

A Model Selection Criterion for Solution of Discrete Ill-Posed Problems Based on the Singular Value Decomposition

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Abstract. *This paper proposes a criterion for selection of the optimal number of components of the singular value decomposition based on an approximation of the reconstruction error of vector data using the estimate of the true signal.*

Keywords

Discrete ill-posed problems, regularization, singular value decomposition.

1 Introduction

Solving ill-posed problems [1, 2] is important for many areas of science and technology. The discrete ill-posed problems [2] emerge, for example, under discretization of integral equations in the areas of spectroscopy, gravimetry, magnetometry and others. There are some approaches to solving discrete ill-posed problems. Some use a randomized approach [3 - 6] based on random projections (that are usually used for other applications, see [7, 8] and refs therein).

One of the methods for solving inverse problems is a solution based on the truncated singular value decomposition [9]. That is, the solution does not use all the components of singular value decomposition (SVD). So it is important to find the optimal number of SVD components when the solution of a discrete ill-posed problem demonstrates stability and maximum accuracy.

In this paper we propose a criterion for selection of the optimal number of components of the singular value decomposition based on an approximation of the reconstruction error of vector data using the estimate of the true signal. We also conduct an experimental study of the accuracy of solutions of discrete ill-posed problems with the use of the proposed criterion.

2 The solution of the inverse problem based on singular value decomposition

Many applications of mathematics, physics, data analysis, etc. require finding an approximate solution of a system of linear equations:

$$\mathbf{Ax} \approx \mathbf{y}, \quad (1)$$

where the matrix $\mathbf{A} \in \mathfrak{R}^{N \times N}$ and the vector $\mathbf{y} = \mathbf{y}_0 + \boldsymbol{\varepsilon}$ distorted by additive noise $\boldsymbol{\varepsilon} \in \mathfrak{R}^N$ are known and it is required to estimate the signal vector $\mathbf{x} \in \mathfrak{R}^N$. The problem of estimating the vector \mathbf{x} by a known vector \mathbf{y} and matrix \mathbf{A} is called an inverse problem. In the case when the matrix \mathbf{A} is very ill-conditioned, SVD is used to obtain a stable evaluation \mathbf{x}' . The solution based on SVD is obtained as follows:

$$\mathbf{x}' = \mathbf{A}_k^+ \mathbf{y}, \mathbf{A}_k^+ = \mathbf{VS}^{-1}\mathbf{U}^T. \quad (2)$$

Here $\mathbf{A}_k = \mathbf{U}\mathbf{S}\mathbf{V}^T$ is the approximation of the matrix \mathbf{A} obtained by k ($k < N$) components of SVD, $\mathbf{U} = (\mathbf{u}_1, \dots, \mathbf{u}_k)$ is the matrix of left singular vectors with orthonormal columns, $\mathbf{V} = (\mathbf{v}_1, \dots, \mathbf{v}_k)$ is the matrix of right singular vectors with orthonormal columns, $\mathbf{S} = \text{diag}(\sigma_1, \dots, \sigma_k)$ is the matrix of singular values, \mathbf{A}^+ is a generalized inverse (pseudoinverse) of the matrix \mathbf{A} . In the case when \mathbf{y} contains noise, the singular values σ_i of matrix \mathbf{A} decay gradually to zero, \mathbf{A} has a large condition number, the problem of estimating \mathbf{x} is called discrete ill-posed problem [2]. Direct truncating of SVD does not work for discrete ill-posed problems since there are no gap in singular values and numerical rank of the matrix is not specified. So finding the number of SVD components corresponding to the optimal solution of discrete ill-posed problem is urgent.

3 The error of true signal and output vector recovery for discrete ill-posed problems solution based on singular value decomposition

The accuracy of the inverse problem solution will be evaluated using the error e_x of the true signal \mathbf{x} recovery. The error is calculated as $e_x = \|\mathbf{x} - \mathbf{x}'_k\| = \|\mathbf{e}_x\|$, where \mathbf{x}'_k is the vector of recovered signal, \mathbf{e}_x is the vector of signal \mathbf{x} recovery error using k components of SVD. Let us write the expression for the error vector \mathbf{e}_x in such a way that the noise vector is explicit:

$$\mathbf{e}_x = \mathbf{A}_k^+(\mathbf{y}_0 + \boldsymbol{\varepsilon}) - \mathbf{x} = \mathbf{A}_k^+\mathbf{y}_0 + \mathbf{A}_k^+\boldsymbol{\varepsilon} - \mathbf{x} = \mathbf{A}_k^+\mathbf{A}_k\mathbf{x} - \mathbf{x} + \mathbf{A}_k^+\boldsymbol{\varepsilon}. \quad (3)$$

Using (3), we write the expression for the true signal recovery error and average it over noise realizations:

$$e_x = \|\mathbf{A}_k^+\mathbf{A}_k\mathbf{x} - \mathbf{x} + \mathbf{A}_k^+\boldsymbol{\varepsilon}\|^2 = \|(\mathbf{A}_k^+\mathbf{A}_k - \mathbf{I})\mathbf{x}\|^2 + \|\mathbf{A}_k^+\boldsymbol{\varepsilon}\|^2 - 2\langle(\mathbf{A}_k^+\mathbf{A}_k - \mathbf{I})\mathbf{x}, \mathbf{A}_k^+\boldsymbol{\varepsilon}\rangle. \quad (4)$$

$$E\{e_x\} = \|(\mathbf{A}_k^+\mathbf{A}_k - \mathbf{I})\mathbf{x}\|^2 + E\|\mathbf{A}_k^+\boldsymbol{\varepsilon}\|^2 - 2E\langle(\mathbf{A}_k^+\mathbf{A}_k - \mathbf{I})\mathbf{x}, \mathbf{A}_k^+\boldsymbol{\varepsilon}\rangle. \quad (5)$$

Given that $E\langle(\mathbf{A}_k^+\mathbf{A}_k - \mathbf{I})\mathbf{x}, \mathbf{A}_k^+\boldsymbol{\varepsilon}\rangle = 0$ and $E\|\mathbf{A}_k^+\boldsymbol{\varepsilon}\|^2 = E(\boldsymbol{\varepsilon}^T \mathbf{A}_k^{+T} \mathbf{A}_k^+ \boldsymbol{\varepsilon}) = \sigma^2 \text{trace}(\mathbf{A}_k^{+T} \mathbf{A}_k^+)$ we get an expression for the mean square error of the true signal recovery:

$$E\{e_x\} = \|(\mathbf{A}_k^+\mathbf{A}_k - \mathbf{I})\mathbf{x}\|^2 + \sigma^2 \text{trace}(\mathbf{A}_k^{+T} \mathbf{A}_k^+). \quad (6)$$

Let us denote the error components as

$$e_{x1} = \|(\mathbf{A}_k^+\mathbf{A}_k - \mathbf{I})\mathbf{x}\|^2, e_{x2} = \sigma^2 \text{trace}(\mathbf{A}_k^{+T} \mathbf{A}_k^+). \quad (7)$$

where e_{x1} is the deterministic component of the error, and e_{x2} is the stochastic one.

Let us estimate the accuracy of the output vector recovery as follows: $e_y = \|\mathbf{y}_0 - \mathbf{y}'_k\| = \|\mathbf{e}_y\|$, where $\mathbf{y}'_k = \mathbf{A}_k \mathbf{A}_k^+ \mathbf{y}$ is the recovered output vector, \mathbf{e}_y is the error vector of output recovery. The expressions for the error vector \mathbf{e}_y and error of output recovery can be written as

$$\mathbf{e}_y = \mathbf{A}_k \mathbf{A}_k^+(\mathbf{y}_0 + \boldsymbol{\varepsilon}) - \mathbf{y}_0 = \mathbf{A}_k \mathbf{A}_k^+ \mathbf{y}_0 - \mathbf{y}_0 + \mathbf{A}_k \mathbf{A}_k^+ \boldsymbol{\varepsilon}, \quad (8)$$

$$e_y = \|\mathbf{A}_k \mathbf{A}_k^+ \mathbf{y}_0 - \mathbf{y}_0 + \mathbf{A}_k \mathbf{A}_k^+ \boldsymbol{\varepsilon}\|^2 = \|\mathbf{A}_k \mathbf{A}_k^+ \mathbf{y}_0 - \mathbf{y}_0\|^2 + \|\mathbf{A}_k \mathbf{A}_k^+ \boldsymbol{\varepsilon}\|^2 - 2\langle\mathbf{A}_k \mathbf{A}_k^+ \mathbf{y}_0 - \mathbf{y}_0, \mathbf{A}_k \mathbf{A}_k^+ \boldsymbol{\varepsilon}\rangle. \quad (9)$$

We average the error of output recovery over noise realizations:

$$E\{e_y\} = \|\mathbf{A}_k \mathbf{A}_k^+ \mathbf{y}_0 - \mathbf{y}_0\|^2 + E\|\mathbf{A}_k \mathbf{A}_k^+ \boldsymbol{\varepsilon}\|^2 - 2E\langle\mathbf{A}_k \mathbf{A}_k^+ \mathbf{y}_0 - \mathbf{y}_0, \mathbf{A}_k \mathbf{A}_k^+ \boldsymbol{\varepsilon}\rangle. \quad (10)$$

As $2E\langle\mathbf{A}_k \mathbf{A}_k^+ \mathbf{y}_0 - \mathbf{y}_0, \mathbf{A}_k \mathbf{A}_k^+ \boldsymbol{\varepsilon}\rangle = 0$ and $E\|\mathbf{A}_k \mathbf{A}_k^+ \boldsymbol{\varepsilon}\|^2 = E(\boldsymbol{\varepsilon}^T \mathbf{A}_k^{+T} \mathbf{A}_k^T \mathbf{A}_k \mathbf{A}_k^+ \boldsymbol{\varepsilon}) = \sigma^2 \text{trace}(\mathbf{A}_k^{+T} \mathbf{A}_k^T \mathbf{A}_k \mathbf{A}_k^+)$, mean squared error of the output recovery is.

$$E\{e_y\} = \left\| (\mathbf{A}_k \mathbf{A}_k^+ - \mathbf{I}) \mathbf{y}_0 \right\|^2 + \sigma^2 \text{trace} (\mathbf{A}_k^{+T} \mathbf{A}_k^T \mathbf{A}_k \mathbf{A}_k^T). \quad (11)$$

Components of the output recovery error are:

$$e_{y1} = \left\| (\mathbf{A}_k \mathbf{A}_k^+ - \mathbf{I}) \mathbf{y}_0 \right\|^2, \quad e_{y2} = \sigma^2 \text{trace} (\mathbf{A}_k^{+T} \mathbf{A}_k^T \mathbf{A}_k \mathbf{A}_k^T), \quad (12)$$

where e_{y1} is the deterministic component of the error, and e_{y2} is the stochastic one.

One approach to solving inverse problems is the approach of model selection. Methods of model selection use different criteria for the selection [10]. Model selection criteria (MSC) are formulated so that they reduce the number of model component for increasing levels of noise. MSC include two components. One of the components is associated with the accuracy of data approximation by the model. The value of this component decreases with increasing the number of components of the model. Another component is associated with noise, it is growing .with the number of model components. Such a construction of criteria achieves their minimum for models that are close to optimal, by a balance between the complexity of the model and the accuracy of approximation. In the case of solutions of discrete ill-posed inverse problems based on SVD, model complexity is the number of SVD components in equation (3). Many existing MSC are based on an approximation of the different types of errors, e.g., Cp of Mallows uses predictive training error [11], whereas AIC of Akaike uses generalization error [12].

In order to develop MSC for solution of discrete ill-posed problem, we studied [13] the behavior of error components (7) and (12) depending on the number of SVD components in the model.

On the basis of the recursive representation of pseudoinverse matrix $\mathbf{A}_k^+ = \mathbf{A}_{k-1}^+ + \mathbf{v}_k \sigma_k^{-1} \mathbf{u}_k^T$, the following expressions for the components of true signal recovery error are obtained. For the deterministic component of the error:

$$e_{x1} = \mathbf{x}^T \mathbf{x} - \mathbf{x}^T \mathbf{Z}_k \mathbf{x} = \mathbf{x}^T \mathbf{x} - \mathbf{x}^T \mathbf{V}_k \mathbf{V}_k^T \mathbf{x} = \mathbf{x}^T \mathbf{x} - \sum_{i=1}^k \mathbf{x}^T \mathbf{v}_i \mathbf{v}_i^T \mathbf{x}. \quad (13)$$

Due to the fact that $\mathbf{x}^T \mathbf{x}$ is constant and $\sum_{i=1}^k \mathbf{x}^T \mathbf{v}_i \mathbf{v}_i^T \mathbf{x}$ increases, the value of the deterministic component of the error e_{x1} decreases with increasing k . The recursive expression for the stochastic component of the error is as follows:

$$e_{x2} = \sigma^2 \text{trace} (\mathbf{A}_{k-1}^{+T} \mathbf{A}_{k-1}^+) + \sigma^2 s_k^{-2} \text{trace} (\mathbf{u}_k \mathbf{u}_k^T). \quad (14)$$

The elements of the diagonal matrix $\mathbf{u}_k \mathbf{u}_k^T$ formed by products $u_i u_i$ are non-negative, so from expression (14) the value of the stochastic component of the error e_{x2} increases with increasing k . For the components of the error of output vector recovery the following expressions were obtained. The expression for the deterministic component of the error:

$$e_{y1} = \mathbf{y}_0^T \mathbf{y}_0 - \mathbf{y}_0^T \mathbf{U}_k \mathbf{U}_k^T \mathbf{y}_0. \quad (15)$$

$\mathbf{U}_k^T \mathbf{y}_0 = [\mathbf{u}_1^T \mathbf{y}_0, \dots, \mathbf{u}_k^T \mathbf{y}_0]$ is a vector with dimensionality increasing with k , so the value of the scalar product $\mathbf{y}_0^T \mathbf{U}_k \mathbf{U}_k^T \mathbf{y}_0$ also increases with increasing k . By virtue of the fact that $\mathbf{y}_0^T \mathbf{y}_0$ is constant and $\mathbf{y}_0^T \mathbf{U}_k \mathbf{U}_k^T \mathbf{y}_0$ increases, the value e_{y1} decreases with increasing k . Given the fact that $\text{trace} (\mathbf{v}_k \mathbf{v}_k^T) = 1$, the expression for the stochastic component of the output vector recovery error is as follows:

$$e_{y2} = \sigma^2 \text{trace} (\mathbf{A}_k^T \mathbf{A}_k \mathbf{A}_k^+ \mathbf{A}_k^{+T}) = \sigma^2 \text{trace} (\mathbf{A}_{k-1}^T \mathbf{A}_{k-1} \mathbf{A}_{k-1}^+ \mathbf{A}_{k-1}^{+T}) + \sigma^2 \text{trace} (\mathbf{v}_k \mathbf{v}_k^T) = \sigma^2 k. \quad (16)$$

The last expression shows that e_{y2} increases with increasing k .

4 The approach to determining the optimal number of SVD components

By the optimal number of SVD components we mean the number k , for which the true signal recovery error is minimized. As in practice it is impossible to calculate the true signal recovery error because of the lack of data about the true signal, we propose to determine the optimal k by using output vector recovery error $\left\| \mathbf{y}' - \mathbf{y}_0 \right\|$.

The expression for the mean square error of output recovery is as follows:

$$e_y = \left\| (\mathbf{A}_k \mathbf{A}_k^+ - \mathbf{I}) \mathbf{y}_0 \right\|^2 + \sigma^2 \text{trace} \left((\mathbf{A}_k \mathbf{A}_k^+)^T \mathbf{A}_k \mathbf{A}_k^+ \right). \quad (17)$$

It is impossible to determine the minimum error directly using the expression (17) due to the presence of the vector \mathbf{y}_0 which is unknown in the wild. Let us replace the unknown vector \mathbf{y}_0 in (17) by a known vector $\mathbf{y} = \mathbf{y}_0 + \boldsymbol{\varepsilon}$ (resulting, for example, from measurements) and average over realizations of the noise:

$$e'_y = \left\| (\mathbf{A}_k \mathbf{A}_k^+ - \mathbf{I}) (\mathbf{y}_0 + \boldsymbol{\varepsilon}) \right\|^2 + \sigma^2 \text{trace} \left((\mathbf{A}_k \mathbf{A}_k^+)^T \mathbf{A}_k \mathbf{A}_k^+ \right), \quad (18)$$

$$\begin{aligned} E\{e'_y\} = & \left\| (\mathbf{A}_k \mathbf{A}_k^+ - \mathbf{I}) \mathbf{y}_0 \right\|^2 + E \left\| (\mathbf{A}_k \mathbf{A}_k^+ - \mathbf{I}) \boldsymbol{\varepsilon} \right\|^2 + 2E \left\langle (\mathbf{A}_k \mathbf{A}_k^+ - \mathbf{I}) \mathbf{y}_0, (\mathbf{A}_k \mathbf{A}_k^+ - \mathbf{I}) \boldsymbol{\varepsilon} \right\rangle + \\ & + \sigma^2 \text{trace} \left((\mathbf{A}_k \mathbf{A}_k^+)^T \mathbf{A}_k \mathbf{A}_k^+ \right). \end{aligned} \quad (19)$$

Given that $2E \left\langle (\mathbf{A}_k \mathbf{A}_k^+ - \mathbf{I}) \mathbf{y}_0, (\mathbf{A}_k \mathbf{A}_k^+ - \mathbf{I}) \boldsymbol{\varepsilon} \right\rangle = 0$ and $E \left\| (\mathbf{A}_k \mathbf{A}_k^+ - \mathbf{I}) \boldsymbol{\varepsilon} \right\|^2 = \sigma^2 \text{trace} \left((\mathbf{A}_k \mathbf{A}_k^+ - \mathbf{I})^T (\mathbf{A}_k \mathbf{A}_k^+ - \mathbf{I}) \right)$, expression () takes the following form:

$$E\{e'_y\} = \left\| (\mathbf{A}_k \mathbf{A}_k^+ - \mathbf{I}) \mathbf{y}_0 \right\|^2 + \sigma^2 \text{trace} \left((\mathbf{A}_k \mathbf{A}_k^+ - \mathbf{I})^T (\mathbf{A}_k \mathbf{A}_k^+ - \mathbf{I}) \right) + \sigma^2 \text{trace} \left((\mathbf{A}_k \mathbf{A}_k^+)^T \mathbf{A}_k \mathbf{A}_k^+ \right). \quad (20)$$

Comparing expression for $E\{e'_y\}$ and the expression for the mean square error of output recovery (), we see that they differ by one term: $\sigma^2 \text{trace} \left((\mathbf{A}_k \mathbf{A}_k^+ - \mathbf{I})^T (\mathbf{A}_k \mathbf{A}_k^+ - \mathbf{I}) \right)$. This allows us to adjust the contribution of noise in the deterministic component of the error estimation based on the noisy output $\left\| (\mathbf{A}_k \mathbf{A}_k^+ - \mathbf{I}) \mathbf{y} \right\|^2$ by subtracting from it $\sigma^2 \text{trace} \left((\mathbf{A}_k \mathbf{A}_k^+ - \mathbf{I})^T (\mathbf{A}_k \mathbf{A}_k^+ - \mathbf{I}) \right)$ and obtain the approximation of the expression (17) that does not contain an unknown vector \mathbf{y}_0 :

$$CR = \left\| (\mathbf{A}_k \mathbf{A}_k^+ - \mathbf{I}) \mathbf{y} \right\|^2 - \sigma^2 \text{trace} \left((\mathbf{A}_k \mathbf{A}_k^+ - \mathbf{I})^T (\mathbf{A}_k \mathbf{A}_k^+ - \mathbf{I}) \right) + \sigma^2 \text{trace} \left((\mathbf{A}_k \mathbf{A}_k^+)^T \mathbf{A}_k \mathbf{A}_k^+ \right). \quad (21)$$

We have obtained expression approximating output error recovery. Instead of the unknown vector \mathbf{y}_0 the expression (21) contains the known vector $\mathbf{y} = \mathbf{y}_0 + \boldsymbol{\varepsilon}$, so it can be used to determine the optimal number of SVD components.

5 Experimental investigation

To study the performance of the proposed MSC we calculated sample means and standard deviation of solution error for determining the optimal number of SVD components using the proposed criterion CR and MSC Cp of Mallows [11], AIC of Akaike [12], minimum description length MDL [14]. An experimental study was carried out for discrete ill-posed problems of Carasso, Phillips, Delves [15]. Table. 1 shows the results of discrete ill-posed problems solutions based on SVD, where the dimension of the matrix was 40×40. The results show that for the proposed CR the error is less than that obtained for other MSC, and the dimension k is closer to the one obtained by e.

Table 1. The average value of the solution error and its standard deviation error, mean and standard deviation of the obtained dimension k for the matrix 40×40.

Задача	M(e)	ско	M(k)	ско	M(e)	ско	M(k)	ско	M(e)	ско	M(k)	ско
Phillips	nl=1E-3				nl=1E-4				nl=1E-5			
e	9.24e-2	2.67e-2	15.5	2.05	1.11e-2	3.37e-3	23.40	2.15	6.38e-4	1.87e-4	32.38	1.31
CR	1.07e-1	3.09e-2	14.4	2.70	1.31e-2	4.74e-3	22.44	2.72	7.66e-4	2.97e-4	31.86	1.80
Cp	1.84e-1	4.69e-2	9.88	0.52	2.38e-2	5.84e-3	17.16	0.55	2.15e-3	3.36e-4	24.96	0.28
AIC	1.33e-1	1.54e-2	11.2	0.77	1.73e-2	2.19e-3	18.30	0.95	2.04e-3	1.24e-4	25.12	0.33
MDL	1.51e-1	2.61e-2	10.4	0.54	7.73e-2	4.67e-2	13.58	3.21	1.54e-2	9.52e-6	18.0	0.0

Carroso	nl=1E-3				nl=1E-4				nl=1E-5			
e	8.37e-4	3.11e-4	11.6	0.49	3.06e-4	3.17e-5	15.7	2.07	2.15e-4	6.22e-6	21.8	1.71
CR	9.89e-4	4.61e-4	11.3	1.04	3.32e-4	5.39e-5	14.04	2.24	2.22e-4	1.21e-5	22.9	2.78
Cp	4.49e-3	1.57e-3	7.52	0.89	3.36e-4	1.39e-5	12.00	0.0	2.32e-4	2.76e-6	17.0	0.0
AIC	1.36e-3	3.46e-4	10.2	1.04	3.50e-4	4.83e-5	12.34	1.14	2.29e-4	6.72e-6	18.1	1.81
MDL	4.41e-3	1.63e-3	7.56	0.91	3.61e-4	1.01e-4	11.94	0.24	3.28e-4	1.27e-6	12.0	0.0
Delves	nl=1E-4				nl=1E-5				nl=1E-6			
e	2.83e-2	3.62e-3	7.96	1.40	1.23e-2	1.30e-3	16.74	2.03	2.87e-3	6.74e-4	36.44	2.67
CR	3.21e-2	5.80e-3	7.22	1.63	1.36e-2	2.28e-3	16.52	2.89	3.29e-3	7.99e-4	34.62	3.83
Cp	4.60e-2	4.33e-3	3.92	0.39	2.17e-2	1.51e-3	8.54	0.65	9.62e-3	7.09e-4	17.20	0.97
AIC	4.16e-2	1.90e-2	6.60	1.57	1.54e-2	1.73e-3	13.06	1.72	7.89e-3	8.47e-4	19.88	1.47
MDL	4.12e-2	3.98e-3	4.52	0.58	2.20e-2	2.08e-3	8.44	0.81	1.81e-2	7.06e-4	10.06	0.37

6 Conclusion

The proposed approximation of the data vector recovery error is close to the true error values. For this reason, the proposed criterion CR for choosing the optimal number of SVD components based on the error approximation can be used in practice. Experimental study of the accuracy of solutions of discrete ill-posed problems with the use of the proposed criterion confirms its quality. Compared to solutions based on such criteria as Cp, AIC, MDL the solutions based on CR demonstrate the highest accuracy

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