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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.

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1. Introduction

The discrete regularization problem in *general form* is the following least squares problem with a quadratic constraint:

$$\min_x \{ \|A\,x - b\|_2^2 + \lambda^2 \|L\,x\|_2^2 \} \tag{1.1a}$$

$$A \in \mathbb{R}^{m \times n} , \quad L \in \mathbb{R}^{p \times n} , \quad m \ge n \ge p , \quad \mathrm{rank}(L) = p , \quad N(A) \cap N(L) = \{0\} . \tag{1.1b}$$

Here, and throughout the paper, $N(\cdot)$ denotes null space and $\|\cdot\|$ denotes the vector and matrix 2-norm $\|\cdot\|_2$. The quantity λ 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 *standard form:*

$$\min_{\bar{x}} \{ \|\bar{A}\,\bar{x} - \bar{b}\|_2^2 + \lambda^2 \|\bar{x}\|_2^2 \} \tag{1.2}$$

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 *singular value decomposition* (SVD) associated with (1.2) and the *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:

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

2) Compute the Q–R factorization of $A\,K_o$:

$$A\,K_o = [H_o, H_q] \begin{bmatrix} T_o \\ 0 \end{bmatrix} . \tag{2.2}$$

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

$$\bar{A} = H_q^T A\,L^+ \quad , \quad \bar{b} = H_q^T b \quad , \quad L^+ = K_p\,R_p^{-T} . \tag{2.3}$$

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:

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

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 $\hat{a} \equiv A\,e/n$ and $\bar{a} \equiv A\,f/n$. If $L = L_1$ is an approximation to the first derivative operator on a uniform net,*

$$L_1 = \begin{bmatrix} 1 & -1 & & & \\ & 1 & -1 & & \\ & & \cdot & \cdot & \\ & & & \cdot & \cdot \\ & & & 1 & -1 \end{bmatrix} \in \mathbb{R}^{p \times n} \quad , \quad p = n - 1 , \tag{2.5}$$

then

$$K_o = n^{-1/2} e \ , \quad H_o = \hat{a} / \| \hat{a} \| \ , \quad T_o = \sqrt{n} \, \| \hat{a} \| \ , \quad K_o \, T_o^{-1} = e / (n \, \| \hat{a} \|) \ . \tag{2.6}$$

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

$$L_2 = \begin{bmatrix} -1 & 2 & -1 & & & & \\ & -1 & 2 & -1 & & & \\ & & \cdot & \cdot & \cdot & & \\ & & & \cdot & \cdot & \cdot & \\ & & & & -1 & 2 & -1 \end{bmatrix} \in \mathbb{R}^{p \times n} \ , \ p = n - 2 \ , \tag{2.7}$$

then

$$K_o = \left[n^{-1/2} e \ , \alpha_n f - \beta_n e \right] \ , \ H_o = \left[\hat{a} / \| \hat{a} \| \ , (\bar{a} - \gamma \hat{a}) / \| \bar{a} - \gamma \hat{a} \| \right] \tag{2.8a}$$

$$T_o = \begin{bmatrix} \sqrt{n} \, \| \hat{a} \| & n \, \| \hat{a} \| (\alpha_n \gamma - \beta_n) \\ 0 & n \, \alpha_n \, \| \bar{a} - \gamma \hat{a} \| \end{bmatrix} \tag{2.8b}$$

$$K_o \, T_o^{-1} = n^{-1} \left[e / \| \hat{a} \| \ , (f - \gamma e) / \| \bar{a} - \gamma \hat{a} \| \right] \tag{2.8c}$$

where

$$\alpha_n = \left[\frac{12}{(n+1) \, n \, (n-1)} \right]^{1/2} \ , \ \beta_n = \left[\frac{3(n+1)}{n \, (n-1)} \right]^{1/2} \ , \ \gamma = \frac{\hat{a}^T \bar{a}}{\| \hat{a} \|^2} \ . \tag{2.8d}$$

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

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_p and R_p 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 $\bar{A}$ and the GSVD of the matrix pair $(A \, , L)$. For convenience, we remind that the SVD of $\bar{A}$ is given by

$$\bar{A} = \bar{U} \, \bar{\Sigma} \, \bar{V}^T \quad , \quad \bar{U} \in \mathbb{R}^{(m-(n-p)) \times p} \quad , \quad \bar{\Sigma}, \bar{V} \in \mathbb{R}^{p \times p} \tag{3.1}$$

in which $\bar{U}^T \bar{U} = \bar{V}^T \bar{V} = I_p$ and $\bar{\Sigma}$ is a diagonal matrix with non-negative diagonal elements $\bar{\sigma}_i$ 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:

$$A = U\,\Sigma\,X^{-1} = [\,U_p\,, U_o\,] \begin{bmatrix} \Sigma_p & 0 \\ 0 & I_o \end{bmatrix} [\,W_p\,, W_o\,]^T \tag{3.2a}$$

$$L = V\,M\,X^{-1} = V\,[\,M_p\,, 0\,]\,[\,W_p\,, W_o\,] = V\,M_p\,W_p^T \tag{3.2b}$$

$$U \in \mathbb{R}^{m \times n}\ , \quad X \in \mathbb{R}^{n \times n}\ , \quad \Sigma_p\,, M_p\,, V \in \mathbb{R}^{p \times p} \tag{3.2c}$$

where $U^T U = I_n$, $V^T V = I_p$, and the diagonal elements σ_i and μ_i of Σ_p and M_p are ordered such that

$$0 \le \sigma_1 \le \cdots \le \sigma_p \le 1\ , \quad 1 \ge \mu_1 \ge \cdots \ge \mu_p > 0\ . \tag{3.2d}$$

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

$$\sigma_i^2 + \mu_i^2 = 1\ , \quad i = 1, \ldots, p\ . \tag{3.3}$$

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, $R(\cdot)$ denotes column space, and we use the notation from Eqs. (3.1) and (3.2)

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

$$N(L) = R(K_o) = R(X_o)\ , \quad R(A\,K_o) = R(H_o) = R(U_o)\ . \tag{3.4}$$

Proof. $N(L) = R(K_o)$ 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

$$W^T X = I_n \quad \Leftrightarrow \quad \begin{bmatrix} W_p^T X_p & W_p^T X_o \\ W_o^T X_p & W_o^T X_o \end{bmatrix} = \begin{bmatrix} I_p & 0 \\ 0 & I_o \end{bmatrix} \tag{3.5}$$

we see that $W_o^T X_o = I_o$ and $W_p^T X_o = 0$ implying that $\mathrm{rank}(X_o) = n - p = \dim(N(L))$ and that $X_o^T W_p = 0 \;\Rightarrow\; R(X_o) \subseteq N(L)$. 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 $R(H_o) = R(A\,K_o) = R(A\,X_o) = R(U_o)$. $\square$

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

$$L^+ = W_p\,(W_p^T W_p)^{-1} M_p^{-1} V^T = P\,X_p\,M_p^{-1} V^T\ . \tag{3.6}$$

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]:

$$L^+ = L^T (L\,L^T)^{-1} = W_p\, M_p\, V^T (V\, M_p\, W_p^T W_p\, M_p\, V^T)^{-1}$$

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

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

$$P\,X_p\,W_p^T W_p = P\,W_p = W_p \quad \Leftrightarrow \quad P\,X_p = W_p\,(W_p^T W_p)^{-1}\ . \qquad \square$$

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

$$X_o = K_o\, T_o^{-1} H_o^T U_o\ . \tag{3.7}$$

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 $A\,K_o = (U_p\,\Sigma_p\,W_p^T + U_o\,W_o^T) K_o = U_o\,W_o^T K_o$. Hence,

$$K_o\,T_o^{-1} H_o^T = K_o\,(A\,K_o)^+ = K_o\,(U_o\,W_o^T K_o)^+ = K_o\,(W_o^T K_o)^{-1} U_o^T$$

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

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

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

$$\bar{U} = H_q^T U_p\,\Pi\ , \quad \bar{\Sigma} = \Pi\,\Sigma_p\,M_p^{-1}\,\Pi\ , \quad \bar{V} = V\,\Pi \tag{3.8}$$

$$U_p = H_q\,\bar{U}\,\Pi\ , \quad U_o = H_o\ , \quad X_o = K_o\,T_o^{-1} \tag{3.9}$$

where $H = [H_o\ ,H_q]$, K_o and T_o are defined in Eqs. (2.1) and (2.2), and $\Pi = \mathrm{antidiag}(1,\dots,1)$ 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

$$\overline{A} = H_q^T A\, L^+ = H_q^T (U_p\, \Sigma_p\, W_p^T + U_o\, W_o^T)\, W_p\, (W_p^T W_p)^{-1} M_p^{-1} V^T$$

$$= H_q^T U_p\, \Sigma_p\, M_p^{-1} V^T = (H_q^T U_p\, \Pi)\, (\Pi\, \Sigma_p\, M_p^{-1}\, \Pi)\, (V\, \Pi)^T \; . \tag{3.10}$$

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,

$$H^T\, U_p = \begin{bmatrix} H_o^T U_p \\ H_q^T U_p \end{bmatrix} = \begin{bmatrix} 0 \\ H_q^T U_p \end{bmatrix} \tag{3.11}$$

and it follows that

$$(H_q^T U_p)^T\, (H_q^T U_p) = (H^T U_p)^T\, (H^T U_p) = U_p^T H\, H^T U_p = U_p^T U_p = I_p \; .$$

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 $\overline{A}$. Next, we shall prove (3.9). From (3.11) we have

$$U_p = H \begin{bmatrix} 0 \\ H_q^T U_p \end{bmatrix} = H_q\, (H_q^T U_p\, \Pi)\, \Pi = H_q\, \overline{U}\, \Pi \; .$$

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 $X_o = K_o\, T_o^{-1}$. □

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 $\overline{A}$ 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 λ. 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 regularization parameter λ. Thus, the transformation (2.4) from $\overline{x}$ back to x need only be done once, when the optimal λ and $\overline{x}$ 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 $\bar{A}$. Our analysis deals only with the matrix U. This is sufficient to illustrate the major drawback 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 $\hat{U}$ 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:

$$\hat{U}\,\hat{\Sigma}\,\hat{X}^{-1} = A + E \tag{4.1}$$

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 ε_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 $\hat{U}$ is given by

$$\sin\Theta(U,\hat{U}) = \|(I_m - U\,U^T)\,\hat{U}\| = \|(I_m - U\,U^T)\,E\,(\hat{\Sigma}\,\hat{X}^{-1})^{-1}\|$$

$$\leq \|E\|\;\|(\hat{\Sigma}\,\hat{X}^{-1})^{-1}\| \approx \|E\|\;\|(\Sigma\,X^{-1})^{-1}\| = \|E\|\;\|A^+\| = \frac{\|E\|}{\|A\|}\,\kappa(A)\,. \tag{4.2}$$

This is the best bound possible; we can not 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 $\bar{A} = H_q^T A\,L^+$. From this expression we would immediately expect that the accuracy of $\tilde{U}_p$ dependes 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 $\bar{A} = H_q^T A\,L^+$ is*

$$\bar{A}^+ = L\,A^+ H_q\,. \tag{4.3}$$

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):

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

$$= V\,M_p\,\Sigma_p^{-1}\,U_p^T H_q = (V\,\Pi)\,(\Pi\,\Sigma_p\,M_p^{-1}\,\Pi)\,(H_q^T U\,\Pi)^T = \bar{V}\,\bar{\Sigma}^{-1}\,\bar{U}^T = \bar{A}^+\,. \qquad \square$$

From this theorem it follows immediately that the condition number of $\bar{A}$ satisfies $\kappa(\bar{A}) \equiv \|\bar{A}\| \, \|\bar{A}^{+}\| \le \kappa(L)\,\kappa(A)$. Now, if we let $\tilde{\bar{U}}$ denote the computed $\bar{U}$, end let $\bar{E}$ represent the influence of rounding errors during the computation of the SVD of $\bar{A}$, then it is easy to show that

$$\sin\Theta(\bar{U},\tilde{\bar{U}}) \le \frac{\|\bar{E}\|}{\|\bar{A}\|}\,\kappa(\bar{A}) \le \frac{\|\bar{E}\|}{\|\bar{A}\|}\,\kappa(L)\,\kappa(A) \tag{4.4}$$

where $\|\bar{E}\| = \bar{c}\,\varepsilon_m\,\|\bar{A}\|$ and $\bar{c}$ is a modest function of $m-p$ and n. Neglecting the errors in the computed H_q, we then obtain:

$$\sin\Theta(U_p,\tilde{U}_p) = \|U_p\,U_p^T - \tilde{U}_p\,\tilde{U}_p^T\| = \|H_q^T(\bar{U}\,\bar{U}^T - \tilde{\bar{U}}\,\tilde{\bar{U}}^T)H_q\|$$

$$\le \|\bar{U}\,\bar{U} - \tilde{\bar{U}}\,\tilde{\bar{U}}^T\| = \sin\Theta(\bar{U},\tilde{\bar{U}}) \le \frac{\|\bar{E}\|}{\|\bar{A}\|}\,\kappa(L)\,\kappa(A)\,. \tag{4.5}$$

This bound is inferior to the bound in (4.2) due to the factor $\kappa(L)$, and we conclude that $\tilde{U}$ 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 $\tilde{U}_p$ in single precision ($\varepsilon_M \approx 9.5\times10^{-7}$) and compared it with U_p computed in double precision ($\varepsilon_M \approx 2.2\times10^{-16}$) 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 resluts are shown in Fig. 1. We see that for $\kappa(L)$ larger than about 10^2, $\sin\Theta(U_p,\tilde{U}_p)$ increases linearly with $\kappa(L)$, while for smaller values of $\kappa(L)$ it is almost a constant, approximately 10^{-5}. 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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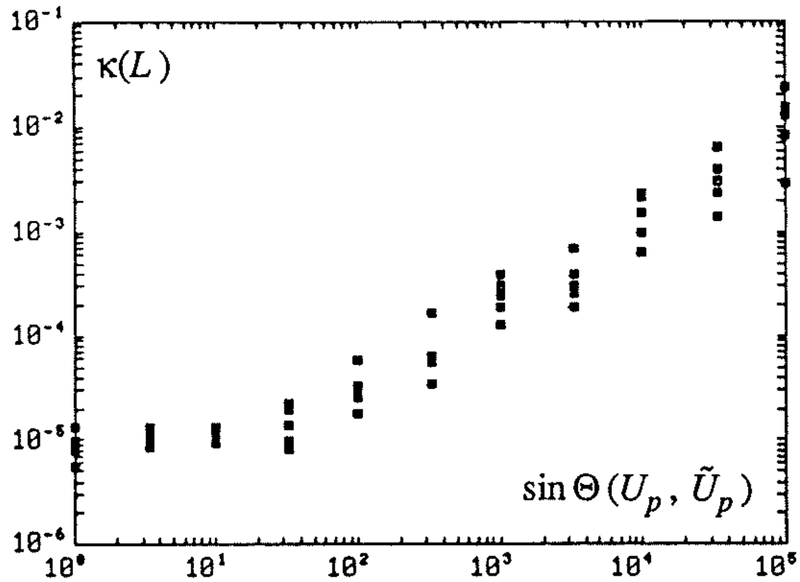

Figure 1. Comparison of computed $\tilde{U}_p$ and true U_p as a function of the condition number $\kappa(L)$. Dimensions: $m = 25$, $n = 10$, $p = 8$.