

# A modified TSVD method for discrete ill-posed problems

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## Discrete ill-posed problems

Consider the computation of an approximate solution of the minimization problem

$$\min_{x \in \mathbb{R}^n} \|Ax - b\|_2, \quad (1)$$

where  $A \in \mathbb{R}^{m \times n}$  is a matrix with many singular values of different size close to the origin.

Minimization problems with a matrix of this kind arise, for example, from the discretization of linear ill-posed problems, such as Fredholm integral equations of the first kind with a smooth kernel.

The vector  $b \in \mathbb{R}^m$  represents error-contaminated data.

Let  $e \in \mathbb{R}^m$  denote the (unknown) error in  $b$ , and let  $\hat{b} \in \mathbb{R}^m$  be the (unknown) error-free vector associated with  $b$ :  $b = \hat{b} + e$ .

# Regularization

We are interested in computing an approximation of the solution  $\hat{x}$  of minimal Euclidean norm of the error-free least-squares problem

$$\min_{x \in \mathbb{R}^n} \|Ax - \hat{b}\|_2.$$

Let  $A^\dagger$  denote the Moore-Penrose pseudoinverse of  $A$ . Because  $A$  has many positive singular values close to the origin,  $A^\dagger$  is of very large norm and the solution of the minimization problem (1),

$$\check{x} = A^\dagger b = A^\dagger(\hat{b} + e) = \hat{x} + A^\dagger e,$$

typically is dominated by the propagated error  $A^\dagger e$  and then is meaningless.

This difficulty can be mitigated by **replacing the matrix  $A$  by a less ill-conditioned nearby matrix**.

This replacement commonly is referred to as *regularization*.

# Truncated Singular Value Decomposition

The TSVD is a popular regularization method for solving linear discrete ill-posed problems with a small to moderately sized matrix  $A$ .

Consider a singular value decomposition of  $A$ , i.e.  $A = U\Sigma V^*$ , where  $U \in \mathbb{R}^{m \times m}$  and  $V \in \mathbb{R}^{n \times n}$  are orthogonal matrices, and the entries of  $\Sigma = \text{diag}[\sigma_1, \sigma_2, \dots, \sigma_n] \in \mathbb{R}^{m \times n}$  are ordered according to

$$\sigma_1 \geq \sigma_2 \geq \dots \geq \sigma_\ell > \sigma_{\ell+1} = \dots = \sigma_n = 0.$$

- The  $\sigma_j$  are the singular values of  $A$ , and  $\ell$  is the rank of  $A$ . For  $k \leq \ell$ , define the matrix  $\Sigma_k = \text{diag}[\sigma_1, \sigma_2, \dots, \sigma_k, 0, \dots, 0] \in \mathbb{R}^{m \times n}$  by setting the singular values  $\sigma_{k+1}, \sigma_{k+2}, \dots, \sigma_n$  to zero.
- Regularization is achieved by **replacing the matrix  $A$  by its rank- $k$  approximant  $A_k = U\Sigma_k V^*$**  and determining the least-square solution of minimal Euclidean norm  $x_k = A_k^\dagger b$ , where  $A_k^\dagger = V\Sigma_k^\dagger U^*$ .

## Singular values and unitarily invariant norms

- It is clear from the SVD that if  $\|\cdot\|$  is a unitarily invariant norm, then  $\|A\| = \|U\Sigma V^*\| = \|\Sigma(A)\|$  is a function only of the singular values of  $A$ .
- The Ky Fan  $p - k$  norms  $N_{k;p} = [\sigma_1(A)^p + \dots + \sigma_k(A)^p]^{1/p}$ , where  $p \geq 1$  and  $1 \leq k \leq n$ , are unitarily invariant norms on  $\mathbb{R}^{m \times n}$  (when  $k = n$ ,  $N_{n;p}$  is often called the Schatten  $p$ -norm);  $N_{1;1}$  is the **spectral norm** and  $N_{n;2}$  is the **Frobenius norm**, i.e. the Schatten 2-norm.
- Let  $A, B \in \mathbb{R}^{m \times n}$  be given. For every unitarily invariant norm  $\|\cdot\|$  on  $\mathbb{R}^{m \times n}$  it can be proved that (see, e.g., Horn and Johnson, *Topics in Matrix Analysis*)

$$\|A - B\| \geq \|\Sigma(A) - \Sigma(B)\|. \quad (2)$$

If  $\text{rank}(B) = k$ ,  $\|A - B\| \geq \|\text{diag}(0, \dots, 0, \sigma_{k+1}(A), \dots, \sigma_n(A))\|$ .

Thus, for  $k \leq \ell$ ,  $A_k = U\Sigma_k V^*$  is the **best rank- $k$  approximation to  $A$  with respect to every unitarily invariant matrix norm.**

## Distances and condition number of $A_k$

- For the spectral and Frobenius norms,

$$\|A_k - A\|_2 = \sigma_{k+1}, \quad \|A_k - A\|_F = \sqrt{\sum_{i=k+1}^n \sigma_i^2},$$

where we define  $\sigma_{n+1} = 0$ .

- The condition number of  $A_k$  with respect to the spectral norm is

$$\kappa_2(A_k) = \frac{\sigma_1}{\sigma_k}.$$

The larger the condition number, the more sensitive can  $x_k = A_k^\dagger b$  be to the error  $e$  in  $b$ .

## The truncation index

- The truncation index  $k$  is a regularization parameter. It determines how close  $A_k$  is to  $A$  and how sensitive the computed solution  $x_k$  is to the error in  $b$ . **The condition number  $\kappa_2(A_k)$  increases and the distance between  $A_k$  and  $A$  decreases as  $k$  increases.**
- It is important to choose a suitable value of  $k$ ; a too large value gives a computed solution  $x_k$  that is severely contaminated by propagated error stemming from the error  $e$  in  $b$ , and a too small value gives an approximate solution that is an unnecessarily poor approximation of the desired solution  $\hat{x}$  because  $A_k$  is far from  $A$ .
- There are many approaches described in the literature to determining the truncation index  $k$ , including the quasi-optimality criterion, the L-curve, generalized cross validation, extrapolation, and the discrepancy principle; see, e.g., Numer. Algorithms papers by Brezinski, Rodriguez, and Seatzu, and by Reichel and Rodriguez.

## A modified TSVD method

- We suggest a modification of the TSVD method in which the matrix  $A_k$  is replaced by a matrix  $\tilde{A}$  that is closer to  $A$  and has the same spectral condition number.
- We show that  $\tilde{x} = \tilde{A}^\dagger b$  may be a more accurate approximation of  $\hat{x}$  than  $x_k = A_k^\dagger b$  furnished by standard TSVD.
- Computed examples illustrate this often to be the case.
- We use the discrepancy principle to determine a suitable value of the regularization parameter  $k$ ; however, our regularization method also can be applied in conjunction with other techniques for determining the regularization parameter.



## A first result

Consider the matrix  $A = U\Sigma V^*$ , and let  $\tilde{\Sigma}$  be of the form

$$\tilde{\Sigma} = \text{diag}[\tilde{\sigma}_1, \tilde{\sigma}_2, \dots, \tilde{\sigma}_n] \in \mathbb{R}^{m \times n}, \quad \tilde{\sigma}_1 \geq \tilde{\sigma}_2 \geq \dots \geq \tilde{\sigma}_n \geq 0.$$

Then

$$\min_{\tilde{U}, \tilde{V}} \|A - \tilde{U}\tilde{\Sigma}\tilde{V}^*\| = \|\Sigma - \tilde{\Sigma}\| \quad (3)$$

for any unitarily invariant matrix norm  $\|\cdot\|$ , where the minimization is over all orthogonal matrices  $\tilde{U} \in \mathbb{R}^{m \times m}$  and  $\tilde{V} \in \mathbb{R}^{n \times n}$ .

**Proof.**

Let  $U$  and  $V$  be the orthogonal matrices in the SVD of  $A$ . Then

$$\min_{\tilde{U}, \tilde{V}} \|A - \tilde{U}\tilde{\Sigma}\tilde{V}^*\| \leq \|A - U\tilde{\Sigma}V^*\| = \|\Sigma - \tilde{\Sigma}\|.$$

The result follows from  $\|A - B\| \geq \|\Sigma(A) - \Sigma(B)\|$  (inequality in (2)). □

## The main result

*A closest matrix to  $A$  in the spectral or Frobenius norms with smallest singular value  $\sigma_k$  is given by*

$$\tilde{A} = U\tilde{\Sigma}V^*$$

where  $\tilde{\Sigma}$  has the entries

$$\begin{aligned}\tilde{\sigma}_j &= \sigma_j, & 1 \leq j \leq k, \\ \tilde{\sigma}_j &= \sigma_k, & k < j \leq \tilde{k}, \\ \tilde{\sigma}_j &= 0, & \tilde{k} < j \leq n,\end{aligned}$$

where  $\tilde{k}$  is determined by the inequalities  $\sigma_{\tilde{k}} \geq \sigma_k/2$  and  $\sigma_{\tilde{k}+1} < \sigma_k/2$ .

# Proof

- We first consider the matrix  $\tilde{\Sigma}$ .
  - If  $\sigma_k = 0$ , then  $\tilde{k} = n$  and  $\tilde{\Sigma} = \Sigma$ ;
  - if  $\sigma_k > 0$ , then a closest matrix  $\tilde{\Sigma}$  to  $\Sigma$  in the spectral or Frobenius norms with smallest singular value  $\sigma_k$  is obtained by modifying each singular value of  $\Sigma$  that is smaller than  $\sigma_k$  as little as possible to be either  $\sigma_k$  or zero. Thus, singular values of  $\Sigma$  that are larger than  $\sigma_k/2$  are set to  $\sigma_k$ , while singular values that are smaller than  $\sigma_k/2$  are set to zero. Singular values that are  $\sigma_k/2$  can be set to either  $\sigma_k$  or zero.
- For  $\tilde{A} = U\tilde{\Sigma}V^*$  one has the equal sign in  $\|A - \tilde{A}\| \geq \|\Sigma - \tilde{\Sigma}\|$  (inequality in (2)), i.e.  $\tilde{A}$  is a minimizer in the minimization problem (3).



## Replacing $A$ with $\tilde{A}$

$$\|A - \tilde{A}\|_2 \leq \frac{\sigma_k}{2}, \quad \|A - A_k\|_2 = \sigma_{k+1},$$

$$\|A - \tilde{A}\|_F \leq \frac{\sigma_k}{2} \sqrt{n-k}, \quad \|A - A_k\|_F = \sqrt{\sum_{i=k+1}^n \sigma_i^2}.$$

- $\|A - A_k\|_2 > \|A - \tilde{A}\|_2$ ,  $\|A - A_k\|_F > \|A - \tilde{A}\|_F$  when  $\sigma_{k+1} > \sigma_k/2$ . The singular values for linear discrete ill-posed problems typically decay slowly to zero for increasing values of  $k$ . Therefore, the latter inequality holds for many problems. Thus, for many discrete ill-posed problems  $\tilde{A}$  is a better approximation of  $A$  than  $A_k$ .
- Moreover,  $\kappa_2(\tilde{A}) = \kappa_2(A_k)$ . The propagated error in the approximation  $\tilde{x} = \tilde{A}^\dagger b$  of  $\hat{x} = A_k^\dagger b$  is not expected to be larger than the propagated error in the TSVD solution  $x_k$ .

## Numerical tests

- The regularization parameter  $k$  is determined by the discrepancy principle. Its application requires a bound  $\varepsilon$  for  $\|e\|_2$  to be known. To compute an approximation of  $\hat{x}$  we first choose the value of  $k$  as small as possible so that

$$\|Ax_k - b\|_2 \leq \varepsilon,$$

where  $x_k$  is defined by TSVD. Then we determine  $\tilde{x}$  with  $\tilde{A}$  given by modified TSVD.

- The examples are obtained by discretizing Fredholm integral equations of the first kind

$$\int_a^b \kappa(s, t)x(t) dt = g(s), \quad c \leq s \leq d,$$

with a smooth kernel  $\kappa$ . The discretizations are carried out by Galerkin or Nyström methods and yield linear discrete ill-posed problems.

## Numerical tests

- In the MATLAB package Regularization Tools by Hansen [Numer. Algorithms, 2007] discretizations  $A \in \mathbb{R}^{n \times n}$  of the integral operators and scaled discrete approximations  $\hat{x} \in \mathbb{R}^n$  of the solution  $x$  are determined.
- We add an error vector  $e \in \mathbb{R}^n$  with normally distributed random entries with zero mean to  $\hat{b} = A\hat{x}$  to obtain the vector  $b$ . The vector  $e$  is scaled to yield a specified noise level  $\|e\|/\|\hat{b}\|$ . In particular,  $\|e\|$  is available and we can apply the discrepancy principle with  $\varepsilon = \|e\|$  to determine the truncation index  $k$  in TSVD.
- We report in every example the average of the relative errors in the computed solution determined by the TSVD and the modified TSVD methods over 1000 runs for each noise level. We let  $n = 200$  in all examples.

## phillips test problem

Fredholm integral equation of the first kind with  $a = c = -6$ ,  $b = d = 6$ ,

$$\phi(t) = \begin{cases} 1 + \cos\left(\frac{\pi t}{3}\right), & |t| < 3, \\ 0, & |t| \geq 3, \end{cases}$$

with kernel, right-hand side function, and solution given by

$$\kappa(s, t) = \phi(s - t), \quad x(t) = \phi(t),$$

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

Noise level	TSVD	$k_{\text{avg}}$	modified TSVD	$\tilde{k}_{\text{avg}}$
10.0%	$7.857 \cdot 10^{-2}$	$6.201 \cdot 10^0$	$7.582 \cdot 10^{-2}$	$6.634 \cdot 10^0$
5.0%	$3.717 \cdot 10^{-2}$	$6.944 \cdot 10^0$	$3.695 \cdot 10^{-2}$	$6.975 \cdot 10^0$
1.0%	$2.585 \cdot 10^{-2}$	$7.046 \cdot 10^0$	$2.620 \cdot 10^{-2}$	$7.082 \cdot 10^0$
0.1%	$1.214 \cdot 10^{-2}$	$9.805 \cdot 10^0$	$1.025 \cdot 10^{-2}$	$1.100 \cdot 10^1$

Table: Average relative errors and average truncation indices.

## *ilaplace* test problem

Fredholm integral equation of the first kind with

$$\kappa(s, t) = \exp(-st), \quad x(t) = \exp(-t/2), \quad g(s) = \frac{2}{2s + 1},$$

and  $a = c = 0$ ,  $b = d = \infty$ .

Noise level	TSVD	$k_{\text{avg}}$	modified TSVD	$\tilde{k}_{\text{avg}}$
10.0%	$2.455 \cdot 10^{-1}$	$4.498 \cdot 10^0$	$2.404 \cdot 10^{-1}$	$4.950 \cdot 10^0$
5.0%	$2.222 \cdot 10^{-1}$	$5.317 \cdot 10^0$	$2.215 \cdot 10^{-1}$	$5.373 \cdot 10^0$
1.0%	$1.881 \cdot 10^{-1}$	$6.830 \cdot 10^0$	$1.881 \cdot 10^{-1}$	$6.830 \cdot 10^0$
0.1%	$1.545 \cdot 10^{-1}$	$9.237 \cdot 10^0$	$1.545 \cdot 10^{-1}$	$9.237 \cdot 10^0$

**Table:** Average relative errors and average truncation indices.



## deriv2 test problem

Fredholm integral equation of the first kind with  $a = c = 0$ ,  $b = d = 1$ , with kernel, solution, and right-hand side given by

$$\kappa(s, t) = \begin{cases} s(t-1), & s < t, \\ t(s-1), & s \geq t, \end{cases}$$

$$x(t) = t,$$

$$g(s) = \frac{s^3 - s}{6}.$$

Noise level	TSVD	$k_{\text{avg}}$	modified TSVD	$\tilde{k}_{\text{avg}}$
10.0%	$3.959 \cdot 10^{-1}$	$4.222 \cdot 10^0$	$3.912 \cdot 10^{-1}$	$5.558 \cdot 10^0$
5.0%	$3.526 \cdot 10^{-1}$	$5.270 \cdot 10^0$	$3.448 \cdot 10^{-1}$	$7.045 \cdot 10^0$
1.0%	$2.680 \cdot 10^{-1}$	$8.841 \cdot 10^0$	$2.544 \cdot 10^{-1}$	$1.198 \cdot 10^1$
0.1%	$1.832 \cdot 10^{-1}$	$1.865 \cdot 10^1$	$1.696 \cdot 10^{-1}$	$2.571 \cdot 10^1$

Table: Average relative errors and average truncation indices.