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THE DISCRETE PICARD CONDITION FOR DISCRETE ILL-POSED PROBLEMS

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Abstract.

We investigate the approximation properties of regularized solutions to discrete ill-posed least squares problems. A necessary condition for obtaining good regularized solutions is that the Fourier coefficients of the right-hand side, when expressed in terms of the generalized SVD associated with the regularization problem, on the average decay to zero faster than the generalized singular values. This is the discrete Picard condition. We illustrate the importance of this condition theoretically as well as experimentally.

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1. Introduction.

By *discrete ill-posed problems*, we mean a particular class of discrete least squares problems

$$\min_{x} \|Ax - b\|_2, \qquad A \in \mathbb{R}^{m \times n}, \qquad m \geq n, \tag{1.1}$$

where the singular values of the matrix A decay gradually to zero in such a fashion that A is very ill-conditioned. Often, due to rounding errors as well as errors in the data, such ill-conditioned matrices have full rank in a strict mathematical sense and the finite-dimensional least squares problem (1.1) is therefore not ill-posed in the original sense due to Hadamard (see e.g. [12, Section 1.1]). However, we feel that it is still practical to use the terminology *discrete ill-posed problems*, partly because many of the difficulties of ill-posed problems carry over to the problem (1.1), and partly because (1.1) often arises when an underlying ill-posed problem – for example a Fredholm integral equation of the first kind – is discretized for computation of a numerical solution.

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For such problems, a variety of direct and iterative numerical regularization methods have been proposed, see e.g. [1, 5, 6, 8, 11, 18, 19, 24, 26, 27, 29] and the surveys in [2, 3, 9, 12, 21, 22, 30, 31]. Common for all these regularization methods is that they replace the ill-posed problem with a "nearby" well-posed problem which is much less sensitive to perturbations. A great deal of these methods have in common that they seek to either compute or approximate a certain regularized solution, namely the solution $\boldsymbol{x}_\lambda$ to the *discrete Tikhonov-regularization problem*

$$\boldsymbol{x}_\lambda = \operatorname{argmin}\{\|A\boldsymbol{x} - \boldsymbol{b}\|_2^2 + \lambda^2 \|L\boldsymbol{x}\|_2^2\}, \tag{1.2}$$

where L typically is either the identity matrix or a well-conditioned discrete approximation to some derivative operator. Although the case $L = I_n$ is easier to treat numerically, it may be necessary to choose $L \neq I_n$ in order to compute a useful solution, see e.g. [3, 30, 31]. Both the matrix L and the regularization parameter λ are used to control the smoothness of the regularized solution $\boldsymbol{x}_\lambda$. An underlying assumption when using these methods is therefore that the exact solution, which one is trying to approximate by $\boldsymbol{x}_\lambda$, is indeed smooth. Another assumption, which is equally important, is that the larger the singular values of A, the smoother the corresponding singular vectors (in the sense: less zero crossings). For a discussion of these aspects, see [30] and [18, Section 2].

There is, however, one more assumption which is not so well understood, and which bears a similarity with the Picard condition for ill-posed problems. Let $K(s,t) = \sum_{i=1}^{\infty} \sigma_i u_i(s) v_i(t)$ be the singular value expansion of the compact operator K, and let the right-hand side g be expressed as $g(s) = \sum_{i=1}^{\infty} \beta_i u_i(s)$. In order that the equation $Kf = g$ have a square integrable least-squares solution f, it is necessary and sufficient that g satisfies the following condition [12, Theorem 1.2.6]:

THE PICARD CONDITION (PC). *The right-hand side g in $Kf = g$ satisfies the PC if*

$$\sum_{i=1}^{\infty} |(u_i, g)/\sigma_i|^2 < \infty, \qquad \sigma_i \neq 0, \tag{1.3}$$

where (u_i, g) denotes the usual inner product between u_i and g.

Eq. (1.3) implies that from a certain point in the summation, the Fourier coefficients (u_i, g) must decay to zero faster than the σ_i. For the finite-dimensional discrete problem (1.1), the equivalent of Eq. (1.3) is always satisfied. Nevertheless, the ratio between the decay of the singular values of A and the decay of the Fourier coefficients of the right-hand side $\boldsymbol{b}$, when expressed in terms of the left singular vectors of A, still plays an important role for the success of discrete Tikhonov regularization, because it determines how well the regularized solution $\boldsymbol{x}_\lambda$ approximates the wanted, but unknown, underlying exact solution. The purpose of this paper is to illustrate this phenomenon, to introduce the *discrete Picard condition*, and to show how this condition is used in practice. A discussion of different choices of L, as well as a careful convergence analysis (which requires a discussion of the

principles for choosing the regularization parameter) are outside the scope of this paper. The work extends and further develops the author's work in [13, 15, 18]. The concept of a discrete Picard condition was first discussed by Varah [30, 31].

The paper is organized as follows. In Section 2 we introduce the generalized SVD, which we use throughout the paper to analyze Tikhonov regularization as well as a related regularization method, truncated GSVD. In sections 3 and 4, we investigate the conditions in which Tikhonov regularization and truncated GSVD will produce reasonable solutions. This analysis leads to the definition of the discrete Picard condition in Section 5, where we also briefly discuss how to test this condition numerically. Finally, in Section 6, we give two numerical examples.

2. Discrete Tikhonov regularization and generalized SVD.

The most convenient tool for analysis of the discrete Tikhonov-regularization problem (1.2) is the *generalized SVD* (GSVD) of the matrix pair (A, L). The GSVD was introduced by Van Loan [28] and further generalized by Paige and Saunders [25]. Here, we use a slightly simpler formulation, which is sufficient for our analysis.

THEOREM 1. *Let the matrix pair (A, L) satisfy*

$$A \in \mathbb{R}^{m \times n}, \qquad L \in \mathbb{R}^{p \times n}, \qquad m \geq n \geq p, \qquad \operatorname{rank}(L) = p. \tag{2.1}$$

Then there exist matrices $U \in \mathbb{R}^{m \times n}$, $V \in \mathbb{R}^{p \times p}$ with $U^T U = I_n$, $V^T V = I_p$ and a nonsingular $X \in \mathbb{R}^{n \times n}$ such that

$$\begin{bmatrix} U & 0 \\ 0 & V \end{bmatrix}^T \begin{bmatrix} A \\ L \end{bmatrix} X = \begin{bmatrix} \Sigma \\ M \end{bmatrix} = \begin{bmatrix} \Sigma_p & 0 \\ 0 & I_0 \\ M_p & 0 \end{bmatrix} \begin{matrix} p \\ n-p \\ p \end{matrix} \tag{2.2}$$

$$\Sigma_p = \operatorname{diag}(\sigma_1, \ldots, \sigma_p) \in \mathbb{R}^{p \times p}, \qquad M_p = \operatorname{diag}(\mu_1, \ldots, \mu_p) \in \mathbb{R}^{p \times p}, \tag{2.3}$$

where $\Sigma_p^2 + M_p^2 = I_p$ and

$$0 \leq \sigma_1 \leq \ldots \leq \sigma_p \leq 1, \qquad 1 \geq \mu_1 \geq \ldots \geq \mu_p > 0. \tag{2.4}$$

The generalized singular values of (A, L) are defined as the ratios $\gamma_i \equiv \sigma_i / \mu_i$, $i = 1, \ldots, p$.

PROOF. See [25, Section 2]. ∎

REMARK. It is no restriction to assume that A and L are scaled such that $\|A\|_2 = \|L\|_2 = 1$. As long as L is well-conditioned and its null-space is spanned by smooth vectors, it can be shown that the σ_i are closely related to the usual singular

values ψ_j of A in the sense that

$$\tfrac{1}{2} \le \frac{\sigma_i}{\psi_{n-i+1}} \lesssim \|L^+\|_2, \qquad i = 1, \ldots, p, \tag{2.5}$$

where L^+ is the pseudoinverse of L [15, Theorem 2.4 and Section 3].

Now, if we define $F_\lambda \equiv \operatorname{diag}(f_1, \ldots, f_p) \in \mathbb{R}^{p \times p}$ as a diagonal matrix with diagonal elements

$$f_i = \gamma_i^2/(\gamma_i^2 + \lambda^2), \qquad i = 1, \ldots, p \tag{2.6}$$

then it is easy to show that the regularized solution $\boldsymbol{x}_\lambda$ to (1.2) can be written as

$$\boldsymbol{x}_\lambda = X \begin{bmatrix} F_\lambda \Sigma_p^+ & 0 \\ 0 & I_0 \end{bmatrix} U^T \boldsymbol{b} = \sum_{i=1}^{p} f_i \frac{\boldsymbol{u}_i^T \boldsymbol{b}}{\sigma_i} \boldsymbol{x}_i + \sum_{i=p+1}^{n} \boldsymbol{u}_i^T \boldsymbol{b} \boldsymbol{x}_i. \tag{2.7}$$

Equations (2.6) and (2.7) show that F_λ basically "filters out" the contributions to $\boldsymbol{x}_\lambda$ corresponding to small γ_i. Since the oscillation property of the singular vectors of A carries over to the columns $\boldsymbol{x}_i$ of X (i.e., the larger the generalized singular values γ_i, the smoother the $\boldsymbol{x}_i$) [15, Theorem 3.2], we see how we can use λ to control the smoothness of the solution. At the same time, λ controls the sensitivity of $\boldsymbol{x}_\lambda$ to perturbations of A and $\boldsymbol{b}$ [16], such that the smoother $\boldsymbol{x}_\lambda$ the less sensitive it is. The "cost" of this regularization is that we neglect a (hopefully) small part of the information in $\boldsymbol{b}$ and that $\boldsymbol{x}_\lambda$ – from a statistical point of view – is not an unbiased estimator.

In connection with our discussion of discrete Tikhonov regularization it is also natural to consider the *truncated GSVD* (TGSVD) solution introduced in [15]. This method is of interest in its own right, and it is also closely related to both Tikhonov regularization and to the well-known truncated SVD method for regularization. For example, if (1.2) is transformed into a problem in standard form (i.e., $L = I_n$) – e.g. by the algorithm due to Eldén [6] – then the truncated SVD solution to the standard-form problem is identical to the TGSVD solution to (1.2) [15, Section 6]. The TGSVD solution $\boldsymbol{x}_k$ is defined as

$$\boldsymbol{x}_k \equiv X \begin{bmatrix} \hat{\Sigma}_k^+ & 0 \\ 0 & I_0 \end{bmatrix} U^T \boldsymbol{b}, \qquad \hat{\Sigma}_p^+ \equiv \operatorname{diag}(0, \ldots, 0, \sigma_{p-k+1}^{-1}, \ldots, \sigma_p^{-1}). \tag{2.8}$$

Since $\gamma_i = \sigma_i/\mu_i = \sigma_i(1 - \sigma_i^2)^{-1/2}$, small γ_i correspond to small σ_i, so TGSVD simply means discarding the $p - k$ smallest γ_i of (A, L). The TGSVD solution $\boldsymbol{x}_k$ is also a regularized solution and is in fact very similar to $\boldsymbol{x}_\lambda$ in many respects, see [15] for more details. For $L = I_n$, TGSVD becomes the truncated SVD method [13, 18, 30]. We include a discussion of $\boldsymbol{x}_k$ in this analysis in order to give an example of how the properties of the regularized solution $\boldsymbol{x}_\lambda$ carry over to other solutions that approximate $\boldsymbol{x}_\lambda$, such as the TGSVD solution. We believe that the same analysis can be carried out for any approximate regularized solution when its expansion in terms of the GSVD is known. See for example the analysis of SIRT and Lanczos type iterative methods in [29].

3. Regularization errors.

One of the central problems in relation to any regularization method is how well the regularized solution approximates the unknown, underlying exact solution [12, Chapter 2]. In this part of the analysis, one therefore ignores the errors in A and $\boldsymbol{b}$ and seeks to give a bound for the mere *regularization error* in the solution.

For both regularization methods considered here, Tikhonov regularization and TGSVD, the above-mentioned exact solution is given by

$$\boldsymbol{x}_0 = X\Sigma^+ U^T \boldsymbol{b}. \tag{3.1}$$

This $\boldsymbol{x}_0$ satisfies $\boldsymbol{x}_0 = \boldsymbol{x}_\lambda$ for $\lambda = 0$ (no Tikhonov regularization) and $\boldsymbol{x}_0 = \boldsymbol{x}_k$ for $k = n$ (no truncation). If A has full rank, then the matrix $X\Sigma^+ U^T$ equals the pseudoinverse A^+ and $\boldsymbol{x}_0 = A^+\boldsymbol{b}$ is the minimum-norm least squares solution to (1.1). If A does not have full rank (which is mainly of theoretical interest), then $X\Sigma^+ U^T$ is, in general, different from A^+ [7, Theorem 2.3], but $\boldsymbol{x}_0 = X\Sigma^+ U^T\boldsymbol{b}$ is still a member of the general solution to (1.1) given by $A^+\boldsymbol{b} + \boldsymbol{x}^*$, where $\boldsymbol{x}^*$ is an arbitrary vector in the null space of A.

For regularization in general form, we are primarily interested in the properties of the quantities $L\boldsymbol{x}_\lambda$ and $L\boldsymbol{x}_k$, because we seek to minimize the seminorms $\|L\boldsymbol{x}_\lambda\|_2$ and $\|L\boldsymbol{x}_k\|_2$. It is therefore natural to compare $L\boldsymbol{x}_\lambda$ and $L\boldsymbol{x}_k$ with the vector $L\boldsymbol{x}_0$, and we define $L(\boldsymbol{x}_0 - \boldsymbol{x}_\lambda)$ and $L(\boldsymbol{x}_0 - \boldsymbol{x}_k)$ as the *Tikhonov regularization error* and the *TGSVD regularization error*, respectively.

We are interested in upper bounds for the norms $\|L(\boldsymbol{x}_0 - \boldsymbol{x}_\lambda)\|_2$ and $\|L(\boldsymbol{x}_0 - \boldsymbol{x}_k)\|_2$. We can easily obtain the naive upper bound $\gamma_1^{-1}\|\boldsymbol{b}\|_2$ for both these norms. However, this bound certainly does not guarantee small regularization errors. Obviously, we must incorporate more information about the right-hand side $\boldsymbol{b}$ into our analysis. I.e., we must analyze upper bounds of the form:

$$\|L(\boldsymbol{x}_0 - \boldsymbol{x}_\lambda)\|_2 \le p^{1/2} \max_{1 \le i \le p} \left\{ \frac{\lambda^2}{\gamma_i^2 + \lambda^2} \frac{|\boldsymbol{u}_i^T\boldsymbol{b}|}{\gamma_i} \right\} \tag{3.2a}$$

$$\|L(\boldsymbol{x}_0 - \boldsymbol{x}_k)\|_2 \le p^{1/2} \max_{1 \le i \le p-k} \{|\boldsymbol{u}_i^T\boldsymbol{b}|/\gamma_i\}. \tag{3.2b}$$

In the light of these bounds, it is easy to see that the upper bounds for the regularization errors are related to the ratios between the Fourier coefficient $\boldsymbol{u}_i^T\boldsymbol{b}$ and the corresponding generalized singular values v_i.

To emphasize this relationship, we use the same strategy as in [18] and assume a simple, but still quite realistic model of the right-hand sides $\boldsymbol{b}$ as they typically appear in discrete ill-posed problems. In this model problem we assume that the Fourier coefficients have the following simple form:

$$\boldsymbol{u}_i^T\boldsymbol{b} = \begin{cases} \gamma_i^\alpha, & i = 1, \ldots, p \\ \gamma_p^\alpha, & i = p+1, \ldots, m \end{cases} \qquad \alpha \ge 0. \tag{3.3}$$

Here, α is a real parameter which controls the decay rate of the Fourier coefficients $\boldsymbol{u}_i^T\boldsymbol{b}$ relative to that of the generalized singular values v_i. Then we have:

THEOREM 2. *Let $\boldsymbol{x}_\lambda$ and $\boldsymbol{x}_k$ denote the regularized solutions* (2.7) *and* (2.8), *and let $\boldsymbol{x}_0$ denote the unregularized solution* (3.1). *Further, let the right-hand side $\boldsymbol{b}$ satisfy Eq.* (3.3). *Then the regularization errors satisfy*

$$\text{(3.4a)} \qquad \frac{\|L(\boldsymbol{x}_0 - \boldsymbol{x}_\lambda)\|_2}{\|L\boldsymbol{x}_0\|_2} \le \begin{cases} p^{1/2}, & 0 \le \alpha < 1 \\ p^{1/2}(\lambda/\gamma_p)^{\alpha-1}, & 1 \le \alpha < 3 \\ p^{1/2}(\lambda/\gamma_p)^2, & 3 \le \alpha \end{cases}$$

$$\text{(3.4b)} \qquad \frac{\|L(\boldsymbol{x}_0 - \boldsymbol{x}_k)\|_2}{\|L\boldsymbol{x}_0\|_2} \le \begin{cases} p^{1/2}, & 0 \le \alpha < 1 \\ p^{1/2}(\gamma_{k-p+1}/\gamma_p)^{\alpha-1}, & 1 \le \alpha. \end{cases}$$

PROOF. The proofs for the theorems in this paper follow the same line as the proofs given in [13] and [15] for the case $L = I_n$. The complete proof for Theorem 2 is given in [17]. ■

REMARK. When $L = I_n \Rightarrow \gamma_{p-k+1} = \psi_k$, $\gamma_p = \psi_1$, Eqs. (3.4a) and (3.4b) are consistent with the results in [18, Theorem 3.1].

In any practical application of Tikhonov regularization and TGSVD, to obtain a reasonable filtering of the small γ_i one always chooses $\lambda < \gamma_p$ and $k < p$. Theorem 2 then shows that in order to guarantee small regularization errors in the model problem, α must be somewhat larger than 1, i.e. the absolute value of the Fourier coefficients, $|\boldsymbol{u}_i^T\boldsymbol{b}|$, must decay to zero *faster* than the generalized singular values γ_i. And the faster the decay, the better $L\boldsymbol{x}_\lambda$ and $L\boldsymbol{x}_k$ approximate $L\boldsymbol{x}_0$. We can conclude that whenever this basic requirement is satisfied by the underlying exact problem, then we can ensure that Tikhonov regularization and TGSVD are able to produce useful approximate solutions.

4. Similarity of Tikhonov regularization and TGSVD.

In this section we take a closer look at the similarity between Tikhonov regularization and TGSVD, and we investigate the conditions in which we can guarantee that $\boldsymbol{x}_\lambda$ and $\boldsymbol{x}_k$ have the same properties. For this purpose, it is convenient to introduce matrices A_λ^I and A_k^I such that $\boldsymbol{x}_\lambda$ and $\boldsymbol{x}_k$ can be written as $\boldsymbol{x}_\lambda = A_\lambda^I\boldsymbol{b}$ and $\boldsymbol{x}_k = A_k^I\boldsymbol{b}$. Eqs. (2.7) and (2.8) show that these matrices are uniquely determined by

$$\text{(4.1)} \qquad A_\lambda^I = X\begin{bmatrix} F_\lambda\Sigma_p^+ & 0 \\ 0 & I_0 \end{bmatrix}U^T \quad \text{and} \quad A_k^I = X\begin{bmatrix} \hat{\Sigma}_k^+ & 0 \\ 0 & I_0 \end{bmatrix}U^T.$$

Then the difference between $L\boldsymbol{x}_\lambda$ and $L\boldsymbol{x}_k$ and the difference between the residuals can be measured by the norms of $LA_\lambda^I - LA_k^I$ and $AA_\lambda^I - AA_k^I$:

THEOREM 3. *Let the matrices A_λ^I and A_k^I be given by* (4.1), *and let* $\omega_k = \gamma_{p-k}/\gamma_{p-k+1}$. *Then for any* $\lambda > 0$ *and any positive* $k < p$:

$$\frac{\omega_k^{1/2}}{1+\omega_k^{1/2}} \le \min_\lambda \frac{\|LA_\lambda^I - LA_k^I\|_2}{\|LA_k^I\|_2} \le \frac{\omega_k^{1/2}}{1+\omega_k^{3/2}}; \tag{4.2a}$$

$$\min_\lambda \|AA_\lambda^I - AA_k^I\|_2 = \frac{\omega_k}{1+\omega_k}. \tag{4.2b}$$

These two minima are attained for $\lambda \approx (\gamma_{p-k+1}^3\gamma_{p-k})^{1/4}$ *and* $\lambda = (\gamma_{p-k+1}\gamma_{p-k})^{1/2}$, *respectively.*

PROOF. See [17]. ■

REMARK. When $L = I_n \Rightarrow \omega_k = \psi_{k+1}/\psi_k$, Eqs. (4.2a) and (4.2b) agree with the results derived in [13, Theorem 5.2].

Theorem 3 guarantees similar results from Tikhonov regularization and TGSVD whenever ω_k is sufficiently small and λ is chosen somewhere between $(\gamma_{p-k+1}\gamma_{p-k})^{1/2}$ and $(\gamma_{p-k+1}^3\gamma_{p-k})^{1/4}$. If the matrix A has well-determined numerical rank, i.e. if there is a distinct gap in the singular value spectrum, and therefore also in the spectrum of generalized singular values γ_i, then $\omega_k = \gamma_{p-k}/\gamma_{p-k+1}$ can always be made small by a proper choice of k. In this case, it is also *natural* to choose this k as the truncation parameter in the TGSVD method. Then Theorem 3 shows that there always exists a λ and a k such that TGSVD produces results similar to those obtained by Tikhonov regularization. This is, in itself, an important result.

However, practical experience with the use of the TGSVD method suggests that it can also be used successfully as a regularization method when A has ill-determined numerical rank, i.e. when the singular values of A, and therefore also the generalized singular values of (A, L), decay gradually to zero without any particular gap in the spectrum (see e.g. [18, 30, 31]). In order to analyze this situation, we must again incorporate information about the right-hand side into our analysis, and we shall again use the simple model problem from the previous section. We shall also assume that λ lies in the interval $[\gamma_{p-k}, \gamma_{p-k+1}]$, since we know from Theorem 3 that $\boldsymbol{x}_\lambda$ and $\boldsymbol{x}_k$ are most similar for such λ.

THEOREM 4. *Let $\boldsymbol{x}_\lambda$ and $\boldsymbol{x}_k$ denote the regularized solutions* (2.7) *and* (2.8), *and let the right-hand side $\boldsymbol{b}$ satisfy Eq.* (3.3). *If* $\gamma_{p-k} \le \lambda \le \gamma_{p-k+1}$, *then*

$$\frac{\|L(\boldsymbol{x}_\lambda - \boldsymbol{x}_k)\|_2}{\|L\boldsymbol{x}_k\|_2} \le \begin{cases} p^{1/2}\omega_k^{\alpha-1}, & 0 \le \alpha < 1 \\ p^{1/2}(\gamma_{p-k+1}/\gamma_p)^{\alpha-1}, & 1 \le \alpha < 3 \\ p^{1/2}(\gamma_{p-k+1}/\gamma_p)^2, & \alpha \ge 3 \end{cases} \tag{4.3a}$$

$$\frac{\|A\boldsymbol{x}_\lambda - A\boldsymbol{x}_k\|_2}{\|\boldsymbol{b}\|_2} \le \begin{cases} p^{1/2}(\gamma_{p-k+1}/\gamma_p)^\alpha, & 0 \le \alpha < 2 \\ p^{1/2}(\gamma_{p-k+1}/\gamma_p)^2, & \alpha \ge 2. \end{cases} \tag{4.3b}$$

PROOF. See [17]. ■

REMARK. When $L = I_n \Rightarrow \gamma_{p-k+1} = \psi_k$, $\gamma_p = \psi_1$, Eqs. (4.3a) and (4.3b) agree with the results in [18, Theorem 3.2].

Theorem 4 supplements the results in Theorem 3: it shows that if α is somewhat larger than one, such that the Fourier coefficients $|\boldsymbol{u}_i^T \boldsymbol{b}|$ decay to zero faster than the γ_i, then there exist λ and k such that $L\boldsymbol{x}_\lambda$ and $L\boldsymbol{x}_k$ are very similar for the model problem, even if there is no particular gap in the singular value spectrum of A. Although we are only able to prove this result for the model problem (3.3), we know from the relations between the singular value expansion, the SVD, and the GSVD [14, 15] that the $|\boldsymbol{u}_i^T \boldsymbol{b}|$ and γ_i are indeed very important in more general circumstances. Finally, it is interesting to notice that practical choices of λ and k, based on e.g. *generalized cross-validation* (GCV) [10], usually produces λ and k satisfying $\gamma_{p-k} \lesssim \lambda \lesssim \gamma_{p-k+1}$, see [13, Section 5]. The conclusion is therefore that whenever Tikhonov regularization produces a satisfactory regularized solution $\boldsymbol{x}_\lambda$, then TGSVD is also guaranteed to produce a satisfactory solution $\boldsymbol{x}_k$ with properties very similar to $\boldsymbol{x}_\lambda$.

5. The discrete Picard condition.

As we have illustrated in the previous sections, the decay rate of the Fourier coefficients indeed plays a central role in connection with discrete ill-posed problems. The key result is that if the Fourier coefficients $|\boldsymbol{u}_i^T \boldsymbol{b}|$ decay to zero faster than the generalized singular values γ_i, then the regularized solutions $\boldsymbol{x}_\lambda$ and $\boldsymbol{x}_k$ are guaranteed to have approximately the same properties as the exact solution $\boldsymbol{x}_0$. The decay of the Fourier coefficients need not be monotonic, as long as $|\boldsymbol{u}_i^T \boldsymbol{b}|$ on the *average* decay to zero faster than γ_i.

There are two important exceptions to this requirement to the Fourier coefficients. The first exception is that the smallest singular values ψ_i of A may be *numerically zero*, i.e. smaller than some threshold ε reflecting the errors in A (typically, ε is an upper bound for the norm of the perturbation matrix). In this case, it is natural to consider generalized singular values γ_i smaller than $\varepsilon \|L^+\|_2$ as being numerically zero, due to (2.5) and the relation $\gamma_i = \sigma_i(1 - \sigma_i^2)^{-1/2} \simeq \sigma_i$ for small σ_i. For those γ_i, the decay of the corresponding $|\boldsymbol{u}_i^T \boldsymbol{b}|$ is unimportant. Instead, the size of these $|\boldsymbol{u}_i^T \boldsymbol{b}|$ largely determines the norm of the residual and therefore, in turn, signals whether the problem (1.1) is consistent or not. This aspect has nothing to do with the existence of a smooth solution, and it is therefore important to restrict the analysis of the decay rates to those Fourier coefficients corresponding to numerically nonzero generalized singular values.

The second exception is that some of the Fourier coefficients of the given right-hand side, $\boldsymbol{u}_i^T \tilde{\boldsymbol{b}}$, themselves may be *numerically zero* with respect to some other threshold δ reflecting the errors in $\tilde{\boldsymbol{b}}$. Often, these $|\boldsymbol{u}_i^T \tilde{\boldsymbol{b}}| < \delta$ represent true zero Fourier coefficients $\boldsymbol{u}_i^T \boldsymbol{b}$, and – as illustrated in the next section – care should be

taken to avoid confusion if such numerically zero Fourier coefficients are intermingled with numerically nonzero coefficients.

This discussion leads to the following definition of a *discrete Picard condition* for discrete ill-posed problems:

THE DISCRETE PICARD CONDITION (DPC). *Let* $\boldsymbol{b}$ *denote an unperturbed right-hand side in* (1.2). *Then* $\boldsymbol{b}$ *satisfies the DPC if, for all numerically nonzero generalized singular values* $\gamma_i > \varepsilon \|L^+\|_2$, *the corresponding Fourier coefficients* $|\boldsymbol{u}_i^T \boldsymbol{b}|$ *on the average decay to zero faster than the* γ_i.

REMARK. When $L = I_n$, simply substitute the ordinary singular values ψ_i for the γ_i in the DPC.

We have chosen the name *discrete Picard condition* because the DPC resembles the PC so much. We stress, however, that while the PC only needs to be satisfied asymptotically, it is important that the DPC be satisfied for preferably all the generalized singular values.

When solving real-world problems, where the right-hand side (and sometimes also the matrix) are contaminated with measurement errors, approximation errors, and rounding errors, then the given perturbed problem rarely satisfies the DPC. However, if the underlying exact problem satisfies the DPC, then by a proper choice of λ or k one can often make the regularized problem satisfy the DPC. I.e., one can regard regularization as a method to derive from the given ill-posed problem a related problem which – in addition to being less sensitive to perturbations [16] – satisfies the DPC and therefore has a regularized solution that approximates the exact, unknown solution.

As a typical example of this situation, let the problem (1.1) be derived from a first kind Fredholm integral equation satisfying the Picard condition. Then, ideally, due to the strong connection between the singular value expansion of the kernel and the SVD of the matrix A [14], the DPC is also satisfied. However, due to data errors as well as approximation errors in setting up the discrete problem, all the $\boldsymbol{u}_i^T \boldsymbol{b}$ generally do not satisfy the DPC. Instead, they typically roll off gradually until they reach an almost constant level, determined by the errors. By means of a proper choice of the Tikhonov regularization parameter λ one can, however, guarantee that the Fourier coefficients for the regularized problem, namely $f_i \boldsymbol{u}_i^T \boldsymbol{b}$, satisfy the DPC. Similarly, for TGSVD, the regularized Fourier coefficients are $\varphi_i \boldsymbol{u}_i^T \boldsymbol{b}$ where $\varphi_i = 0$ for $i \leq p - k$ and $\varphi_i = 1$ for $i \geq p - k + 1$, and obviously one can always choose a truncation parameter k such that $\varphi_i \boldsymbol{u}_i^T \boldsymbol{b}$ satisfy the DPC.

If, on the other hand, the underlying problem does not satisfy the DPC (or even the PC), then it is generally not possible to compute a satisfactory solution by means of Tikhonov regularization or any related method. See [4] for an example of this situation.

Having introduced the discrete Picard condition as defined above, a natural question is: how does one check numerically whether the DPC is satisfied? Of

course, a visual inspection of a plot of the Fourier coefficients $|\boldsymbol{u}_i^T \boldsymbol{b}|$ and the generalized singular values γ_i will often reveal this and, at the same time, guide the user in choosing a suitable k or λ. But we believe that an automatic check for satisfaction of the DPC may also be required, partly because the amount of data may be large, and partly because one might want a more specific test than just a visual inspection (as is the case for both the discrepancy method [12, Section 3.3] and the GCV method for choosing the optimal regularization parameters λ and k).

From the discussion leading to the DPC, it is evident that satisfaction of the DPC in practice is a local phenomenon, taking place only in that part of the spectrum with the large generalized singular values γ_i. Hence, the check for satisfaction of the DPC should also be based on the use of local information in the sequences $|\boldsymbol{u}_i^T \boldsymbol{b}|$ and γ_i, only. We could, for example, fit cubic splines to the $|\boldsymbol{u}_i^T \boldsymbol{b}|$ and the γ_i and then check the first derivative of these splines. However, a much simpler and easy-to-use approach seems to be sufficient.

Since we are interested in information about the decay of the data, it is the *ratios* of nearby coefficients $|\boldsymbol{u}_i^T \boldsymbol{b}|$ and γ_i – rather than their absolute values – that is important. Therefore, we propose to base the numerical check for satisfaction of the DPC on the *moving geometric mean:*

$$\rho_i \equiv \gamma_i^{-1} \left(\prod_{j=i-q}^{i+q} |\boldsymbol{u}_j^T \boldsymbol{b}|\right)^{1/(2q+1)}, \qquad i = q+1, \ldots, n-q \tag{5.1}$$

where q is a small integer, thus ensuring the locality of the ρ_i. Note that ρ_i should only be computed for numerically nonzero γ_i, i.e. for $\gamma_i > \varepsilon \|L^+\|_2$, and that special care should also be taken if some of the $|\boldsymbol{u}_i^T \boldsymbol{b}|$ are numerically zero in the sense that $|\boldsymbol{u}_i^T \boldsymbol{b}| < \delta$. Note the two different thresholds δ and ε. Based on our experiments, we find that q equal to 1, 2 or 3 gives good results, and we will say that the DPC is satisfied when all the ρ_i defined by (5.1), corresponding to numerically nonzero $|\boldsymbol{u}_i^T \boldsymbol{b}|$ and γ_i, decay monotonically to zero.

6. Numerical examples.

In this section we illustrate, by two numerical examples, the important role the discrete Picard condition plays in the analysis of discrete ill-posed problems. Both examples are obtained from discretizations of Fredholm integral equations of the first kind:

$$\int_a^b K(s,x)\,dx = g(s), \qquad c \le s \le d. \tag{6.1}$$

Our first example is the classical integral equation devised by Phillips [27] with $[a,b] = [c,d] = [-6,6]$, and with K and g given by:

$$K(s,x) = f(s-x) \equiv \begin{cases} 1 + \cos[(s-x)\pi/3], & |s-x| \le 3 \\ 0, & |s-x| > 3 \end{cases} \tag{6.2a}$$

(6.2b) $$g(s) = (6 - |s|)\left[1 + \tfrac{1}{2}\cos\frac{\pi s}{3}\right] + \frac{9}{2\pi}\sin\frac{\pi|s|}{3}.$$

This integral equation satisfies the Picard condition, and the square integrable solution is simply $f(x)$ as given in (6.2a). We discretized the integral equation using the trapezoidal quadrature rule as described in [23] with $m = 78$ and $n = 49$, and as regularization matrix L we chose an approximation to the second derivative operator,

(6.3) $$L = \begin{bmatrix} -1 & 2 & -1 & & & & \\ & -1 & 2 & -1 & & & 0 \\ & & \ddots & \ddots & \ddots & & \\ & & & \ddots & \ddots & \ddots & \\ 0 & & & & -1 & 2 & -1 \end{bmatrix} \in \mathbb{R}^{p \times n}, \qquad p = n - 2.$$

In order to simulate measurement errors in the right-hand side $\tilde{\boldsymbol{b}}$, we then added to $\boldsymbol{b}$ a random perturbation vector with elements from a normal distribution with zero mean and standard deviation 10^{-5}. The corresponding threshold is therefore $\delta = 10^{-5}$.

The perturbed Fourier coefficients $|\boldsymbol{u}_i^T \tilde{\boldsymbol{b}}|$ and the generalized singular values γ_i are shown in Fig. 1. Notice the "reverse" ordering of γ_i as compared to the usual singular

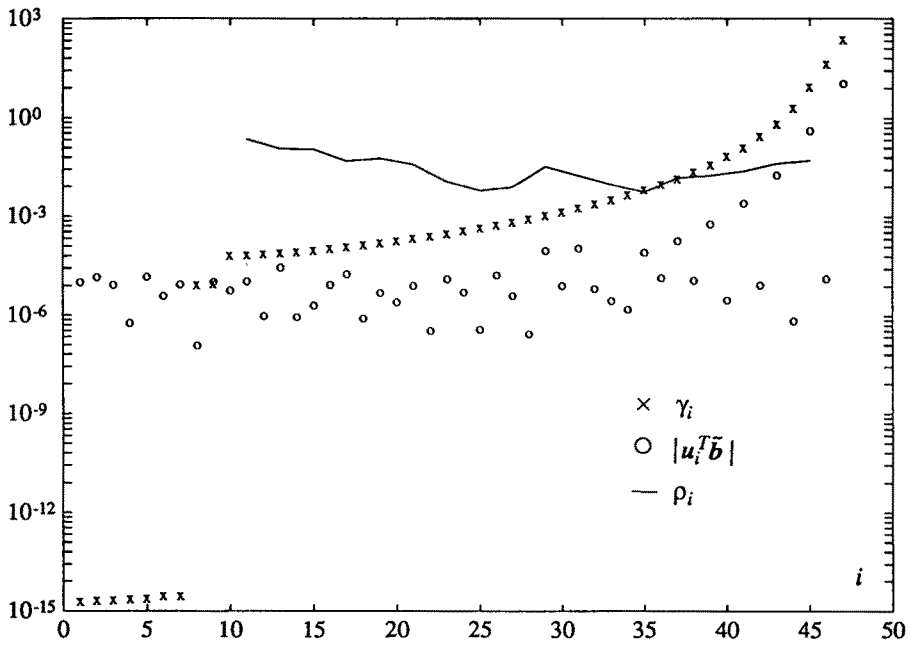

Fig. 1. The generalized singular values (crosses), Fourier coefficients $|\boldsymbol{u}_i^T \tilde{\boldsymbol{b}}|$ (circles), and means ρ_i (solid line) for example one with $m = 78$, $n = 49$ and $p = 47$. Note that there are $p = 47$ generalized singular values. The DPC is satisfied for $i = 45, 44, \ldots, 35$.

values ψ_i. All the singular values of the kernel K in (6.2b) are nonzero, but due to the particular discretization method the matrix A has 7 numerically zero singular values ψ_i of the order $\varepsilon = 10^{-15}$. Hence, there are also 7 numerically zero generalized singular values γ_i of (A, L) of order 10^{-15}, while the rest of the γ_i are numerically nonzero and decay monotonically with decreasing i. The corresponding Fourier coefficients $|\boldsymbol{u}_i^T \boldsymbol{b}|$ also tend to decay with decreasing i until they level off at about 10^{-5}, which is the noise level δ caused by our random errors. The particular Fourier coefficients corresponding to the numerically zero $\gamma_i \simeq \varepsilon$ are of the same size as δ, and the problem is therefore consistent within the noise.

For this particular problem, all the Fourier coefficients $|\boldsymbol{u}_i^T \tilde{\boldsymbol{b}}|$ with *even* index i are actually numerically zero (i.e., of the same size as δ). As mentioned in Section 5, these numerically zero $|\boldsymbol{u}_i^T \tilde{\boldsymbol{b}}|$ should not be included in the analysis of the DPC, and we therefore only computed ρ_i for *odd* values of i. These ρ_i, computed with $q = 1$, are shown by the solid line in Fig. 1. We see that for $i = 45, 44, \ldots, 35$ the values ρ_i decay monotonically, and for $i < 35$ they start growing again for decreasing values of i. From such a plot, we conclude that the underlying, exact problem seems to satisfy the discrete Picard condition. We also see that the perturbed problem satisfies the DPC if it is regularized in such a way that the terms $(\boldsymbol{u}_i^T \tilde{\boldsymbol{b}}/\gamma_i)\boldsymbol{x}_i$ are damped or truncated for $i < 35$.

To illustrate this in another way, we have plotted the seminorms $\|L\boldsymbol{x}_\lambda\|_2$ and $\|L\boldsymbol{x}_k\|_2$ versus the residual norms $\|A\boldsymbol{x}_\lambda - \boldsymbol{b}\|_2$ and $\|A\boldsymbol{x}_k - \boldsymbol{b}\|_2$ in Fig. 2. Such a plot clearly illustrates the tradeoff between minimization of the (semi)norm of the solution and the residual norm. We also immediately see that the solutions computed by means of Tikhonov regularization and TGSVD are indeed very similar. As

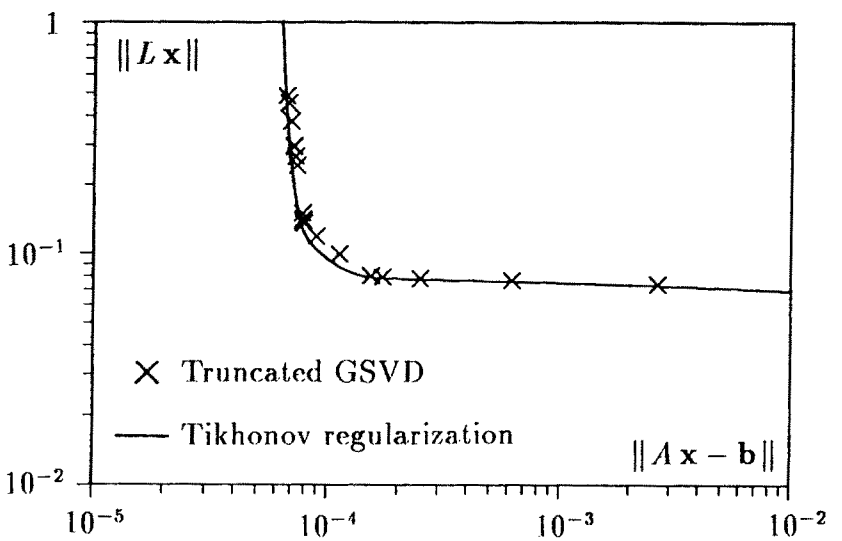

Fig. 2. The seminorm of the regularized solutions versus the residual norms for Tikhonov regularization (solid line) and TGSVD (crosses).

shown in [18, Section 5], there is a distinct L-shaped corner on the $(\|Ax_\lambda - b\|_2, \|Lx_\lambda\|_2)$-curve, and the optimal parameters λ and k produce solutions near this corner. For smaller values of λ (and larger values of k), the solution is dominated by oscillating contributions from the perturbation of the right-hand side, while for larger values of λ (and smaller values of k) the solution is over-regularized, i.e. the regularization error is too large. Fig. 2 suggests an optimal truncation parameter k equal to 16 or 18, while inspection of plots of the TGSVD solutions (not shown here) indicates that $k = 14$ is optimal.

In this connection, we would like to emphasize that we do not encourage the choice of λ or k being based solely on the ρ_i-curve. Rather, we see this curve as a useful aid to analyzing discrete ill-posed problems. To choose λ and k, we will advocate the use of several simultaneous strategies, such as inspection of the γ_i, $|u_i^T \tilde{b}|$ and ρ_i, plotting the (semi)norm of the solution versus the residual norm, using GCV, etc.

The second example is a model of the transient transport across the blood-retina barrier in the human eye [20]. A simple version of this model, assuming the eye to be a sphere, was refined to allow for a more realistic geometry of the eye where the front half deviates from spherical form. The kernel and right-hand side of the integral equation (6.1) are then given by:

$$\text{(6.4a)} \quad K(s,x) = 2\pi \sin x D(x)[D(x)^2 + [dD(x)/dx]^2]^{1/2} E(s^2 + D(x)^2 - 2sD(x)\cos x)$$

$$\text{(6.4b)} \quad g(s) = F(\beta s + (\beta - 1)a_0), \qquad \beta = \tfrac{1}{2}(3 + \alpha)/(1 + \alpha)$$

where $[a,b] = [0,\pi]$, $[c,d] = [-\alpha_0, \alpha a_0]$, and

$$\text{(6.5c)} \quad D(x) = \begin{cases} \tfrac{1}{2}(\alpha - 1)a_0 \cos 3x + \tfrac{1}{2}(\alpha + 1)a_0, & 0 \le x < \pi/3 \\ a_0 \quad , & \pi/3 \le x \le \pi \end{cases}$$

$$\text{(6.5d)} \quad E(t) = \exp(-s_0 t^{1/2})/t^{1/2}, \qquad F(t) = 2\exp(-a_0 s_0)\sinh(s_0 t)/t.$$

The parameters were $a_0 = 1.2\,\text{cm}$ (radius of the spherical back half of the eye), $\alpha = 0.9$ (deformation from spherical form of the front half of the eye), and $s_0 = 0.316$ (time constant for the diffusion through the blood-retina barrier). We discretized the integral equation by means of the moment method with $m = n$ using piecewise constant approximations (see e.g. [14] for more details), and we used $L = I_n$. This leads us to considering the usual singular values ψ_i, the Fourier coefficients $|u_i^T \tilde{b}|$ (where u_i are the usual left singular vectors of A), and the moving geometric mean $\rho_i = \psi_i^{-1}[\prod_{j=i-q}^{i+q} |u_j^T \tilde{b}|]^{1/(2q+1)}$.

When the order n of the matrix is smaller than about 100, the DPC does not seem to be satisfied, because all the Fourier coefficients decay to zero slower than the singular values. However, if n is greater than 100, then the DPC is in fact satisfied for $i < i_0$ (i.e., for the larger singular values), and the number i_0 increases with the order n. This behavior of i_0 implies that the growth of ρ_i for $i > i_0$ is primarily due to the approximation errors caused by the rough piecewise constant approximations. A plot of the first 30 coefficients for the case $n = 256$ is shown in Fig. 3, using $q = 3$.

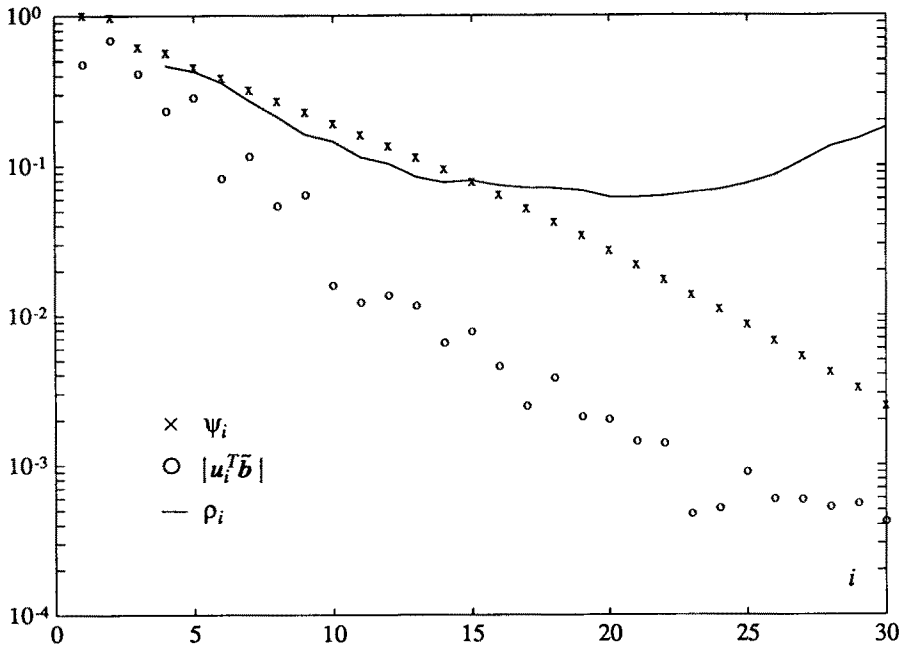

Fig. 3. The first 30 singular values ψ_i (crosses), Fourier coefficients $|\boldsymbol{u}_i^T \tilde{\boldsymbol{b}}|$ (circles), and means ρ_i (solid line) for example two with $m = n = 256$. The DPC is satisfied for $i < i_0 = 20$.

From these results, we can conclude that the underlying, exact problem seems to satisfy the DPC, which means that the integral equation is a satisfactory model. Use of more sophisticated approximation functions would increase the quality of the discrete solution.

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