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# Regularization of Large-scale Ill-conditioned Least Squares Problems

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**Abstract** Ill-conditioned problems arise in important areas like geophysics, medical imaging and signal processing. The fact that the ill-conditioning is an intrinsic feature of these problems makes
it necessary to develop special numerical methods to treat them. Regularization methods belong to this class. In this paper, we compare some regularization methods.

**Keywords** Discrete ill-posed problem, Tikhonov regularization, truncated singular value decomposition, discrepancy principle, regularization matrix

## 1. Introduction

Ill-conditioned problems arise in important areas like geophysics, medical imaging and signal processing. Common problems in these areas are inverse problems which attempt to determine the structure of a system from the system's behavior.

Inverse problems are a natural source of ill-posed problems. The numerical solution of these problems usually involves some kind of discretization which in turn originates a class of problems known as discrete ill-posed problems which are very ill-conditioned.

The fact that the ill-conditioning is an intrinsic feature of these problems makes it necessary to develop special numerical methods to treat them. Regularization methods belong to this class.

A regularization method computes an approximate solution, the regularization solution, to an ill-conditioned problem through a regularization parameter. A complete regularization method must address these two aspects.

When ill-conditioned systems or least squares problems are encountered, the usual recommendation is not to trust any computed solution and to try to replace the coefficient matrix by a nearby well-conditioned one.

According to [1], we can distinguish two main classes of ill-conditioned problems based on the properties of their coefficient matrices.

Rank-deficient problems are characterized by the coefficient matrices $A$ having a cluster of small singular values, and there is a well-determined gap between large and small singular values. This implies that one or more rows and columns of $A$ are nearly linear combinations of some or all of the remaining rows and columns. Therefore, the matrix $A$ contains almost redundant information, and the key to the numerical treatment of such problems is to extract the linearly independent information in $A$, to arrive at another problem with a well-conditioned matrix.

Discrete ill-posed problems arise from the discretization of ill-posed problems such as Fredholm integral equations of the first kind. Here all the singular values of the coefficient matrix $A$, as well as the SVD components of the solution, on the average, decay gradually to zero, and we say that a discrete Picard condition (see in [1]) is satisfied. Since there is no gap in the singular value spectrum, there is no notion of a numerical rank for these matrices. For discrete ill-posed problems, the goal is to find a balance between the residual norm and the size of the solution that matches the errors in the data as well as one's expectations to the computed solution. Here, "size" should be interpreted in a rather broad sense; e.g., size can be measured by a norm, a seminorm, or a Sobolev norm.

Since standard methods fail to produce a meaningful solution for ill-conditioning, it is necessary to use other approaches to treat this kind of problems. One of such approaches is numerical regularization, which attempts to compute a more stable (or regularized) approximate solution by using additional information about the unknown exact solution.

The existing numerical regularization methods are designed for rank-deficient and discrete ill-posed problems. For other kinds of ill-conditioned problems, these methods are not suitable and we must use other techniques like iterative refinement, extended precision iterative refinement or preconditioning for the large-scale case.

## 2. The SVD and Its Generalizations

The superior numerical "tools" for analysis of discrete ill-posed problems are the (ordinary) SVD of $A$ and its generalization to two matrices, the generalized SVD (GSVD) of the matrix pair( $A, L$ ). The SVD reveals all the difficulties associated with the ill-conditioning of the matrix $A$, while the GSVD of ( $A, L$ ) yields important insight into regularization problems involving both the matrix $A$ and the regularization matrix $L$ .

### 2.1. The (ordinary) SVD

Let $A \in R^{m \times n}$ be a rectangular or square matrix, and assume for ease of presentation that $m > n$. Then the SVD of $A$ is a decomposition of the form

$$A = U \sum V^T = \sum_{i=1}^{n} u_i \sigma_i v_i^T \ , \quad (1)$$

where $U = (u_1, \cdots, u_n) \in R^{m \times n}$ and $V = (v_1, \cdots, v_n) \in R^{n \times n}$ are matrices with orthonormal columns, $U^T U = V^T V = I_n$, and the diagonal matrix $\sum = diag(\sigma_1, \cdots, \sigma_n)$ has nonnegative elements appearing in nonincreasing order such that

$$\sigma_1 \geq \sigma_2 \geq \cdots \geq \sigma_n \geq 0 . \quad (2)$$

The numbers $\sigma_i$ are called the singular values of $A$, while the vectors $u_i$ and $v_i$ are the left and right singular vectors of $A$, respectively. The decomposition in (1) is called the "thin SVD" in [2], because $U$ is rectangular when $m > n$. The SVD is defined for any $m$ and $n$; if $m < n$, we can apply (1) to $A^T$ and interchange $U$ and $V$ .

Form the relations $A^T A = V \sum^2 V^T$ and $AA^T = U \sum^2 U^T$, we can see that the SVD of $A$ is strongly linked to the eigenvalue decompositions of the symmetric semidefinite matrices $A^T A$ and $AA^T$ . This shows that the SVD is unique for a given matrix $A$, up to a sign change in the pair $(u_i, v_i)$ ---except for singular vectors associated with multiple singular values, where only the spaces spanned by the vectors are unique. In connection with discrete ill-posed problems, Wing and his workers in a series of papers [3], [4] and [5] studied two characteristic features of the SVD .

1. The singular values $\sigma_i$ decay gradually to zero with no particular gap in the spectrum. An increase of the dimensions of $A$ will increase the number of small singular values.

2. The left and right singular vectors $u_i$ and $v_i$ tend to have more sign changes in their elements as the index $i$ increases, i.e., as $\sigma_i$ decreases.

### 2.2. The GSVD

The GSVD of the matrix pair $(A, L)$ is a generalization of the SVD of $A$ in the sense that the generalized singular values of $(A, L)$ are essentially the square roots of the generalized eigenvalues of the matrix pair $(A^T A, L^T L)$. We assume that the dimensions of $A \in R^{m \times n}$ and $L \in R^{p \times n}$ satisfy $m \geq n \geq p$, which is always the case in connection with discrete ill-posed problems. We also assume that $N(A)\cap N(L)=0$ and that $L$ has full row rank. Then the GSVD is a decomposition of $A$ and $L$ in the form

$$A=U\begin{pmatrix}\Sigma & 0\\ 0 & I_{n-p}\end{pmatrix}X^{-1}, L=V(M,0)X^{-1}. \quad (3)$$

Where the columns of $U\in R^{m\times n}$ and $V\in R^{p\times p}$ are othonormal, $UU^T=I_n$ and $V^TV=I_p$; $X\in R^{n\times n}$ is nonsingular. $\Sigma$ and $M$ are $p\times p$ diagonal matrices: $\Sigma=diag(\sigma_1,\cdots\sigma_p)$ . Moreover, the diagonal elements of $\Sigma$ and $M$ are nonnegative and ordered such that

$$0\le\sigma_1\le\cdots\sigma_p\le1,1\ge\mu_1\ge\cdots\mu_p>0,$$

and they are normalized such that

$$\sigma_i^2+\mu_i^2=1, i=1,\cdots,p.$$

Then the generalized singular values $\gamma_i$ of $(A,L)$ are defined as the ratios

$$\gamma_i=\frac{\sigma_i}{\mu_i}, i=1,\cdots,p,$$

and they obviously appear in nondecreasing order.

## 3. Methods for Discrete Ill-posed Problems

Consider the computation of an approximate solution of the minimization problem

$$\min_{x\in R^n}\|Ax-b\|, \quad (4)$$

where $\|\cdot\|$ denotes the Euclidean vector norm. Let $e\in R^m$ denote the (unknown) error in $b$ , and let $\hat{b}\in R^m$ be the (unknown) error-free vector associated with $b$ , i.e.,

$$b=\hat{b}+e.$$

We sometimes will refer to the vector $e$ as "noise". We assume that a bound $\|e\|\le\varepsilon$ is available and the (unavailable) linear system of equations with
error-free right-hand side,

$$Ax=\hat{b},$$

is assumed to be consistent; however, we do not require the least-squares problem with error-contaminated data $b$ (3) to be consistent. Let $\hat{x}$ denote a desired solution of, e.g., the solution of minimal Euclidean norm. We seek to determine an approximation of $\hat{x}$ by computing an approximate solution of the available linear system of equations (3).

### 3.1. Regularization by truncated singular value decomposition

The Moore-Penrose pseudoinverse of $A$ is given by

$$A^+=\sum_{j=1}^{l}\sigma_j^{-1}v_ju_j^T, l=rank(A),$$

the difficulty of solving (3) without regularization stems from the fact that the matrix $A$ has "tiny" positive singular values and the computation of (3) involves division by these tiny singular values. This results in severe propagation of the error $e$ in $b$ and of round-off errors introduced during the calculations into the computed solution of (3).

The truncated SVD method uses the singular value decomposition (1) to determine the approximate solution

$$x_k = \sum_{j=1}^{k} \frac{u_j{}^T b}{\sigma_j} v_j, k = 1, 2, \cdots, l, l = \text{rank}(A), \quad (4)$$

here $k(1 \le k \le n)$ is the truncated parameter.

We note that $x_k \in span\{v_1, \cdots, v_k\}$. The singular values $\sigma_j$ and the Fourier coefficients $u_j{}^T b$ provide valuable insight into the properties of the linear discrete ill-posed problem (3); see, e.g., Hansen [1,7] for a discussion on the application of the TSVD to linear discrete ill-posed problems.

**3.2. Tikhonov regularization**

Tikhonov regularization replaces the linear system of equations (3) by the minimization problem of the form

$$\min_{x \in R^n} \left\{ \|Ax - b\|^2 + \|L_\mu x\|^2 \right\}. \quad (5)$$

Here and throughout this paper $\|\cdot\|$ denotes the Euclidean vector norm or the associated induced matrix norm. This replacement is commonly referred to as regularization. The matrix $L_\mu \in R^{p \times n}, p \le n$, is referred to as the regularization matrix. The scalar $\mu > 0$ is the regularization parameter. The minimization problem (5) is said to be in *standard form* when $L = I$ and in *general form* otherwise. Many examples of regularization matrices can be found in [8,9,10,11,15].

The matrix $L_\mu$ is assumed to be chosen so that system of equations (5) by the minimization problem of the form

$$N(A) \cap N(L_\mu) = 0.$$

Then the Tikhonov minimization problem (5) has the unique solution

$$x_\mu = (A^T A + L_\mu{}^T L_\mu)^{-1} A^T b \quad (6)$$

see,e.g., Hansen [1] and Engl et al.[6] for discussions on Tikhonov regularization.

We apply the discrepancy principle to determine a suitable value of the truncation index $k$ and the regularization parameter $\mu$. It prescribes that $k$ be chosen so that the associated solution (4) satisfies

$$\|Ax_k - b\| \le \eta\varepsilon, \quad (7)$$

and $\mu$ be chosen so that the associated solution (6) satisfies

$$\|Ax_\mu - b\| = \eta\varepsilon, \quad (8)$$

where $\eta > 1$ is usually chosen to be fairly close to unity is a user-specified constant independent of $\varepsilon$. Thus, $k$ is such that

$$\sum_{j=k+1}^{n} (u_j{}^T b)^2 \le (\eta\varepsilon)^2 \le \sum_{j=k}^{n} (u_j{}^T b)^2.$$

Properties of this method are discussed in [6].

We can use a zero-finder, such as Newton's method to get the desired value of $\mu$, further discussion can be found in [1,6,12].

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