nontrivial ways when their rows or columns are multiplied by constants. For example, let the \( n \times p \) matrix \( X \) be partitioned in the form

\[ X = \begin{pmatrix} X_1 & X_2 \end{pmatrix}, \]

and for \( 1 \geq t \geq 0 \) define**

\[ X_t = \begin{pmatrix} X_1 & tX_2 \end{pmatrix}. \]

Let

\[ X_t = U_t S_t V_t^T \]

be the singular value decomposition of \( X_t \) (see [4] for definitions). The columns of \( U_t \) and \( V_t \) (the singular vectors of \( X_t \)) and the diagonal elements of \( S_t \) (the singular values) are nonlinear functions of \( t \), and there is no simple way of obtaining, say, \( S_t \) from \( S_1 \).

One purpose of this paper is to derive expansions for the singular value decomposition of \( X_t \) as \( t \) approaches zero. An application of these expansions is the following. When \( t \) is small, the ratio of the largest to the smallest singular values of \( X_t \) will be large, and from this one might conclude that problems associated with \( X_t \) are ill-conditioned. In order to determine whether this apparent ill-conditioning is real, it is necessary to have precise information about the singular value decomposition of \( X_t \) (see [3] for an example).

A related problem concerns the QR factorization of a matrix. Partition \( X \) in the form

\[ X = \begin{bmatrix} X_{11} & X_{12} \\ X_{21} & X_{22} \end{bmatrix}, \]

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**There is an ambiguity in this notation, since \( X_t \) can mean either the first element in the partition (1.1) or the matrix \( X_1 \) for \( t = 1 \). To resolve it, we let \( X_1 \) refer only to the former.
where $X_{11}$ is square, and write

\[(1.5)\]

\[
X_t = \begin{bmatrix}
X_{11} & X_{12} \\
\tau X_{21} & \tau X_{22}
\end{bmatrix}
\]

[note the different definitions of $X_t$ in (1.2) and (1.5)]. Matrices such as (1.5) with small $\tau$ arise in the numerical solution of constrained least squares problems [1, Chapter 22]. The approach is to down-weight the problem [represented by $(X_{21} X_{22})$] compared to the constraints [represented by $(X_{11} X_{12})$]. The best method for solving constrained problems in this way uses the QR factorization $X_t = Q_t R_t$, in which $Q_t$ has orthonormal columns and $R_t$ is upper triangular. In Section 3 we will derive asymptotic expressions for $Q_t$ and $R_t$.

2. The Singular Value Decomposition. We begin by observing that null vectors of $X$ behave in a simple manner under scaling. If $Xv = 0$ and

\[
v = \begin{bmatrix}
v_1 \\
v_2
\end{bmatrix}
\]

is partitioned conformally with (1.1), then

\[
v_t = \begin{bmatrix}
\tau v_1 \\
v_2
\end{bmatrix}
\]

is a null vector of $X_t$. Thus null vectors behave linearly under transformations of the form (1.2), and there is no need to treat them here. We shall therefore assume that $X$ has no null vectors.

The main result is summarized in the following theorem.

**Theorem 2.1.** Let the $n \times p$ matrix $X$ have rank $p$, and let $X$ be partitioned as in (1.1). Let $X_t$ be defined by (1.2). Let

\[(2.1)\] $B = (X_t^T X_t)^{-1} X_t^T X_2,
\]

and

\[(2.2)\] $\bar{X}_2 = X_2 - X_1 B.$

To each singular value $s_1$ of $X_1$ there is associated a unique singular value $s_1^{(t)}$ of $X_t$ which satisfies

\[(2.3)\] $s_1^{(t)} = s_1 + O(\tau^2).
\]

If $s_1$ is simple and its right singular vector is denoted by $v_1$, then the corresponding right singular vector of $X_t$ satisfies

\[(2.4)\] $v_1^{(t)} = \begin{bmatrix}
v_1 + O(\tau^2) \\
\tau B v_1 + O(\tau^3)
\end{bmatrix}.$

Moreover, if the left singular vector of $s_1$ is denoted by $u_1$, then the corresponding left singular vector of $X_t$ satisfies

\[(2.5)\] $u_1^{(t)} = u_1 + O(\tau^2).
\]

To each singular value $s_2$ of $\bar{X}_2$ there is associated a unique singular value $s_2^{(t)}$ of $X_t$ which satisfies

\[(2.6)\] $s_2^{(t)} = t s_2 + O(\tau^3).$
If $\tilde{\sigma}_2$ is simple and its right singular vector is denoted by $\tilde{v}_2$, then the corresponding right singular vector of $X_t$ satisfies

$$
(2.7) \quad \tilde{v}_2^{(t)} = \begin{bmatrix}
-tB\tilde{v}_2 + O(t^3) \\
\tilde{v}_2 + O(t^2)
\end{bmatrix}.
$$

Moreover, if the left singular vector of $\tilde{\sigma}_2$ is denoted by $\tilde{u}_2$, then the corresponding left singular vector of $X_t$ satisfies

$$
(2.8) \quad u_2^{(t)} = \tilde{u}_2 + O(t^2).
$$

Proof. We shall use the fact that the right singular vectors of $X_t$ are the eigenvectors of

$$
A_t = X_t^T X_t = \begin{bmatrix}
A_{11} & tA_{21}^T \\
tA_{21} & t^2A_{22}
\end{bmatrix},
$$

and the singular values are the nonnegative square roots of the corresponding eigenvalues. The matrix $A_0$ has two invariant subspaces corresponding to its partitioning. Specifically the columns of

$$
\begin{bmatrix}
I \\
0
\end{bmatrix}
$$

span an invariant subspace whose eigenvalues are those of $A_{11}$, while the columns of

$$
\begin{bmatrix}
0 \\
I
\end{bmatrix}
$$

span an invariant subspace whose eigenvalues are zero. The idea of the proof is to use the perturbation theory in [2] to derive expressions for the corresponding invariant subspaces of $A_t$. Expressions for the individual singular values and singular vectors may then be obtained from the expressions for the invariant subspaces.

Since $X$ has full column rank, $A_{11}$ is nonsingular. It follows [2] that for all sufficiently small $t$ there is a matrix $P$ satisfying

$$
(2.9) \quad (-P I) A_t \begin{bmatrix} I \\ P \end{bmatrix} = 0
$$

and

$$
P = O(t)
$$

such that

$$
\begin{bmatrix}
I \\
P
\end{bmatrix}
$$

spans an invariant subspace of $A_t$. If (2.9) is expanded and terms of order greater than $t$ are dropped, the result is

$$
(2.10) \quad P = tA_{21}A_{11}^{-1} + O(t^3) = tB^T + O(t^3).
$$

The eigenvectors of $A_t$ in the invariant subspace have the form

$$
(2.11) \quad \begin{bmatrix}
I \\
P
\end{bmatrix} v,
$$

where $v$ is an eigenvector of

$$
(2.12) \quad (I + P^T P)^{-1/2} (I P^T) A \begin{bmatrix}
I \\
P
\end{bmatrix} (I + P^T P)^{-1/2} = A_{11} + O(t^2).
$$
If \( v_1 \) is a singular vector of \( X \) with singular value \( s_1 \), then it is an eigenvector of \( A_{11} \) with eigenvalue \( s_1^2 \). The order \( t^2 \) perturbation in (2.12) perturbs \( s_1^2 \) by terms of order \( t^2 \), from which (2.3) follows. If \( s_1 \) is simple, the order \( t^2 \) perturbation in (2.12) induces an order \( t^2 \) perturbation in \( v_1 \). Thus we may take \( v = v_1 + O(t^2) \) in (2.11), and (2.4) follows from (2.10). Finally (2.5) follows from the relation

\[
 u^{(t)}_1 = s_1^{(t)} X X_1 v^{(t)}_1.
\]

In order to establish (2.6), (2.7), and (2.8), note that the orthogonal complement of the space spanned by the columns of \((I PT)^T\) is the complementary invariant subspace of \( A_t \). This subspace is spanned by

\[
\begin{bmatrix}
  -P^T \\
  I
\end{bmatrix} = \begin{bmatrix}
  -tB + O(t^3) \\
  I
\end{bmatrix}.
\]

As above, the eigenvectors and eigenvalues of the invariant subspace are to be found from the matrix

\[
(I + PP^T)^{-1/2}(-P I) A \begin{bmatrix}
  -P^T \\
  I
\end{bmatrix} (I + PP^T)^{-1/2}
\]

(2.13)

\[
= t^2(-B^T A_{11} B - B^T A_{21}^T - A_{12} B + A_{22}) + O(t^4)
\]

\[
= t^2(X_2 - X_1 B)^T (X_2 - X_1 B) + O(t^4)
\]

\[
= t^2 X_2^T X_2 + O(t^4).
\]

The results now follow from (2.13) by reasoning as above.

Theorem 2.1 divides the singular values of \( X \) into two classes. The first consists of the singular values of \( X_1 \) perturbed by terms of \( O(t^2) \). The initial components of the corresponding right singular vector approach the right singular vector \( v_1 \) of \( X_1 \), while the last components approach zero linearly with \( t \) along the direction \( B^T v_1 \). The left singular vector is the left singular vector of \( X_1 \) up to terms of order \( t^2 \).

Singular values of the second class approach zero linearly with \( t \). However, they are to be sought in the matrix \( tX_2 \), not \( tX_2 \). From (2.1) and (2.2), it follows that

\[
\bar{X}_2 = \left[ I - X_1 \left( X_1^T X_1 \right)^{-1} X_1^T \right] X_2.
\]

From this it is seen that \( \bar{X}_2 \) is the projection of \( X_2 \) onto the orthogonal complement of the column space of \( X_1 \). Singular vectors of the second class behave like those of the first class, except that it is the first components of the right singular vectors that approach zero.

A particularly satisfying feature of these expansions is that the error in any expression is \( O(t^2) \) times the order of the expression itself. This suggests that one can expect the asymptotic behavior to set in very quickly.

3. The QR Decomposition. In this section we shall derive expressions for the asymptotic form of the QR decomposition of the matrix \( X \) defined by (1.5). The results are summarized in the following theorem.

**Theorem 3.1.** Let \( X \) be of full column rank and be partitioned as in (1.4), where \( X_{11} \) is square. Let

\[
R_{11}^T R_{11} = X_{11}^T X_{11}
\]
be the Cholesky factorization of $X_{11}^T X_{11}$. Let
\[
\begin{bmatrix}
X_{11} & X_{12} \\
tX_{21} & tX_{22}
\end{bmatrix}
= \begin{bmatrix}
Q_{11}^{(t)} & Q_{21}^{(t)} \\
Q_{12}^{(t)} & Q_{22}^{(t)}
\end{bmatrix}
\begin{bmatrix}
R_{11}^{(t)} & R_{12}^{(t)} \\
0 & R_{22}^{(t)}
\end{bmatrix}
\]
be the QR factorization of $X_t$. Let
\[
X_{22} = X_{22} - X_{21} X_{11}^{-1} X_{12},
\]
and let
\[
\bar{X}_{22} = \bar{Q}_{22} \bar{R}_{22}
\]
be the QR factorization of $\bar{X}_{22}$. Then
\[
\begin{bmatrix}
R_{11}^{(t)} & R_{12}^{(t)} \\
0 & R_{22}^{(t)}
\end{bmatrix}
= \begin{bmatrix}
R_{11} + O(t^2) & R_{11}^{-1} X_{12} + O(t^2) \\
0 & tR_{22} + O(t^3)
\end{bmatrix}.
\]
Moreover,
\[
\begin{bmatrix}
Q_{11}^{(t)} \\
Q_{21}^{(t)}
\end{bmatrix}
= \begin{bmatrix}
X_{11} R_{11}^{-1} + O(t^2) \\
tX_{21} R_{11}^{-1} + O(t^3)
\end{bmatrix},
\]
and
\[
\begin{bmatrix}
Q_{12}^{(t)} \\
Q_{22}^{(t)}
\end{bmatrix}
= \begin{bmatrix}
-tX_{11}^T X_{21}^T + O(t^3) \\
I + O(t^3)
\end{bmatrix} \bar{Q}_{22}.
\]

Proof. We use the fact that the $R$-factor of the QR factorization of a matrix $X$ is
the Cholesky factor of $X^T X$. In particular,
\[
R_{11}^{(t)T} R_{11}^{(t)} = \begin{bmatrix}
X_{11}^T \\
tX_{21}^T
\end{bmatrix}^T \begin{bmatrix}
X_{11} \\
tX_{21}
\end{bmatrix} = X_{11}^T X_{11} + O(t^2).
\]

Since the Cholesky decomposition of a nonsingular matrix is a differentiable
function of its elements, it follows from (3.5) that $R_{11}^{(t)} = R_{11} + O(t^2)$. Since $R_{12}^{(t)} = R_{11}^{-1} X_{12}$ we have $R_{12}^{(t)} = R_{11}^{-1} X_{12} + O(t^2)$. This takes care of the first row of (3.2).
We will return to the expression for $R_{22}^{(t)}$ later. The expression (3.3) is derived from
the relation
\[
\begin{bmatrix}
Q_{11}^{(t)} \\
Q_{21}^{(t)}
\end{bmatrix}
= \begin{bmatrix}
X_{11} \\
tX_{21}
\end{bmatrix} R_{11}^{(t)-1}.
\]

In order to derive (3.4) and an expression for $R_{22}^{(t)}$, we use the fact that
\[
\begin{bmatrix}
Q_{12}^{(t)} \\
Q_{22}^{(t)}
\end{bmatrix}
R_{22}^{(t)}
\]
is the projection of $(X_{11}^T tX_{21}^T)^T$ onto the orthogonal complement of the space
spanned by $(X_{11}^T tX_{21}^T)^T$. The projection matrix has the form $I - P$, where
\[
P = \begin{bmatrix}
X_{11} \\
tX_{21}
\end{bmatrix} (X_{11}^T X_{11} + t^2 X_{21}^T X_{21})^{-1} (X_{11}^T tX_{21}^T)
= \begin{bmatrix}
I \\
tC
\end{bmatrix} (I + t^2 C^T C)^{-1} (I tC^T),
\]
where we have written \( C = X_{21}X_{11}^{-1} \). After some manipulation it follows that

\[
(I - P) \begin{bmatrix} X_{12} \\ tX_{22} \end{bmatrix} = \begin{bmatrix} -t^2C^T\bar{X}_{22} + O(t^4) \\ t\bar{X}_{22} + O(t^3) \end{bmatrix}.
\]

Thus \( R^{(t)}_{22}R^{(t)}_{22} = t^2\bar{X}^T_{22}\bar{X}_{22} + O(t^4) \), from which it follows that \( R^{(t)}_{22} = t\bar{R}_{22} + O(t^3) \). Equation (3.4) follows from (3.6) and the fact that

\[
\begin{bmatrix} Q^{(t)}_{12} \\ Q^{(t)}_{22} \end{bmatrix} = (I - P) \begin{bmatrix} X_{12} \\ tX_{22} \end{bmatrix} R^{(t)}_{22}^{-1}.
\]

Theorem 3.1 has some analogies with Theorem 2.1. In both theorems the decomposition is divided into two parts, one having a nonzero limit, and the other having a zero limit. In both theorems the first part is obtained from the constant part of the original matrix [e.g., \( (X_{11}X_{12}) \)], while the vanishing part is obtained from a modification of the vanishing part of the original decomposition (e.g., from \( \bar{X}_{22} \)). In Theorem 2.1 the row space of \( X \) is divided into two orthogonal subspaces which become uncoupled in the natural coordinate system of the partition [see (2.4) and (2.7)]. In Theorem 3.1 the same thing happens to the column space of \( X \).

The matrix \( \bar{X}_{22} \), defined by (3.1) is a generalization of the Schur complement of \( X_{11} \) in \( X \). For square matrices, the Schur complement is what is left over after Gaussian elimination has been performed on \( X_{11} \). Its appearance here can be related to the solution by elimination of the constrained least squares problem

\[
\begin{align*}
\text{minimize} & \quad \| y - (X_{21}X_{22}) \begin{bmatrix} b_1 \\ b_2 \end{bmatrix} \| \\
\text{subject to} & \quad (X_{11}X_{12}) \begin{bmatrix} b_1 \\ b_2 \end{bmatrix} = c.
\end{align*}
\]

If (3.8) is solved for \( b_1 \) and the result is substituted into (3.7), the result is the problem

\[
\begin{align*}
\text{minimize} & \quad \| (y - X_{21}X_{11}^{-1}c) - \bar{X}_{22}b_2 \|.
\end{align*}
\]

On the other hand, the solution may be approximated as in [1] by solving

\[
\begin{align*}
\text{minimize} & \quad \| \begin{bmatrix} c \\ ty \end{bmatrix} - X_tb_t \|
\end{align*}
\]

for small \( t \). From (3.2) and (3.4) the solution is seen to be

\[
b_2^{(t)} = \bar{R}_{22}^{-1}\bar{Q}_{22}^T (y - X_{21}X_{11}^{-1}c) + O(t^2).
\]

Since \( \bar{R}_{22}^{-1}\bar{Q}_{22}^T \) is the pseudo-inverse of \( \bar{X}_{22} \), a comparison of (3.9) and (3.10) shows that \( b_2^{(t)} \) differs from \( b_2 \) by terms of \( O(t^2) \). Thus the solution by weighting is seen as an approximation to the solution by elimination.

This relation throws light on an interesting piece of folklore: namely, that pivoting on column size must be used when solving weighted least squares problems of the form (3.10). The dicta is usually justified by an appeal to the numerical properties of the particular algorithm used to compute the QR decomposition. An alternative line of reasoning goes as follows. The method of elimination will not work if \( X_{11} \) is
singular, and it can be expected to produce inaccurate results when $X_{11}$ is nearly singular. Since the method of weights mimics the method of elimination, the columns $X_i$ should be interchanged to make $X_{11}$ well-conditioned. Pivoting on column size during the computations of the QR decomposition is an adaptive algorithm for doing just this.

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