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Regularization, GSVD and Truncated GSVD

Per Christian Hansen

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Engineering Physics and Mathematics Division

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REGULARIZATION, GSVD AND TRUNCATED GSVD

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ABSTRACT

The generalized singular value decomposition (GSVD) is used to analyze two alternative methods for solving ill-posed problems: regularization in general form, and truncated SVD. We give conditions in which suitable solutions can be found, discuss the perturbation theory, and show that the optimum regularization and truncation parameters can be computed via generalized cross-validation. Our analysis also sheds light on a particular method, based on a transformation to standard form, that avoids the numerical difficulties associated with computation of the GSVD.

1. INTRODUCTION

The purpose of this report is to analyze regularization in general form by means of *generalized SVD* (GSVD) in the same spirit as SVD is used to analyze standard-form regularization [8]. We also define a Truncated GSVD solution, which has interest in its own right, and which sheds light on regularization as well. Attention is primarily put on least squares problems derived from the numerical treatment of Fredholm integral equations of the first kind, but the theory holds for ill-posed problems in general.

We start by reminding that the *regularized solution* x_λ is the solution to:

$$\min \{ \| Ax - b \|^2 + \lambda^2 \| Lx \|^2 \} . \tag{1.1}$$

This x_λ is obviously a least squares solution to the equivalent problem:

$$\min \left\| \begin{bmatrix} A \\ \lambda L \end{bmatrix} x - \begin{bmatrix} b \\ 0 \end{bmatrix} \right\| . \tag{1.2}$$

Here, and throughout the report, $\|\cdot\| = \|\cdot\|_2$. If $L = I_n$, then (1.1) is said to be in standard form. The problem (1.1) usually occurs in connection with the numerical solution of ill-posed problems where A is an ill-conditioned matrix derived from a compact operator,

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and where the right-hand side b is contaminated by errors. The singular values of A are associated with the singular values of the underlying operator, and A *must* therefore be ill-conditioned [6,14]. The standard least squares solution A^+b is useless because it is dominated by rapid oscillations due to the errors. Hence, in (1.1), one adds a term $\| Lx \|^2$ where L typically is a discrete approximation to some derivative operator, and the *regularization parameter* λ controls the weight given to minimization of $\| Lx \|^2$ relative to minimization of $\| Ax - b \|^2$.

Throughout the report we shall use the notations $R(\cdot)$ and $N(\cdot)$ for range and null space, respectively, and use P_S to denote the orthogonal projection matrix onto the subspace S. We shall make the following assumptions about the problem (1.1):

$$A \in R^{m \times n} \quad , \quad L \in R^{p \times n} \quad , \quad m \geqslant n \geqslant p \quad , \quad \text{rank}(L) = p \tag{1.3a}$$

$$\| A \| \approx 1 \quad , \quad \| L \| \approx 1 \tag{1.3b}$$

$$N(A) \cap N(L) = \{0\} \quad \Longleftrightarrow \quad \text{rank}\left(\begin{bmatrix} A \\ L \end{bmatrix} \right) = n \ . \tag{1.3c}$$

Assumption (1.3b) is simply a convenient scaling of the problem, and assumption (1.3c) ensures that there is a *unique* solution x_λ to (1.1) for all $\lambda > 0$. Notice that there is no assumption on the rank of A. By setting up the normal equations associated with (1.2) it is easy to see that x_λ is given by:

$$x_\lambda = A_\lambda^I b \quad , \quad A_\lambda^I \equiv (A^T A + \lambda^2 L^T L)^{-1} A^T \ . \tag{1.4}$$

The matrix A_λ^I is only a $\{3,4\}$-inverse of A [15] and therefore not really an inverse.

In section 2 we introduce the GSVD as a convenient tool for analysis of (1.1), and we define the Truncated GSVD solution. Section 3 discusses the requirements L and b must satisfy in order to be able to compute reasonable solutions, and Section 4 gives the perturbation theory for regularization and truncated GSVD. In Section 5 we discuss the Generalized Cross-Validation as a method for choosing the regularization parameter and truncation parameter. Finally, in Section 6 we show how the solution can be computed efficiently via transformation of (1.1) to standard form as suggested by Eldén [2], thus avoiding explicit computation of the GSVD.

2. THE GSVD OF (A, L)

In this section we introduce the GSVD of the pair of matrices (A, L) and prove some relations associated with it. We also write x_λ in terms of the GSVD and define the Truncated GSVD solution.

Theorem 2.1. *Let the matrix pair (A, L) satisfy (1.3a-c). Then there exist matrices $U \in R^{m \times n}$, $V \in R^{p \times p}$ with $U^T U = I_n$, $V^T V = I_p$ and a nonsingular $X \in R^{n \times n}$ such that:*

$$A = U \Sigma X^{-1} \quad , \quad L = V [M, 0] X^{-1} , \tag{2.1}$$

where

$$\Sigma = \operatorname{diag}(\sigma_1, \ldots, \sigma_p, 1, \ldots, 1) \in R^{n \times n} \tag{2.2a}$$

$$M = \operatorname{diag}(\mu_1, \ldots, \mu_p) \in R^{p \times p} , \tag{2.2b}$$

and such that

$$0 \leqslant \sigma_1 \leqslant \cdots \sigma_p \leqslant 1 \quad , \quad 1 \geqslant \mu_1 \geqslant \cdots \mu_p > 0 \tag{2.2c}$$

$$\sigma_i^2 + \mu_i^2 = 1 \quad , \quad i = 1, \ldots, p . \tag{2.2d}$$

Proof. See e.g. [1, Theorem 22.2]. □

In connection with the GSVD it is convenient to split the matrices U, Σ and X as follows:

$$U = [U_p, U_o] \quad , \quad \Sigma = \begin{bmatrix} \Sigma_p & 0 \\ 0 & I_o \end{bmatrix} \quad , \quad X = [X_p, X_o] \tag{2.3}$$

where U_p and X_p have p columns, and when Σ_p is $p \times p$. The subscript 'o' is a shorthand notation for $n - p$. It is also convenient to let $\sigma_i = 1$ for $i = p+1, \ldots, n$.

The quantities σ_i / μ_i are termed the *generalized singular values* of (A, L). Notice that if one knows their ratios, then σ_i and μ_i can be computed from:

$$\gamma_i = \sigma_i / \mu_i \quad => \quad \begin{cases} \sigma_i = \gamma_i (\gamma_i^2 + 1)^{-1/2} \\ \mu_i = (\gamma_i^2 + 1)^{-1/2} . \end{cases} \tag{2.4}$$

The σ_i and μ_i are related to the usual singular values of A and L as shown in the following theorem:

Theorem 2.2. *Let $\psi_i(A)$ and $\psi_j(L)$ denote the usual singular values of A and L, respectively, and let $Z^T = [A^T, L^T]$. Then for all $\psi_i(A)$, $i = 1, \ldots, n$ and $\psi_j(L)$, $j = 1, \ldots, p$:*

$$\rho_p \leqslant \frac{1}{\| Z^+ \|} \leqslant \frac{\psi_i(A)}{\sigma_{n-i+1}} \leqslant \| Z \| \leqslant \| A \| + \| L \| \tag{2.5a}$$

$$\rho_p \leqslant \frac{1}{\| Z^+ \|} \leqslant \frac{\psi_j(L)}{\mu_j} \leqslant \| Z \| \leqslant \| A \| + \| L \| . \tag{2.5b}$$

where:

$$\rho_p = \begin{cases} \min\{ \psi_p(L), \inf(A P_{N(L)}) \} & , p < n \\ \psi_n(L) & , p = n . \end{cases} \tag{2.5c}$$

Here, $\inf(AP_{N(L)})$ denotes the smallest nonzero singular value of $AP_{N(L)}$.

Proof. For a product of two matrices, one has $\psi_i(AB) \leqslant \psi_i(A)\cdot\|B\|$ [10, p. 89]. This relation and Eq. (2.1) lead to:

$$\psi_i(A) = \psi_i(U\,\Sigma\,X^{-1}) \leqslant \psi_i(\Sigma)\cdot\|X^{-1}\| = \sigma_{n-i+1}\,\|X^{-1}\|$$

$$\sigma_{n-i+1} = \psi_i(\Sigma) = \psi_i(U^T A\,X) \leqslant \psi_i(A)\cdot\|X\|$$

(the relation $\sigma_{n-i+1} = \psi_i(\Sigma)$ is due to the ordering in (2.2c)), and thus:

$$\frac{1}{\|X\|} \leqslant \frac{\psi_i(A)}{\sigma_{n-i+1}} \leqslant \|X^{-1}\| .$$

The bounds for $\psi_j(L)/\mu_j$ are derived analogously. The upper bounds in (2.5a-b) follow from the relation $\psi_i(X^{-1}) = \psi_i(Z)$ [1, Theorem 22.2], so that $\|X^{-1}\| = \|[A^T, L^T]\| \leqslant \|A\| + \|L\|$. Concerning the lower bound, the same relation also leads to $\|X\|^{-1} = \psi_n(Z)$. The interlacing inequalities for singular values [1, Theorem 3.5] immediately lead to:

$$\psi_i(Z) \geqslant \psi_i([0, L^T]) = \psi_i(L) , \qquad i = 1, \ldots, p .$$

Further, we have $\psi_i([0, L^T]) = 0$ for $i = p+1, \ldots, n$, and from [11] it thus follows that:

$$\psi_i(Z) \geqslant \inf\left(P_{R^{\perp}([0,L^T])}[A^T, 0]\right) , \; i = p+1, \ldots, n ,$$

where we consider $[A^T, 0]$ a perturbation at $[0, L^T]$. Since $R^{\perp}([0,L^T]) = R^{\perp}(L^T) = N(L)$, the right-hand side becomes $\inf(A\,P_{N(L)})$. Thus, we can take

$$\psi_i(Z) \geqslant \begin{cases} \psi_i(L) & \text{for} \quad i = 1, \ldots, p \\ \inf(A\,P_{N(L)}) & \text{for} \quad i = p+1, \ldots, n \end{cases} .$$

Hence, a lower bound for $\psi_n(Z)$ is $\psi_n(L)$ for $p = n$, and $\min\{\psi_p(L), \inf(A\,P_{N(L)})\}$ for $p < n$. □

These relations between σ_i and μ_i and the singular values of A and L are used in the following sections. In the above proof, bounds were derived for the norms of X and X^{-1}, and they lead to bounds for the condition number of X:

Corollary 2.3. *The condition number $\kappa(X)$ of X is bounded by:*

$$\kappa(X) = \|X\|\,\|X^{-1}\| \leqslant \frac{\|A\| + \|L\|}{\rho_p} \tag{2.6}$$

and for the particular case $p = n$:

$$\kappa(X) \leqslant \kappa(L)\left(1 + \frac{\|A\|}{\|L\|}\right). \tag{2.6a}$$

Using the GSVD (2.1) for A and L, it is easy to derive the following expression for A_λ^I in (1.4):

$$A_\lambda^I = X \begin{bmatrix} F & 0 \\ 0 & I_o \end{bmatrix} \Sigma^+ U^T = X_p F \Sigma_p^+ U_p^T + X_o U_o^T \tag{2.7}$$

where $F = \mathrm{diag}(f_i) \in R^{p \times p}$ is given by:

$$f_i = \begin{cases} 0 & \text{for} \quad \sigma_i = 0 \\ \dfrac{(\sigma_i / \mu_i)^2}{(\sigma_i / \mu_i)^2 + \lambda^2} & \text{for} \quad \sigma_i \neq 0 . \end{cases} \tag{2.8}$$

A straightforward extension of Truncated SVD (TSVD) [5] to general-form regularization is easily derived from Eqs. (2.7) and (2.8). We introduce the *Truncated GSVD solution* x_k by substituting for F in (2.7) a diagonal matrix with k unit elements corresponding to the k largest σ_i in Σ_p and otherwise 0's, thus simply neglecting the contributions corresponding to the $p-k$ smallest σ_i [9].

Definition 2.4. *Define the matrix* $\hat{\Sigma}_k^+$ *by:*

$$\hat{\Sigma}_k^+ \equiv \mathrm{diag}(0, \ldots, 0, \sigma_{p-k+1}^{-1}, \ldots, \sigma_p^{-1}) . \tag{2.9}$$

Then the Truncated GSVD (TGSVD) solution x_k *to (1.1), defined by neglecting the components of* $X_p \Sigma_p^+ U^T$ *corresponding to the* $p-k$ *smallest* σ_i, *is given by:*

$$x_k = A_k^I \quad . \quad A_k^I \equiv X \begin{bmatrix} \hat{\Sigma}_k^+ & 0 \\ 0 & I_0 \end{bmatrix} U^T = X_p \hat{\Sigma}_k^+ U_p^T + X_o U_o^T . \tag{2.10}$$

The matrix A_k^I is a $\{2,3\}$-inverse of A.

3. THE REQUIREMENTS ON L AND b

In this section we use the GSVD of (A, L) to analyze some of the properties of the regularized solution x_λ to (1.1). First of all, it follows immediately from Eq. (2.7) that x_λ is given by:

$$x_\lambda = x_\lambda^{(1)} + x_\lambda^{(2)} \quad , \quad x_\lambda^{(1)} = X_p F \Sigma_p^+ U^T b \quad , \quad x_\lambda^{(2)} = X_o U_o^T b . \tag{3.1}$$

We see that x_λ actually consists of a smoothed component $x_\lambda^{(1)}$ and a nonsmoothed component $x_\lambda^{(2)}$. The latter component is associated with $N(L)$ which is spanned by the columns of X_o, and it vanishes for $p = n$. Concerning the smoothed component $x_\lambda^{(1)}$, the basic idea in regularization is to use F to dampen the contributions to the solution corresponding to the small σ_i. A general observation is that the columns x_i of X tend to be increasingly oscillating for decreasing σ_i, and the regularized solution x_λ will therefore

automatically be 'smoother' than without the factor F.

It is of interest to analyze the behavior of x_λ for $\lambda \to \infty$ and for $\lambda \to 0$. In the former case, $F \to 0$ for $\lambda \to \infty$, so that:

$$x_\lambda \to x_\lambda^{(2)} \quad \text{for} \quad \lambda \to \infty, \tag{3.2}$$

i.e., x_∞ is identical to the unregularized part $x_\lambda^{(2)}$ of x_λ. In the second case, for $\lambda \to 0$, F consists of 0's and 1's, and thus:

$$x_\lambda \to x_o \equiv X\,\Sigma^+ U^T b = A_{IL}^\dagger b \quad \text{for} \quad \lambda \to 0 \tag{3.3}$$

where $A_{IL}^\dagger$ is the weighted pseudoinverse of A as defined in [3]. Notice that if A is rank deficient then $A_{IL}^\dagger \neq A^+$, and thus $x_o \neq A^+ b$. Eq. (3.3) shows that x_o is a least squares solution to (1.2), with $\lambda = 0$, and if A is rank deficient then x_o is not the minimum norm solution since it has a component in $N(A)$ and $N(L)$, via the matrix X. In connection with general-form regularization (1.1) it is therefore natural to define the *unregularized solution* to be x_o (instead of the usual least squares solution $A^+ b$). Notice that for $k = p$ (i.e., no truncation), the TGSVD solution x_k is identical to x_o.

Eq. (3.1) shows that L must satisfy several requirements in order to obtain a satisfactory regularized solution x_λ. First, it is common experience that the noise e present in the right-hand side is usually '*white*' in the sense that all the coefficients $|u_i^T e|$ are of the same magnitude. Hence, the filter coefficients in F must dampen the contributions corresponding to the small $\sigma_i \neq 0$ which appear as σ_i^{-1} in Σ_p^+. This again requires that the corresponding generalized singular values σ_i / μ_i must also be small when σ_i is small, so that f_i (2.8) is small. Hence, all the μ_i should preferably be as large as possible, and according to Theorem 2.2 this means that L should be *well-conditioned*, and A^T must have a *large component in* $N(L)$. Second, x_λ is expressed in terms of the columns of X, and one must therefore require that $\|X\|$ be small in order to keep the norm of x_λ small. Since $\|X^{-1}\| = \|Z\|$, which is of order 1, this leads to the requirement that the condition number $\kappa(X) = \|X\|\,\|X^{-1}\|$ of X be small. Corollary 2.3 then leads to the same requirements on L as above.

Fortunately, the matrices L most frequently used in regularization, such as approximations to the first and second derivative operators, are well-conditioned as long as the grid defining the solution is not too irregular. Further, for these matrices the null space $N(L)$ either vanishes or is spanned by very 'smooth' vectors such that $\|A\,P_{N(L)}\|$ is large for all practical A. For example, for

$$L_1 = \text{bidiag}(1, -1) \in R^{(n-1)\times n} \tag{3.4}$$

the null space $N(L_1)$ is spanned by the vector $e = [1, 1, \ldots, 1]^T$.

Throughout the rest of the report we shall assume that L is properly chosen so that it is well-conditioned and, when $p < n$, so that $\inf(A\ P_{N(L)})$ is not large. Practical experience then shows that the vectors u_i of U in (2.1) have behavior very similar to the usual left singular vectors of A: the smaller the σ_i, the more oscillations are present in the corresponding u_i. Similar observations hold for the oscillations in the columns x_i of X and in the columns v_i of V. In order to be able to compute reasonable solutions, i.e. solutions that are sufficiently 'smooth', a necessary condition is that the solution to the *unperturbed* problem (with exactly given b) is reasonably smooth for $\lambda \to 0$ (no regularization) and for $k = p$ (no truncation). This essentially means that the norm of x_o (3.3) must not be large, which can only be satisfied if X is well-conditioned (so that $\| X \|$ is not large) and if none of the coefficients $| u_i^T b | / \sigma_i$ in the expression:

$$x_o = \sum_{i=1}^{p} \frac{u_i^T b}{\sigma_i} x_i + \sum_{i=p+1}^{n} u_i^T b\ x_i \tag{3.5}$$

are significantly larger than the others. The first requirement is satisfied when L is chosen properly, but the second requirement puts a bound on allowable right-hand sides. A careful analysis can be applied to the differences $x_\lambda - x_o$ and $x_k - x_o$, by analogy with the technique used in [7] (via a transformation of variables to $\xi = X^{-1}x$), and the conclusion is that in order for x_λ as well as x_k to be close to x_o, the unperturbed b must satisfy the following condition:

The Discrete Picard Condition (DPC). *Let b denote an unperturbed right-hand side in (1.1). Then b satisfies the Discrete Picard condition if the coefficients $\beta_i = u_i^T b$ satisfy:*

$$\frac{| \beta_i |}{\sigma_i} = \frac{| u_i^T b |}{\sigma_i} \lesssim \frac{\| b \|}{\| A \|} \quad , \quad i = 1, \ldots, n \ . \tag{3.6}$$

Due to the above mentioned analogy between the u_i and the usual left singular vectors of A, the DPC is satisfied if the problem underlying (1.1) - usually a Fredholm integral equation of the first kind - satisfies the Picard condition, (see [6]).

Notice that the existence of a satisfactory solution does not depend on the presence of a particular gap in the σ_i-spectrum associated with A. Instead, the DPC requires that the coefficients $| \beta_i |$ must decay to zero at least as fast as the σ_i. This requirement applies to regularization as well as TGSVD.

4. PERTURBATION ANALYSIS

In this section we give the perturbation bounds for the TGSVD solution x_k (2.10) and for the regularized solution x_λ (1.4). We restrict ourselves to the case when only the

right-hand side is perturbed. This is the common situation in connection with integral equations.

Theorem 4.1. *Let e denote the perturbation of the right-hand side $\tilde{b} = b + e$. Then the relative perturbations of x_k and x_λ are bounded as:*

$$\frac{\| \tilde{x}_k - x_k \|}{\| x_k \|} \leqslant \frac{1}{\sigma_{p-k+1}} \kappa(X) \frac{\| e \|}{\| b_k \|} \tag{4.1}$$

$$\frac{\| \tilde{x}_\lambda - x_\lambda \|}{\| x_\lambda \|} \leqslant \phi_\lambda \, \kappa(X) \frac{\| e \|}{\| b_\lambda \|} \tag{4.2}$$

where $b_k = Ax_k$, $b_\lambda = Ax_\lambda$, and ϕ_λ is given by:

$$\phi_\lambda = \begin{cases} 1 & \text{for} \quad \lambda > 1/\sqrt{2} \\ \frac{1}{2\lambda}(1-\lambda^2)^{-1/2} & \text{for} \quad \lambda \leqslant 1/\sqrt{2}\,. \end{cases} \tag{4.3}$$

Proof. The norm of b_k satisfies:

$$\| b_k \| \leqslant \| A \| \| x_k \| \leqslant \| U \| \| \Sigma \| \| X^{-1} \| \| x_k \| = \| X^{-1} \| \| x_k \|$$

and similarly $\| b_\lambda \| \leqslant \| X^{-1} \| \| x_\lambda \|$. From (2.10) we have:

$$\tilde{x}_k - x_k = X \begin{bmatrix} \hat{\Sigma}_k^T & 0 \\ 0 & I_o \end{bmatrix} U^T e \quad \Rightarrow$$

$$\| \tilde{x}_k - x_k \| \leqslant \| X \| \max \{ \| \hat{\Sigma}_k^+ \|, 1 \} \| U^T \| \| e \| = \| X \| \frac{1}{\sigma_{p-k+1}} \| e \| .$$

This immediately leads to Eq. (4.1). Similarly, for the regularized solution, (2.7) yields:

$$\tilde{x}_\lambda - x_\lambda = X \begin{bmatrix} F \, \Sigma_p^+ & 0 \\ 0 & I_o \end{bmatrix} U^T e \quad \Rightarrow$$

$$\| \tilde{x}_\lambda - x_\lambda \| \leqslant \| X \| \max \{ \| F \, \Sigma_p^+ \|, 1 \} \| e \|$$

in which

$$F \, \Sigma_p^+ = \operatorname{diag} \left(\frac{(\sigma_i / \mu_i)^2}{(\sigma_i / \mu_i)^2 + \lambda^2} \cdot \frac{1}{\sigma_i} \right) = \operatorname{diag} \left(\frac{\gamma_i}{\gamma_i^2 + \lambda^2} (\gamma_i^2 + 1)^{1/2} \right)$$

where we have set $\gamma_i = \sigma_i / \mu_i$ and used (2.4). If we define the function $g(\gamma, \lambda) = \gamma (\gamma^2 + 1)^{1/2} (\gamma^2 + \lambda^2)^{-1}$, then $\| F \, \Sigma_p^+ \| \leqslant \max_\gamma g(\gamma, \lambda)$ for all $\lambda \geqslant 0$. It is straightforward to show that $\max_\gamma g(\gamma, \lambda) = \phi_\lambda$ given in (4.3), and since $\phi_\lambda > 1$, we have proved (4.2). □

From Theorem 4.1 we see that the condition numbers associated with TGSVD and regularization are

$$\kappa_k = \frac{\kappa(X)}{\sigma_{p-k+1}} \quad , \quad \kappa_\lambda = \phi_\lambda \kappa(X) , \tag{4.4}$$

respectively. Since we assume L is well-conditioned, Corollary 2.3 shows that $\kappa(X)$ is small, and the condition numbers depend primarily on the choice of k and λ. We see that it is always possible to choose parameters that improve the condition of the problem, compared to the condition of the original problem: $\min \| Ax - b \|$.

Following the reasoning that led to Definition 2.4 of the TGSVD solution, one would usually choose a regularization parameter λ or a truncation parameter k such that damping or filtering, respectively, of the σ_i sets in at about the same level. From Eq. (2.8) we see that this is the case when $\lambda \approx \sigma_k / \mu_k$. Now, since the μ_i are guaranteed to be of the order 1 (Theorem 2.2 and well-conditioned L), this roughly corresponds to choosing $\lambda \approx \sigma_k \cdot \| L \| = \sigma_k$. Eq. (4.3) then shows that when TGSVD and regularization produce approximately the same solution, $x_k \approx x_\lambda$, both these solutions are approximately equally sensitive to perturbations in b.

The condition numbers κ_k and κ_λ in (4.4) are consistent with the corresponding condition numbers $\bar{\kappa}_k$ and $\bar{\kappa}_\lambda$ for TSVD and standard-form regularization [7]:

$$\bar{\kappa}_k = \frac{\sigma_1}{\sigma_k} \quad , \quad \bar{\kappa}_\lambda = \frac{\sigma_1}{2\lambda} . \tag{4.5}$$

These condition numbers follow from (4.1) and (4.2) when replacing $\sigma_1 = 1$ with $\psi_1(A) = \| A \|$, σ_{p-k+1} with $\psi_k(A)$, and using the facts that $L = I_n \Rightarrow \kappa(X) = 1$ and ϕ_λ simply becomes $1/(2\lambda)$. The proper choice of λ and k is determined mainly by the size of the errors $\| e \|$ (cf. Section 5), and λ and k would therefore be practically the same for all methods (standard-form/general regularization and TSVD/TGSVD). This leads to the conclusion that the sensitivity of the solutions to perturbations of the right-hand side is approximately the same for $L = I_n$ and $L \neq I_n$ (still provided that L is chosen properly). The argument for using an $L \neq I_n$ is therefore primarily associated with L's properties, in connection with the choice of λ or k, as a filter of the errors e.

5. THE CHOICE OF λ AND k

In this section we briefly discuss the behavior of the solutions x_k and x_λ, and this enables us to choose the appropriate values of k and λ. We assume the following realistic 'model' for the right-hand side:

$$\tilde{b} = b + e \tag{5.1}$$

where b represents the underlying exact data while e denotes the errors. We assume that

b satisfies the DPC (3.6) and that e is 'white noise'. To visualize this, consider the usual case in connection with Fredholm integral equations of the first kind, where A has ill-determined numerical rank, i.e. all its singular values decay gradually towards zero. Then the coefficients $|u_i^T b|$ and $|u_i^T e|$ typically appear as shown in Fig. 1. When one starts with $k = 1$ and increases k, the TGSVD solution x_k contains increasing amounts of the 'signal' (from b) until the noise starts to dominate; then x_k starts to oscillate and $\|x_k\|$ grows rapidly. The proper choice of k is obviously the one for which $|u_k^T b| \approx |u_i^T e|$, i.e. where the signal-to-noise ratio in the solution is best. The same conclusion holds for any σ_i-spectrum of A as long as the DPC is satisfied.

Consider now the regularized solution. For the case $L = I_n$, Hansen [5] proved that once the DPC (3.6) is satisfied, there always exists a $\lambda \in [\sigma_{k+1}, \sigma_k]$ such that $x_\lambda \approx x_k$. The proof carries immediately over to the case $L \neq I_n$ whenever L is properly chosen. Consequently, the behavior of x_λ as a function of λ is roughly the same as the behavior of x_k as outlined above, and the optimum λ is therefore roughly given by $\lambda \approx \sigma_k$, where k is the optimum truncation parameter.

Concerning the behavior of the residuals $\tilde{r}_k = \tilde{b} - A\tilde{x}_k$ and $\tilde{r}_\lambda = \tilde{b} - A\tilde{x}_\lambda$, one should look at the functions:

$$V(k) = \frac{\|\tilde{r}_k\|^2}{\operatorname{trace}(I_m - AA_k^I)} = \frac{\|\tilde{r}_k\|^2}{m-k-(n-p)} \tag{5.2}$$

$$V(\lambda) = \frac{\|\tilde{r}_\lambda\|^2}{\operatorname{trace}(I_m - AA_\lambda^I)} = \|\tilde{r}_\lambda\|^2 \left[m-n + \sum_{i=1}^{p} \frac{\lambda^2}{(\sigma_i/\mu_i)^2 + \lambda^2} \right]^{-1} . \tag{5.3}$$

In (5.2), $k+(n-p)$ is the number of terms in the expression (2.10) for $\tilde{x}_k$, and $m-k-(n-p)$ is therefore the number of degrees of freedom in $\tilde{r}_k$. Thus, with our 'model' of $\tilde{b}$, $V(k)$ will behave as follows: when k is increased from 1, $V(k)$ is an overall decreasing function until it settles at a level where it stays almost constant. Then most of the 'signal' is extracted, and $V(k)$ becomes an estimate for the variance $\|e\|/m$ of the noise. Similar arguments hold for $V(\lambda)$. The optimum k and λ are exactly those for which $V(k)$ and $V(\lambda)$ start to level off.

A computationally attractive method for determining these optimum values of k and λ is to compute the minimizers of the *generalized cross-validation* (GCV) functions [4], defined as:

$$G(k) \equiv \frac{V(k)}{m-k-(n-p)} \quad , \quad G(\lambda) \equiv \frac{V(\lambda)}{\operatorname{trace}(I_m - AA_\lambda^I)} . \tag{5.4}$$

Since the denominators of these functions are slowly increasing functions of k and λ, $G(k)$ and $G(\lambda)$ will have a *minimum* at the optimal k and λ where $V(k)$ and $V(\lambda)$ start

to level off. Notice that there are several other statistical reasons for choosing k and λ as the minimizers of the GCV functions, cf. [12,13].

6. SOLUTION VIA TRANSFORMATION TO STANDARD FORM

We conclude this report by investigating a particular numerical method, due to Eldén [2], for solving (1.1) via a transformation to a standard-form problem:

$$\min \{ \| \bar{A}\, \bar{x} - \bar{b} \|^2 + \lambda^2 \| \bar{x} \|^2 \} . \tag{6.1}$$

The algorithm can be summarized as follows:

1) Compute the Q-R decomposition of L^T:

$$L^T = [\, K_p , K_o \,] \begin{bmatrix} R_p \\ 0 \end{bmatrix} \quad , \quad K_p \in R^{n \times p} \quad , \quad K_o \in R^{n \times (n-p)} . \tag{6.2}$$

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

$$A\, K_o = [\, H_o , H_1 \,] \begin{bmatrix} T_o \\ 0 \end{bmatrix} \quad , \quad H_o \in R^{m \times (n-p)} \quad , \quad H_1 \in R^{m \times (m-(n-p))} . \tag{6.3}$$

3) Solve the standard-form problem (6.1) with:

$$\bar{A} = H_1^T A L^+ \quad , \quad L^+ = K_p R_p^{-T} \quad , \quad \bar{b} = H_1^T b . \tag{6.4}$$

4) Compute the solution to (1.1) as:

$$x = L^+ \bar{x} + K_o T_o^{-1} H_o (b - A L^+ \bar{x}) . \tag{6.5}$$

One might suppose that there is a connection between the standard-form regularized solution $\bar{x}_\lambda$ to (6.1) and the regularized solution x_λ to (1.1). One may also expect a connection between the TSVD solution $\bar{x}_k$ to (1.1) and the TGSVD solution x_k to (1.1). That this is indeed the case is demonstrated by the following theorem.

Theorem 6.1. *Let the SVD of $\bar{A}$ (6.4) be given by:*

$$\bar{A} = \bar{U} \Psi \bar{V}^T \tag{6.6}$$

and let the GSVD of (A , L) be given by (2.1)-(2.3). Then:

$$\bar{U} = H_1^T U_p \Pi \quad , \quad \Psi = \Pi \Sigma_p M^{-1} \Pi \quad , \quad \bar{V} = V \Pi \tag{6.7}$$

where $\Pi = [\, e_p , \ldots , e_1 \,]$ is the p-by-p exchange matrix. Further, let $\bar{x}_k$ and $\bar{x}_\lambda$ denote the TSVD and regularized solutions to (6.1),

$$\bar{x}_k = \bar{V} \Psi_k^+ \bar{U}^T \bar{b} \quad , \quad \bar{x}_\lambda = \bar{V} \operatorname{diag} \left(\frac{\psi_i^2}{\psi_i^2 + \lambda^2} \right) \Psi^+ \bar{U}^T \bar{b} . \tag{6.8}$$

Then the solutions obtained by inserting these $\bar{x}_k$ and $\bar{x}_\lambda$ into (6.5) are exactly the TGSVD and regularized solutions x_k (2.10) and x_λ (1.4).

Proof. Eq. (6.7) is proved in [9, Theorem 1]. The relations between $\bar{x}_k$ and x_k, and between $\bar{x}_\lambda$ and x_λ, follow immediately by insertion of (6.7) into (6.8) and noting that $\mathrm{diag}(\psi_i^2/(\psi_i^2+\lambda^2)) = F$. □

Theorem 6.1 shows that when (6.1) is solved by means of standard-form regularization, then the solution obtained via insertion of $\bar{x}_\lambda$ into (6.5) is *exactly* the regularized solution x_λ to (1.1). Likewise, when the TSVD solution $\bar{x}_k$ is inserted into (6.5), one is *guaranteed* to obtain the TGSVD solution x_k as defined in (2.10). We remind the reader that in both $\bar{x}_k$ and x_k, $p-k$ is the number of neglected (generalized) singular values.

In order to determine the optimum parameters k and λ, one may of course compute the GCV-functions $G(k)$ and $G(\lambda)$ (5.4) via insertion of $\bar{x}_k$ or $\bar{x}_\lambda$ into (6.5). However, the optimum parameters can be determined *directly* from the problem (6.1) without reference to the original problem. This is an attractive feature that simplifies the numerical procedure for solving (1.1) via (6.1). The result relies on the following theorem:

Theorem 6.2. *Let r_k and $\bar{r}_k$ denote the residuals corresponding to x_k and $\bar{x}_k$, respectively:*

$$r_k = b - A\,x_k \quad , \quad \bar{r}_k = \bar{b} - \bar{A}\,\bar{x}_k \ . \tag{6.9a}$$

Similarly, let r_λ and $\bar{r}_\lambda$ denote the residuals:

$$r_\lambda = b - A\,x_\lambda \quad , \quad \bar{r}_\lambda = \bar{b} - \bar{A}\,\bar{x}_\lambda \ . \tag{6.9b}$$

Then:

$$\|\bar{r}_k\| = \|r_k\| \quad \text{and} \quad \|\bar{r}_\lambda\| = \|r_\lambda\| \ . \tag{6.10}$$

Proof. First, we extend the matrix $U = [U_p, U_o]$ in (2.3) with U_q to an orthogonal matrix:

$$\hat{U} \equiv [U_p, U_o, U_q] \in R^{m\times m} \ .$$

Since $R(H_o) = R(U_o)$ [9], $H_1^T U_o = 0$. And since $H^T\hat{U}$ is orthogonal, the matrix $H_1^T[U_p, U_q]$ must also be orthogonal. If we define $b = [\beta_1, \ldots, \beta^m]^T$, then insertion of (2.1) and (2.10) into r_k (6.9a) yields:

$$r_k = \hat{U}[\beta_1, \ldots, \beta_{p-k}, 0, \ldots, 0, \beta_{n+1}, \ldots, \beta_m]^T \quad \Rightarrow$$

$$\|r_k\|^2 = \beta_1^2 + \cdots + \beta_{p-k}^2 + \beta_{n+1}^2 + \cdots + \beta_m^2 \ .$$

Concerning $\bar{r}_k$, Eqs. (6.4), (6.7) and (6.8) lead to $\bar{A}\,\bar{x}_k = H_1^T U_p \Pi \Psi \Psi_k^+ (\bar{U}^T \bar{b})$, where:

$$\bar{U}^T \bar{b} = (H_1^T U_p \Pi)^T H_1^T b = \Pi (H_1 H_1^T U_p)^T b = \Pi U_p^T b \ ,$$

such that $\bar{A}\,\bar{x}_k$ becomes:

$$\bar{A}\,\bar{x}_k = H_1^T\,\hat{U}[0,\ldots,0,\beta_{k+1},\ldots,\beta_p,0,\ldots,0]^T\ .$$

Inserting this relation and $\bar{b} = H_1^T\,b = H_1^T\,\hat{U}\beta$ into (6.9a), we get:

$$\bar{r} = H_1^T\,\hat{U}[\beta_1,\ldots,\beta_k,0,\ldots,0,\beta_{p+1},\ldots,\beta_m]^T$$

$$= H_1^T[U_p,U_q][\beta_1,\ldots,\beta_k,0,\ldots,0,\beta_{n+1},\ldots,\beta_m]^T$$

because $H_1^T U_o = 0$. Since $H_1^T[U_p,U_q]$ is orthogonal, we see that $\|\bar{r}_k\| = \|r_k\|$. The same argumentation and the fact that $\bar{x}_\lambda = \bar{V}\,F\,\Psi^+\,\bar{U}^T\bar{b}$, with F given by (2.8), lead to the second result $\|\bar{r}_\lambda\| = \|r_\lambda\|$. □

Consider now the GCV-function $\bar{G}(k)$ associated with the TSVD solution $\bar{x}_k$:

$$\bar{G}(k) = \frac{\|\bar{r}_k\|^2}{[\mathrm{trace}\,(I_{m-(n-p)} - \bar{A}\,\bar{A}_k^+)]^2} = \frac{\|\bar{r}_k\|^2}{[m-(n-p)-k]^2}\ . \tag{6.11}$$

Due to Theorem 6.2, $\|\bar{r}_k\| = \|r_k\|$, which shows that $\bar{G}(k)$ is identical to the original GCV function $G(k)$ in (5.4). It is easy to show that a similar result holds for the GCV functions associated with $\bar{x}_\lambda$ and x_λ. Thus:

$$\bar{G}(k) = G(k) \quad , \quad \bar{G}(\lambda) = G(\lambda) \tag{6.12}$$

and the minimizer of $\bar{G}(\cdot)$ is therefore identical to the minimizer of $G(\cdot)$. This shows that the truncation parameter k or the regularization parameter λ, chosen by the GCV method applied directly to the standard-form problem (6.1), is identical to the parameter that would be obtained by application of GCV to the original problem (1.1). The same argument shows that the variance $\|e\|^2/\,m$ of the errors can be estimated directly from (6.1).

In this connection we would like to emphasize the TSVD solution because of its simplicity and because the SVD of the transformed problem sheds light on both $\bar{x}_k$ and on the original problem, due to the strong connection between the SVD of $\bar{A}$ and the GSVD of $(A\,,L)$. We stress that the success of TSVD relies only on satisfaction of the DPC (3.6) and not on the singular value spectrum of A. For more details on these aspects, see [8] where several efficient methods for computing $\bar{x}_k$ are also discussed.

7. CONCLUSION

The first part of our investigations deals with the properties of the regularized and TGSVD solutions to (1.1), and we have derived conditions on L and b which are necessary to ensure a satisfactory solution. The main conclusion is that if L is well-conditioned and if b satisfies the Discrete Picard Condition (3.6), then both methods lead to reasonable solutions which are approximately identical and approximately equally

sensitive to perturbations.

The second part of our investigations shows that if (1.1) is transformed into standard form (6.1), then it is not necessary to transform the solutions back to the form (1.1) in order to determine the appropriate k or λ, since these can be determined directly from the standard-form problem.

Finally, we stress that in order to understand the different filter properties of $L \neq I_n$ and $L = I_n$, more investigations have to be carried out. It is necessary to get a better understanding of the similarities between the singular vectors of A and the generalized singular vectors of (A, L).

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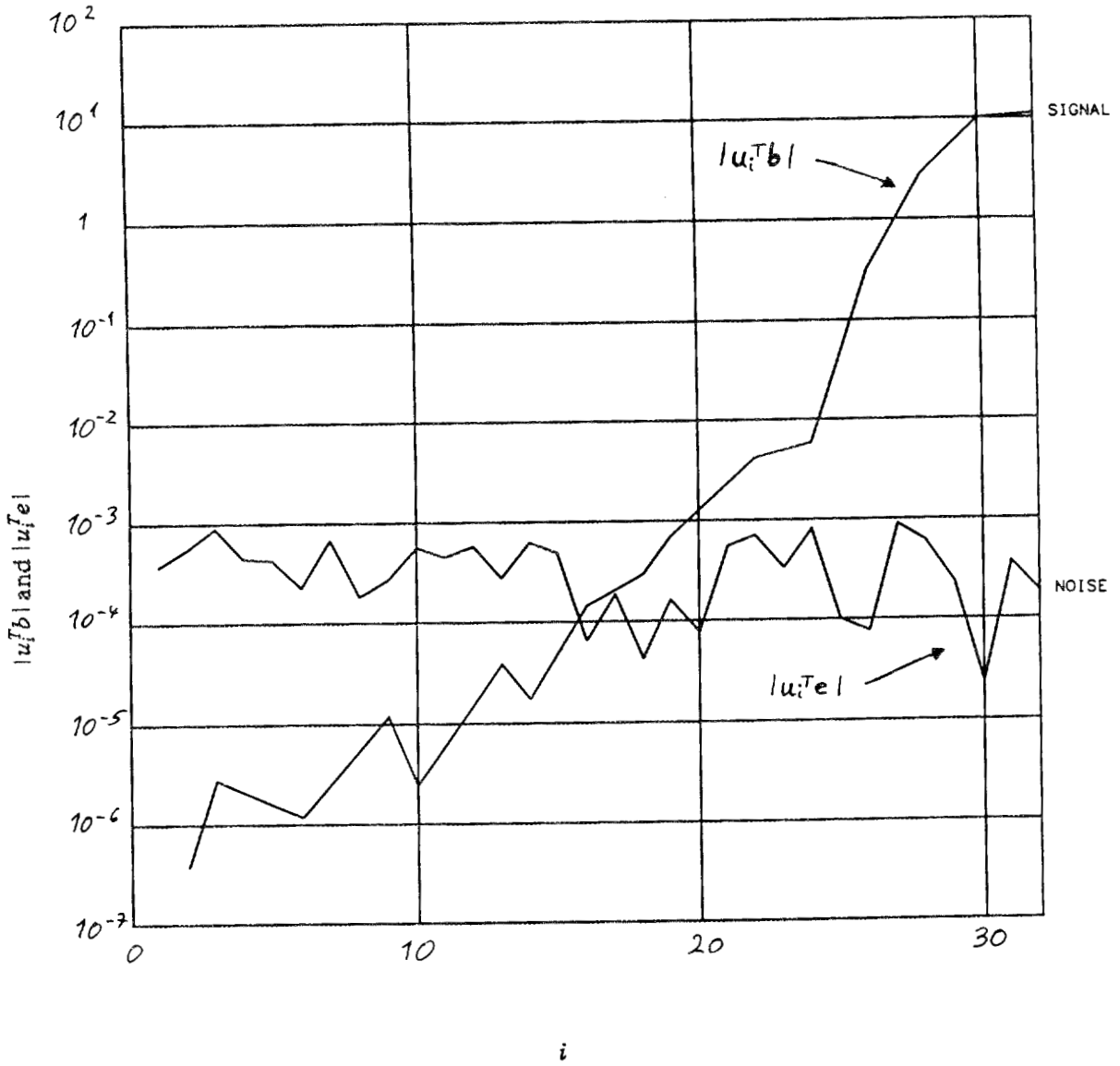

Figure 1. Typical appearance of the quantities $|\boldsymbol{u}_i^T \boldsymbol{b}|$ and $|\boldsymbol{u}_i^T \boldsymbol{e}|$.

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