Relations Between SVD and GSVD of Discrete Regularization Problems in Standard and General Form

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ABSTRACT

We consider an algorithm, due to Eldén, that transforms general discrete regularization problems into standard form. We derive a simple relationship between the SVD associated with the standard-form problem and the GSVD associated with the general problem, and we discuss the accuracy of the GSVD computed via this transformation.


Keywords: SVD and generalized SVD, regularization, transformation to standard form.

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1. Introduction

The discrete regularization problem in \textit{general form} is the following least squares problem with a quadratic constraint:

\[
\min_x \left( \| A x - b \|_2^2 + \lambda^2 \| L x \|_2^2 \right) \tag{1.1a}
\]

\[A \in \mathbb{R}^{m \times n}, \quad L \in \mathbb{R}^{p \times n}, \quad m \geq n \geq p, \quad \text{rank}(L) = p, \quad N(A) \cap N(L) = \{0\}. \tag{1.1b}
\]

Here, and throughout the paper, \( N(\cdot) \) denotes null space and \( \| \cdot \| \) denotes the vector and matrix 2-norm \( \| \cdot \|_2 \). The quantity \( \lambda \) is the regularization parameter which, together with the regularization matrix \( L \), controls the ‘smoothness’ of the solution. The last condition in (1.1b) ensures a unique solution to (1.1). Discrete regularization problems in general form arise in numerous technical applications such as e.g. early vision [1], computerized tomography [14] and electrocardiography [5].

Instead of dealing with (1.1) directly, it is often advantageous to transform the general problem into a problem in \textit{standard form}:

\[
\min_x \left( \| A \vec{x} - \vec{b} \|_2^2 + \lambda^2 \| \vec{x} \|_2^2 \right) \tag{1.2}
\]

The advantage of doing this is that there already exist very efficient methods for solving (1.2) numerically, such as bidiagonalization [3,6,7] and truncated SVD [4,9,12]. See also the survey of methods given in [10].

In this paper we focus on an efficient numerical algorithm for transforming (1.1) into (1.2) described by Eldén [6]. The transformation is summarized in Section 2. In Section 3 we derive a simple relation between the \textit{singular value decomposition} (SVD) associated with (1.2) and the \textit{generalized SVD} (GSVD) associated with (1.1). This relation lets one perform an analysis of (1.1), via its GSVD, merely from the SVD of (1.2) which is simpler to compute. Finally, in Section 4 we discuss the accuracy of the GSVD when computed via the transformation to standard form.

2. The transformation to standard form

We shall here briefly summarize Eldén’s method for transforming the general problem (1.1) into standard form (1.2). More details can be found in [6] and [2, Section 26]. The algorithm has the following four steps (where, for clarity, the subscripts ‘\( p \)’, ‘\( o \)’ and ‘\( q \)’ denote matrices with \( p \), \( n - p \) and \( m - (n - p) \) columns, respectively):
1) Compute the $Q-R$ factorization of $L^T$:

$$L^T = [K_p, K_o] \begin{bmatrix} R_p \\ 0 \end{bmatrix}. \quad (2.1)$$

2) Compute the $Q-R$ factorization of $A K_o$:

$$A K_o = [H_o, H_q] \begin{bmatrix} T_p \\ 0 \end{bmatrix}. \quad (2.2)$$

3) Solve the standard-form problem (2) with:

$$\bar{A} = H_q^T A L^+ , \quad \bar{b} = H_q^T b , \quad L^+ = K_p R_p^{-T}.$$

Notice that $A K_o$ can be computed simultaneously with $R_p$, and that the orthogonal transformations constituting $H = [H_o, H_q]$ can be saved for later multiplications with $H_o^T$ and $H_q^T$.

4) Compute the solution to (1.1) as:

$$x = L^* \bar{x} + K_o T_o^{-1} H_o^T (b - A L^* \bar{x}). \quad (2.4)$$

The matrix $A L^+$ should be computed only if $\bar{A}$ is explicitly required to solve (1.2). If $A$ is sparse or has a special structure (e.g. Hankel or Toeplitz) then iterative methods may be used to solve (1.2) without forming $\bar{A}$. Similarly, if $L$ is sparse or has a special structure then multiplication with $L^+$ should preferably be performed as described in [3, Eq. (6.4)], in which case $K_p$ and $R_p$ are not required.

In the two important cases when $L$ is a discrete approximation to either the first or second derivative operator on a uniform net, some of the above-mentioned quantities can be computed a priori, thus simplifying the method.

**Theorem 1.** Let $e = [1, 1, \ldots, 1]^T \in \mathbb{R}^n$, $f = [1, 2, \ldots, n]^T \in \mathbb{R}^n$ and define $\tilde{a} = A e / n$ and $\bar{a} = A f / n$.

If $L = L_1$ is an approximation to the first derivative operator on a uniform net,

$$L_1 = \begin{bmatrix} 1 & -1 \\ 1 & -1 \\ \ddots & \ddots \\ 1 & -1 \end{bmatrix} \in \mathbb{R}^{p \times n}, \quad p = n - 1,$$

then
\[ K_0 = n^{-1} e, \quad H_o = \hat{a} / \| \hat{a} \|, \quad T_o = \sqrt{n} \| \hat{a} \|, \quad K_o T_o^{-1} = e / (n \| \hat{a} \|). \quad (2.6) \]

If \( L = L_2 \) is an approximation to the second derivative operator on a uniform net,

\[
L_2 = \begin{bmatrix}
-1 & 2 & -1 \\
-1 & 2 & -1 \\
0 & \cdots & \cdots \\
-1 & 2 & -1 \\
\end{bmatrix} \in \mathbb{R}^{p \times p}, \quad p = n - 2.
\]  

(2.7)

then

\[
K_o = \begin{bmatrix}
\frac{1}{n} & \frac{\alpha_s f - \beta_s e}{n} \\
0 & \frac{\alpha_s \gamma - 2 \beta_s}{n} \\
\end{bmatrix}, \quad H_o = \frac{\hat{a} / \| \hat{a} \|, (\hat{a} - \gamma \hat{a}) / \| \hat{a} - \gamma \hat{a} \|}{\alpha_s \gamma - 2 \beta_s / \| \hat{a} \|},
\]  

(2.8a)

\[
T_o = \begin{bmatrix}
\sqrt{n} \| \hat{a} \| & n \| \hat{a} \| (\alpha_s \gamma - 2 \beta_s) \\
0 & n \alpha_s \| \hat{a} - \gamma \hat{a} \|
\end{bmatrix}
\]  

(2.8b)

\[
K_o T_o^{-1} = n^{-1} \begin{bmatrix}
\frac{e / \| \hat{a} \|, (f - \gamma e) / \| \hat{a} - \gamma \hat{a} \|}{\alpha_s \gamma - 2 \beta_s / \| \hat{a} \|}
\end{bmatrix}
\]  

(2.8c)

where

\[
\alpha_s = \left( \frac{12}{(n+1)n(n-1)} \right)^{\frac{1}{2}}, \quad \beta_s = \left( \frac{3(n+1)}{n(n-1)} \right)^{\frac{1}{2}}, \quad \gamma = \frac{\hat{a}^T \hat{a}}{\| \hat{a} \|^2}.
\]  

(2.8d)

Proof. By straightforward insertion it is easy to verify that \( L K_o = 0, \quad K_o^T K_o = H_o^T H = I_o, \quad H_o T_o = A K_o \) and that \( K_o T_o^{-1} \) is given by (2.8d). \( \Box \)

The condition numbers of \( L_1 \) (2.5) and \( L_2 \) (2.7) are approximately 0.64 \( n \) and 0.41 \( n^2 \), respectively. The matrices \( K_o \) and \( R_o \) are not required since both \( L_1 \) and \( L_2 \) are band matrices. We shall need the matrix \( K_o T_o^{-1} \) in Theorem 2 in the next section.

3. Comparison of the general and standard forms

Our main result in this paper is a simple relation between the SVD of \( \tilde{A} \) and the GSVD of the matrix pair \( (A, L) \). For convenience, we remind that the SVD of \( \tilde{A} \) is given by

\[
\tilde{A} = \tilde{U} \tilde{\Sigma} \tilde{V}^T, \quad \tilde{U} \in \mathbb{R}^{m \times (m-p)} \tilde{\Sigma}, \tilde{V} \in \mathbb{R}^{p \times p}
\]  

(3.1)

in which \( \tilde{U}^T \tilde{U} = \tilde{V}^T \tilde{V} = I_p \) and \( \tilde{\Sigma} \) is a diagonal matrix with non-negative diagonal elements \( \tilde{\sigma} \) appearing in non-increasing order. Using the same convention about subscripts 'p' and 'o' as before, the
GSVD of \((A, L)\) in (1.1) can be written as:

\[
A = U \Sigma X^{-1} = [U_p, U_o] \begin{bmatrix} \Sigma_p & 0 \\ 0 & I_o \end{bmatrix} [W_p, W_o]^T 
\]

\[ (3.2a) \]

\[
L = V M X^{-1} = V [M_p, 0] [W_p, W_o] = VM_p W_p^T 
\]

\[ (3.2b) \]

\[
U \in \mathbb{R}^{m \times \infty}, \quad X \in \mathbb{R}^{\infty \times \infty}, \quad \Sigma_p, M_p, V \in \mathbb{R}^{p \times p} 
\]

\[ (3.2c) \]

where \(U^T U = I_n, V^T V = I_p\), and the diagonal elements \(\sigma_i\) and \(\mu_i\) of \(\Sigma_p\) and \(M_p\) are ordered such that

\[
0 \leq \sigma_1 \leq \cdots \leq \sigma_p \leq 1, \quad 1 \geq \mu_1 \geq \cdots \geq \mu_p > 0. 
\]

\[ (3.2d) \]

The relation \(\mu_p > 0\) follows from the fact that \(L\) has full rank. We have set \(W^T = [W_p, W_o]^T = X^{-1} = [X_p, X_o]^{-1}\), and \(X\) is chosen such that

\[
\sigma_i^2 + \mu_i^2 = 1, \quad i = 1, \ldots, p. 
\]

\[ (3.3) \]

The GSVD was introduced in [16] with a slightly different notation than used here. For more details about the present formulation and about SVD and GSVD in general, see e.g. [2, Chapters II and IV].

Before we present the main theorem, we need the following three lemmas. Throughout, \(R()\) denotes column space, and we use the notation from Eqs. (3.1) and (3.2)

**Lemma 1.** If \(L\) has full row rank, then

\[
N(L) = R(X_o) = R(X_o), \quad R(A X_o) = R(H_o) = R(U_o). 
\]

\[ (3.4) \]

**Proof.** \(N(L) = R(X_o)\) follows immediately from (2.1). Since both \(M_p\) and \(V\) have full rank, \(R(L^T) = R(W_p M_p V^T) = R(W_p)\). From the relation

\[
W^T X = I_n \iff \begin{bmatrix} W^T X \sigma_o & W^T X \sigma_p \\ \sigma_o^2 W^T X \sigma_p & \sigma_p^2 W^T X \sigma_o \end{bmatrix} = \begin{bmatrix} I_p & 0 \\ 0 & I_o \end{bmatrix} 
\]

\[ (3.5) \]

we see that \(W^T X \sigma_o = I_o\) and \(W^T X \sigma_p = 0\) implying that rank \((X_o) = n - p = \dim(N(L))\) and that \(X^T W_p = 0 \Rightarrow R(X_o) \subseteq N(L)\). Together, these equations lead to \(N(L) = R(X_o)\). To prove the second relation in (3.4) we use \(A X_o = U_o\) and \(R(K_o) = N(L)\) to show that \(R(H_o) = R(A X_o) = R(A X_o) = R(U_o)\). \(\square\)

**Lemma 2.** If \(L\) has full row rank, then the pseudoinverse of \(L\) is given by

\[
L^+ = W_p (W_p^T W_p)^{-1} M_p^{-1} V^T = P X_p M_p^{-1} V^T. 
\]

\[ (3.6) \]
in which $P$ is the orthogonal projection matrix onto $R(L^T)$.

Proof. The first part of (3.6) follows immediately from (3.2b) and the fact that $L$ has full row rank such that [2, Remark 4.3]:

$$
L^* = L^T (L L^T)^{-1} = W_p M_p V^T (V M_p W_p^TW_p M_p V^T)^{-1}
$$

$$
= W_p M_p V^T V M_p^{-1} (W_p^TW_p)^{-1} M_p^{-1} V^T = W_p (W_p^TW_p)^{-1} M_p^{-1} V^T .
$$

To show the last part of (3.6) we have $P = P X W^T = P X_p W_p W_p^T$, and since $R(L^T) = R(W_p)$, we get

$$
P X_p W_p^TW_p = P W_p W_p^T \iff P X_p = W_p (W_p^TW_p)^{-1} .
$$

$\square$

Lemma 3. The submatrix $X_o$ in $X = [X_p, X_o]$ (3.2) is given by

$$
X_o = K_o T_o^{-1} H_o^T U_o .
$$

(3.7)

Proof. Since $R(K_o) = N(L)$ and $K_o K_o^T$ is the projection matrix for orthogonal projection onto $N(L)$, it follows that

$$
(W_o^T K_o) (K_o^T X_o) = W_o^T K_o K_o^T X_o = W_o^T X_o = I_o
$$

where we have used Lemma 2 and (3.5). Thus, $(W_o^T K_o)^{-1} = K_o^T X_o$. Lemma 2 also implies that $W_p^T K_o = 0$ such that $A K_o = (U_p \Sigma_o W_p^T + U_o \hat{W}_o^T) K_o = U_o \hat{W}_o^T K_o$. Hence,

$$
K_o T_o^{-1} H_o^T = K_o (A K_o)^* = K_o (U_o \hat{W}_o^T K_o)^* = K_o (W_o^T K_o)^{-1} U_o^T
$$

$$
= K_o K_o^T X_o U_o^T - X_o U_o^T \Rightarrow X_o = K_o T_o^{-1} H_o^T U_o . \quad \square
$$

We are now ready to present the relation between the GSVD of $(A, L)$ and the SVD of $\tilde{A}$ derived from $A$ and $L$ as described in the previous section.

Theorem 2. Let $A$, $L$ and $\tilde{A}$ be given by Eqs. (1.1) and (2.3), and let the SVD of $\tilde{A}$ and the GSVD of $(A, L)$ be given by (3.1)-(3.3). Then:

$$
\bar{U} = H_q^T U_p \Pi , \quad \bar{\Sigma} = \Pi \Sigma_p M_p^{-1} \Pi , \quad \bar{V} = V \Pi
$$

(3.8)

$$
U_p = H_q \bar{U} \Pi , \quad U_o = H_o , \quad X_o = K_o T_o^{-1}
$$

(3.9)

where $H = [H_o, H_q]$, $K_o$ and $T_o$ are defined in Eqs. (2.1) and (2.2), and $\Pi = \text{an} \text{diag}(1, ..., 1)$ is the $p \times p$ exchange matrix.
Proof. We shall first prove (3.8). Using (2.3), (3.2) and Lemmas 1 and 2, we obtain

\[ \bar{A} = H_q^T A L^* = H_q^T (U_p \Sigma_p W_p^T + U_o W_o^T) W_p (W_p^T W_p)^{-1} M_p^{-1} V^T \]
\[ = H_q^T U_p \Sigma_p M_p^{-1} V^T = (H_q^T U_p \Pi) (\Pi \Sigma_p M_p^{-1} \Pi) (V \Pi)^T . \]  

(3.10)

Since \( A K_o = U_o W_o^T K_o \) (see the proof for Lemma 3), and \( W_o^T K_o \) has full rank, we have \( R(H_o) = R(A K_o) = R(U_o) \). Thus,

\[ H^T U_p = \begin{bmatrix} H_q^T U_p \\ H_o^T U_p \end{bmatrix} = \begin{bmatrix} 0 \\ H_q^T U_p \end{bmatrix} \]

(3.11)

and it follows that

\[ (H_q^T U_p)^T (H_q^T U_p) = (H^T U_p)^T (H^T U_p) = U_q^T H H^T U_p = U_q^T U_p = I_p . \]

I.e., the columns of \( H_q^T U_p \) are orthonormal. Returning to (3.10), we now see that \( H_q^T U_p \Pi \) has orthonormal columns, \( \Pi \Sigma_p M_p^{-1} \Pi \) is a diagonal matrix with non-negative entries appearing in non-increasing order, and \( V \Pi \) is orthogonal. Hence, (3.10) constitutes the SVD of \( \bar{A} \). Next, we shall prove (3.9).

From (3.11) we have

\[ U_p = H \begin{bmatrix} 0 \\ H_q^T U_p \end{bmatrix} = H_q (H_q^T U_p \Pi) \Pi = H_q \bar{U} \Pi . \]

The matrix \( U_o \) is not unique (it corresponds to multiple \( \sigma_i = 1 \)) and we can therefore always choose \( U_o = H_o \). Lemma 3 then immediately yields \( X_o = K_o T_o^{-1} \). \( \square \)

Theorem 2 has theoretical as well as practical value. First of all, it shows that most of the quantities in the GSVD of \( (A, L) \) can be computed (or estimated) directly from \( \bar{A} \) and \( H_q \) without the need for an explicit GSVD computation. This is very important when analyzing and solving (1.1) numerically, because the generalized singular values and vectors reveals crucial information about the ill-posed problem (see [11,17]). For example, such an analysis will reveal whether a solution at all exists and whether it can be computed by means of regularization. Theorem 2 is also fundamental in connection with the choice of regularization parameter \( \lambda \). By means of Theorem 2, it is proved in [11] that application of generalized cross-validation [8] to either (1.1) or (1.2) leads to the same optimal regularisation parameter \( \lambda \). Thus, the transformation (2.4) from \( \bar{X} \) back to \( x \) need only be done once, when the optimal \( \lambda \) and \( \bar{X} \) has been computed.
4. The accuracy of the computed GSVD

In this section we shall briefly consider the accuracy of the GSVD when computed by means of the transformation to standard form, Eqs. (2.1)-(2.3), followed by computation of the SVD (3.1) of $\tilde{A}$. Our analysis deals only with the matrix $U$. This is sufficient to illustrate the major drawbacks of this approach to computing the GSVD, namely that the accuracy depends on the product $\kappa(A)\kappa(L)$, where $\kappa(A)$ and $\kappa(L)$ are the condition numbers of $A$ and $L$.

Let $\tilde{U}$ denote the computed version of the mathematical quantity $U$ in (3.2a), computed by a backward stable GSVD-algorithm such as [13] or [15]. Then:

$$\tilde{U} \tilde{X}^{-1} = A + E$$

(4.1)

in which $E$ represents the influence of rounding errors during the computation of the GSVD. The norm of $E$ satisfies $\|E\| = c \varepsilon_M \|A\|$, where $c$ is a modest function of $m$ and $n$, and $\varepsilon_M$ is the machine precision. Assuming that $A$ has full rank, it follows from (4.1) that the subspace angle between the column spaces of $U$ and $\tilde{U}$ is given by

$$\sin \Theta(U, \tilde{U}) = \|U_m - U U^T \tilde{U}\| = \|U_m - U U^T E (\tilde{X}^{-1})^{-1}\|$$

$$\leq \|E\| \|\tilde{X}^{-1}\|^{-1} = \|E\| \|X^{-1}\|^{-1} = \|E\| \|A^+\| = \|E\| \kappa(A).$$

(4.2)

This is the best bound possible; we cannot avoid the factor $\|A^+\|$ which is equal to the reciprocal of the smallest singular value of $A$.

Next, let $\tilde{U}_p$ denote the computed version of $U_p$ as computed via the SVD of $\tilde{A} = H_q^T A L^+$. From this expression we would immediately expect that the accuracy of $\tilde{U}_p$ depends on the product $\kappa(A)\kappa(L)$. This is confirmed by the following theorem:

Theorem 3. If $A$ has full rank then the pseudoinverse of $\tilde{A} = H_q^T A L^+$ is

$$\tilde{A}^+ = L A^+ H_q.$$  

(4.3)

Proof. We remind that the relation $(G H)^+ = H^+ G^+$ is not valid in general. To prove Eq. (4.3) we use the results in Theorem 2 and the fact that $A^+ = X \Sigma^{-1} U^T$ (since $A$ has full rank):

$$L A^+ H_q = V M X^{-1} X \Sigma^{-1} U^T H_q = V [M_p, 0] \begin{bmatrix} \Sigma_p^{-1} & 0 \\ \Pi & I_0 \end{bmatrix} \begin{bmatrix} U_p^T \\ U_o^T \end{bmatrix} H_q = V [M_p \Sigma_p^{-1}, 0] \begin{bmatrix} U_p^T H_q \\ U_o^T H_q \end{bmatrix}$$

$$= V M_p \Sigma_p^{-1} U_p^T H_q = (V \Pi) (\Pi M_p^{-1} \Pi) (H_q^T U \Pi)^T = \tilde{V} \tilde{\Sigma}^{-1} \tilde{U}^T = \tilde{A}^+.$$
From this theorem it follows immediately that the condition number of \( \widetilde{A} \) satisfies
\[
\kappa(\widetilde{A}) = \frac{||\widetilde{A}||}{||\widetilde{A}^+||} \leq \kappa(L) \kappa(A).
\]
Now, if we let \( \widetilde{U} \) denote the computed \( \overline{U} \), end let \( \overline{E} \) represent the influence of rounding errors during the computation of the SVD of \( \overline{A} \), then it is easy to show that
\[
\sin \Theta(\overline{U}, \widetilde{U}) \leq \frac{||\overline{E}||}{||\overline{A}||} \kappa(\overline{A}) \leq \frac{||\overline{E}||}{||\overline{A}||} \kappa(L) \kappa(A) \tag{4.4}
\]
where \( ||\overline{E}|| = \varepsilon \varepsilon_m ||\overline{A}|| \) and \( \varepsilon \) is a modest function of \( m-p \) and \( n \). Neglecting the errors in the computed \( H_q \), we then obtain:
\[
\sin \Theta(U_p, \widetilde{U}_p) = ||U_p U_p^T - \widetilde{U}_p \widetilde{U}_p^T|| = ||H_q^T (\overline{U} \overline{U}^T - \overline{U} \overline{U}^T) H_q||
\]
\[
\quad \leq ||\overline{U} \overline{U} - \overline{U} \overline{U}^T|| = \sin \Theta(\overline{U}, \widetilde{U}) \leq \frac{||\overline{E}||}{||\overline{A}||} \kappa(L) \kappa(A). \tag{4.5}
\]
This bound is inferior to the bound in (4.2) due to the factor \( \kappa(L) \), and we conclude that \( \overline{U} \) is only reliable if \( L \) is a well-conditioned matrix such as e.g. \( L_1 \) (2.5) or \( L_2 \) (2.7) for moderate \( n \).

To verify and illustrate the bound in Eq. (4.5) we computed \( \overline{U}_p \) in single precision (\( \varepsilon_M = 9.5 \times 10^{-7} \)) and compared it with \( U_p \) computed in double precision (\( \varepsilon_M = 2.2 \times 10^{-16} \)) for a variety of matrices \( L \) with different condition numbers \( \kappa(L) \). For simplicity, the condition number of \( A \) was held constant, \( \kappa(A) = 15 \). The dimensions were \( m = 25, n = 10, p = 8 \), and both \( A \) and \( L \) were random dense matrices with constant ratios between their singular values. The results are shown in Fig. 1. We see that for \( \kappa(L) \) larger than about \( 10^2 \), \( \sin \Theta(U_p, \overline{U}_p) \) increases linearly with \( \kappa(L) \), while for smaller values of \( \kappa(L) \) it is almost a constant, approximately \( 10^{-3} \). We conclude that for these small values of \( m \) and \( n \), the accuracy of the computed GSVD is acceptable for condition numbers of \( L \) less than, say, \( 10^3 \).

5. Conclusion

It is shown that if a discrete regularization problem in general form is transformed into a problem in standard form by Eldén's method, then the SVD associated with the standard form problem is related in a simple way to the GSVD of the original problem. Thus, computation of the SVD gives important information not only about the standard-form problem, but also about the original general-form problem. This is very important when analyzing and solving discrete ill-posed problems. The accuracy of the GSVD computed in this fashion depends on the condition number of the regularization matrix \( L \) and is therefore accurate only if \( L \) is well-conditioned.
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References


![Graph](image)

**Figure 1.** Comparison of computed $\bar{U}_p$ and true $U_p$ as a function of the condition number $\kappa(L)$. Dimensions: $m = 25$, $n = 10$, $p = 8$. 