*Journal of Mathematical Chemistry Vol. 29, No. 2, 2001*

# Numerical comparison between Tikhonov regularization and singular value decomposition methods using the $L$ curve criterion

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Received 16 June 2000

Many problems in chemistry, physics and engineering requires the inversion of a Fredholm integral equation of first order. To find the solution of this problem one has to deal with ill-posed problem and special techniques have to be used. In this paper two of the most common methods, the Tikhonov regularization and the singular value decomposition, are compared when finding the solution of a model integral equation. The regularization parameter in the Tikhonov regularization and the dimension of the subspaces in the singular value decomposition were chosen using the $L$ curve criterion. The analytical solution of the model integral equation was taken as a reference to analyze the results. The advantages of each method, with the presence of errors in the data, is presented and it is argumented the superiority of the singular value decomposition when dealing with this kind of problem.

**KEY WORDS:** singular value decomposition, Tikhonov regularization, $L$ curve

## 1. Introduction

The Fredholm integral equation of first order [1],

$$\int_a^b K(x, y) f(y)\,\mathrm{d}y = g(x), \quad c \leqslant x \leqslant d, \tag{1}$$

with $K$, $f$ and $g$ functions of $x$ and $y$ can represent a large variety of problems in science. A short list of the occurrence of this equation can be given in the areas of geophysics [2], electromagnetism in soils [3], thermodynamics [4], inverse scattering [5], etc. References [6,7] give a much more complete list of examples. Equation (1) can be interpreted as $f(y)$ being an input, $K(x, y)$ being an apparatus, and $g(x)$ an output. For a given $K(x, y)$ and $f(y)$ calculation of $g(x)$ is a simple problem. On the other hand, calculation of $f(y)$ from $K(x, y)$ and $g(x)$ is a much more elaborate problem to be solved, representing a class of problem known as an ill-posed problems. Since equation (1) is linear in the unknown this ill-posed problem is also known as a linear inverse problem.



0259-9791/01/0200-0151$19.50/0 

In what follows it will be assumed that a representation of (1), in the form $\mathbf{Kf} = \mathbf{g}$, has been found with $\mathbf{f} \in \mathbb{R}^n$, $\mathbf{g} \in \mathbb{R}^m$, and $\mathbf{K} \in \mathbb{R}^{m\times n}$.

In 1932 Hadamard [8] defined a problem as ill-posed whenever one of three conditions: (a) for every $\mathbf{f} \in \mathbb{R}^n$ there *exists* a $\mathbf{g} \in \mathbb{R}^m$ such that $\mathbf{Kf} = \mathbf{g}$, (b) the solution of the problem, $\mathbf{f}$, is *unique* in $\mathbb{R}^n$, and (c) the dependence of $\mathbf{f}$ on $\mathbf{g}$ is *continuous*, is not satisfied. It is clear, therefore, that the nature of an ill-posed problem depends not only on the transformation under consideration but also on the structure of the subspaces $\mathbb{R}^n$ and $\mathbb{R}^m$. Finding the solution of the Fredholm integral equation of first order is an ill-posed problem. As will be seen, the condition number of $\mathbf{K}$ is very large. Therefore any small changes in $\mathbf{g}$, such as those from the experimental work, or even the ones when finding the appropriate representation, will be largely amplified by the $\mathbf{K}^{-1}$. A more intuitive way to see the ill-posed nature of (1), using $f(y) = \cos(ny)$, can be seen in [1].

Among the several methods used to find the solution of an ill-posed problem the Tikhonov regularization [9,10] and the singular value decomposition (SVD) [11] are the most often used. In the present work the efficiency of these two numerical methods will be tested against an analytical solvable Fredholm integral equation of first order [12,13]. In both of these methods there will appear a parameter to be choosen, called the regularization parameter, as will be discussed later. The $L$ curve criterion, used by the first time in [14], will be the criterion to be used here to decided which regularization parameter has to be taken. Although this is the criterion that is most widespread, other methods are available [1]. The $L$ curve approach has been used very often in the literature, for example, in [3–5]. A critical analysis of the Tikhonov regularization and the singular value decomposition method, using the $L$ curve analysis, is the main objective of this paper.

## 2. The Tikhonov regularization

The problem to find the solution for the inverse linear ill-posed problem, represented by the Fredholm integral equation of first order, will be discussed here in two aspects: (i) one by removing the singularity, and (ii) by finding appropriate subspaces in $\mathbb{R}^n$ and $\mathbb{R}^m$ such that the inverse operator can be computed.

In the Tikhonov regularization [9,10] the problem to be solved is

$$\min_{\mathbf{f}} \|\mathbf{Kf} - \mathbf{g}\|_2^2 \tag{2}$$

subject to the restriction

$$\|L\mathbf{f}\|_2^2 \leqslant \delta^2, \tag{3}$$

where $\delta$ is a small positive number. The operator $L$ is generally given by

$$L\mathbf{f} = a_0 \left\| \mathbf{f} - \widehat{\mathbf{f}} \right\|_2^2 + a_1 \left\| \frac{\mathrm{d}\mathbf{f}}{\mathrm{d}\mathbf{x}} \right\|_2^2 + a_2 \left\| \frac{\mathrm{d}^2\mathbf{f}}{\mathrm{d}\mathbf{x}^2} \right\|_2^2 \tag{4}$$

with $a_0$, $a_1$, $a_2$ assuming values equal to 1 or 0, depending on the condition to be impossed. The function $\widehat{\mathbf{f}}$ is an initial guess for the solution itself

The solution of (2) with the restriction (3) can be transformed into a problem to find the minimum of the functional

$$\Phi(\mathbf{f}) = \|\mathbf{K}\mathbf{f} - \mathbf{g}\|_2^2 + \lambda\|L\mathbf{f}\|_2^2, \tag{5}$$

where $\lambda$ is a parameter to be determined, called the regularization parameter. This will give the solution [15]

$$\big(\mathbf{K}^{\mathrm{T}}\mathbf{K} + \lambda(a_0\mathbf{I} + a_1\mathbf{H}_1 + a_2\mathbf{H}_2)\big)\mathbf{f} = \mathbf{K}^{\mathrm{T}}\mathbf{g} + \lambda\widehat{\mathbf{f}} \tag{6}$$

with $\mathbf{I}$ being the identity matrix,

$$\mathbf{H}_1 = \begin{pmatrix} 1 & -1 & & & \\ -1 & 2 & -1 & & \\ & \ddots & \ddots & \ddots & \\ & & -1 & 2 & -1 \\ & & & -1 & 1 \end{pmatrix} \tag{7}$$

and

$$\mathbf{H}_2 = \begin{pmatrix} 1 & -2 & 1 & & & & \\ -2 & 5 & -4 & 1 & & & \\ 1 & -4 & 6 & -4 & 1 & & \\ & \ddots & \ddots & \ddots & \ddots & \ddots & \\ & & 1 & -4 & 6 & -4 & 1 \\ & & & 1 & -4 & 5 & -2 \\ & & & & 1 & -2 & 1 \end{pmatrix}. \tag{8}$$

The solution (6), therefore, satisfies the restrictions (2) and (3). Clearly, the problem is not completely solved since the regularization parameter has not been found. This parameter should properly balance the two contributions, a minimum residual norm, $\Omega = \|\mathbf{K}\mathbf{f} - \mathbf{g}\|_2$, and minimum solution norm, $\rho = \|\mathbf{f}\|_2$. The right balance between these quantities forms the basic idea for the $L$-curve method.

## 3. The singular value decomposition

The singular value decomposition of $\mathbf{K}$ is a decomposition of the form [11]

$$\mathbf{K} = \mathbf{U}\boldsymbol{\Sigma}\mathbf{V}^{\mathrm{T}}, \tag{9}$$

where $\mathbf{U} \in \mathbb{R}^{m\times m}$, $\boldsymbol{\Sigma} \in \mathbb{R}^{m\times n}$ and $\mathbf{V} \in \mathbb{R}^{n\times n}$. The matrices $\mathbf{U}$ and $\mathbf{V}$ are orthogonal matrices whereas $\boldsymbol{\Sigma}$ is a diagonal matrix whose positive elements, $\sigma_i$, appear in a decreasing order in the diagonal. The elements $\sigma_1, \sigma_2, \ldots, \sigma_n$ are unique; however, the matrices $\mathbf{U}$ and $\mathbf{V}$ are not.

Applying the singular value decomposition to $\mathbf{Kf} = \mathbf{g}$ one obtains [16]

$$\mathbf{f} = \sum_{j=1}^{n} \frac{\mathbf{u}_j^{\mathrm{T}}\mathbf{g}}{\sigma_j}\mathbf{v}_j, \tag{10}$$

where the index $j$ refers to the column of the matrix. The above solution, using SVD method has two important features [17]: (a) it minimizes $\|\Omega\|_2^2 = \|\mathbf{Kf} - \mathbf{g}\|_2^2$, and (b) the singular value decomposition solution is the solution with minimum norm. Here also the problem is not completely solved, since, in the presence of errors in $\mathbf{g}$, a point to stop the series (10) has to be choosen. This cutoff point, say $k$, is analogous to the regularization parameter in the Tikhonov regularization. The way it is going to be found will be also using the $L$ curve analysis.

## 4. The model Fredholm integral equation

The numerical comparison between the Tikhonov regularization and the singular value decomposition will be analyzed using a Fredholm integral equation in the form [12]

$$\int_a^b \left(\frac{1}{x+y}\right)\frac{1}{y}\,\mathrm{d}y = \frac{1}{x}\ln\left(\frac{1+x/a}{1+x/b}\right) \tag{11}$$

with $1 \leqslant x \leqslant 5, a = 1$ and $b = 5$. The exact answer for this inverse problem, i.e., $f(y) = 1/y$ will be used to test the two above mentioned methods. Other models for the Fredholm integral of first kind could be used, such as an integral for the representation of the second virial coefficient [4], but the one above provide a simple example of this kind of integral. Also it will avoid thermodynamics, geophysics, or other definitions, being a model easy to handle. The integral (11) has also been used to implement the Tikhonov regularization [12] but no critical analysis of the regularization parameter was discussed, being determined by a trial and error procedure.

The integral (11) was represented in a rectangular basis with $N$ being the number of discretized points. With $N = 32$ one obtains $\|\mathbf{Kf} - \mathbf{g}\|_2^2 = 1.985 \cdot 10^{-6}$, $\mathrm{rank}(\mathbf{K}) = 10$ and $\mathrm{cond}(\mathbf{K}) = 8.92 \cdot 10^{11}$, which make clear the ill-posed nature of the problem. Although with $N = 32$ there is a small error in the representation of the integral, an exact value of $\mathbf{g}$ was generated from the computed values of $\mathbf{K}$ and $\mathbf{f}$. The error was then introduced in $\mathbf{g}$ by the addition of a noise. In the discussion of the Tikhonov regularization and singular value decomposition methods, and for $N = 32$, an average error of 3% was introduced into the exact solution. A first example, with $N = 8$, and treating the discretization error as noise will also be used.

Inversion in the Tikhonov regularization was performed using a Gaussian elimination [11,16]. The algorithm presented in 1970 by Golub and Reinsch [17], as implemented by Forsythe et al. [16], was the one used in this work for the calculating the singular value decomposition.

## 5. Results and discussions

A first attempt to find $\mathbf{f}$ could be by direct inverting $\mathbf{K}$ in the equation $\mathbf{Kf} = \mathbf{g}$. The result for $N = 8$ and treating the discretization error as a noise, $\|\mathbf{Kf}-\mathbf{g}\|_2 = 1.142\cdot 10^{-2}$, is presented in figure 1. It is clear that the computed solution is not acceptable. The small noise in $\mathbf{g}$ and the very high condition of $\mathbf{K}$, $\mathrm{cond}(\mathbf{K}) = 8.9704 \cdot 10^{11}$, are sufficient to amplify the error in the solution. The norm of the exact result in this case is 1.250 whereas the norm of the calculated solution is 126.8. Another approach to this problem, by truncating the singular value expansion, will be discussed later.

A second attempt to find a $f(y)$ such that $\int_a^b K(x, y) f(y)\,\mathrm{d}y = g(x)$ can be tried by setting $a_0 = a_1 = a_2 = 0$ and the regularization parameter also equal to zero in equation (6), which is, in fact, equivalent to the least square method. Again using the inverse of $\mathbf{K}^{\mathrm{T}}\mathbf{K}$ the solution obtained is not better than before since $\mathbf{K}^{\mathrm{T}}\mathbf{K}$ and $\mathbf{K}$ have the same rank. From these two examples it is clear that one has to give some extra information to the original problem or, instead, decompose the problem into subspaces.

The extra information to be given in this work will be the one to minimize, not only the residual norm, but also the norm of the solution itself. No initial guess for $\mathbf{f}$ will be assumed and due to the nature of the solution the conditions $a_1 = 0$ and $a_2 = 0$ will be further imposed. Under these conditions one has that $\Omega = \|\mathbf{Kf} - \mathbf{g}\|_2$ and $\rho = \|\mathbf{f}\|_2$ are function of the regularization parameter, i.e., $\Omega = \Omega(\lambda)$ and $\rho = \rho(\lambda)$. The next step in the Tikhonov regularization is to find the regularization parameter, $\lambda$.

The right balance between $\Omega = \Omega(\lambda)$ and $\rho = \rho(\lambda)$ can be done analyzing the graphics of $\log(\rho) \times \log(\Omega)$, for several values of $\lambda$, as given in figure 2. Due to its peculiar form, this parametric curve is called the $L$-curve. The estimation of the optimal $\lambda$,

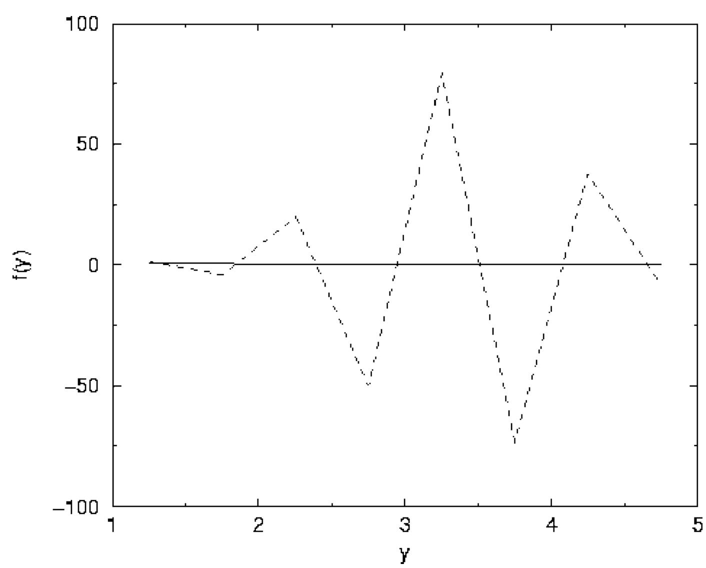


Figure 1. Calculated value (dashed line) and exact value (solid line) of $f(y)$.

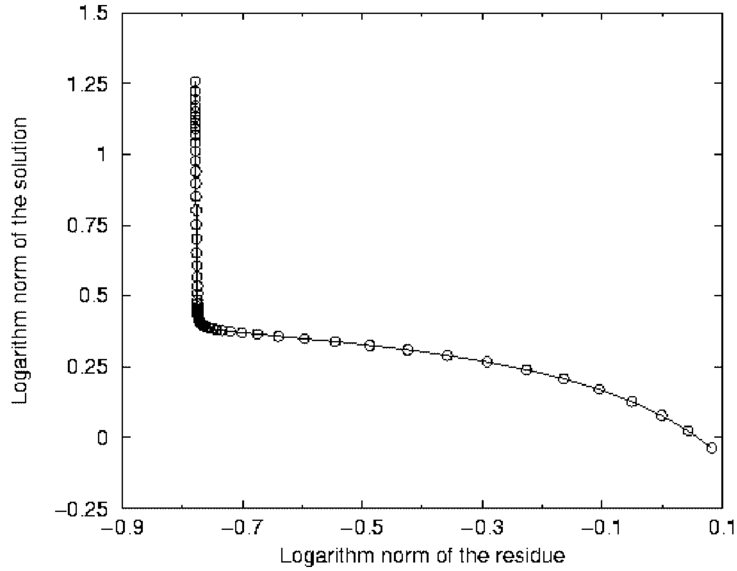


Figure 2. Regularized solution and norm (in logarithm form) for several regularized parameter.

say $\lambda^*$, can be obtained by calculating the point of maximum curvature in the $L$-curve which correspond to the maximum of the curve [13],

$$\kappa(\lambda) = \frac{\rho'\Omega'' - \rho''\Omega'}{((\rho')^2 + (\Omega')^2)^{3/2}}, \tag{12}$$

where the primes represent derivative with respect to $\lambda$ . This maximum gives the right balance between the residual and solution norm. Figure 3 shows the graphic of $\kappa(\lambda) \times \lambda$ from which it is obtained the regularization parameter. The maximum curvature occurs at $\lambda^* = 1.2590 \cdot 10^{-2}$. For this value one has $\Omega(\lambda^*) = 0.17824$ and $\rho(\lambda^*) = 2.4262$. Since for this case the exact value for $\Omega$ is 2.5278 one might conclude that the solution is a good estimate for the problem. But this is not the case since the residual norm is not a small number.

The solution for $\lambda^* = 1.2590 \cdot 10^{-2}$ is given in figure 4 where one can see why the residual norm for the solution has a value close to the correct value. Contribution of the norm to the left and to the right of the intersection point makes the two norm to be close one to the other. Analogous situation has also happen, for example, when applying Tikhonov regularization in field soils [3] and thermodynamics [4], being in fact an expected tendency since the solution found has to be close to the true solution. Under the $L$-curve criterion, this is the best one can do to find the solution of the above ill-posed problem using the Tikhonov regularization.

Applying the singular value decomposition to $\mathbf{Kf} = \mathbf{g}$ the solution can be computed as in equation (10). The answer, as in the first example for the Tikhonov regularization, is also done for $N = 8$. Again, due to the presence of errors in the discretizing the

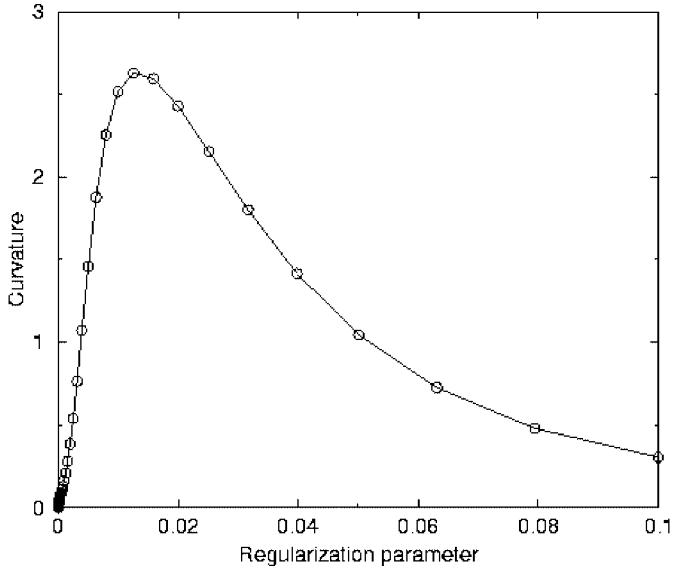


Figure 3. $L$-curve curvature as a function of the regularization parameter.

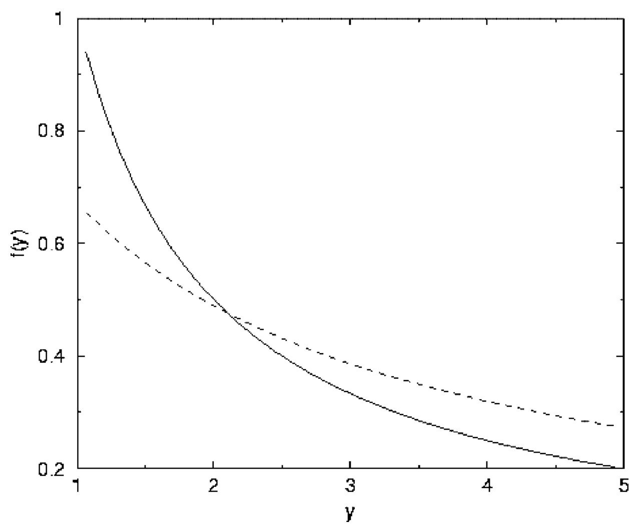


Figure 4. Exact value (solid line) and calculated value from Tikhonov regularization (dashed line) of the function $f(y)$.

integral equation, the answer is not acceptable. In fact, using the complete basis for the $\mathbb{R}^n$ space the answer is exactly the same as the Tikhonov solution, presented in figure 1.

The singular value decomposition provides a clear interpretation of the above wrong results. One has first to realize the importance of the singular values when computing a solution of an ill posed problem. The singular values for $N = 8$ are presented in table 1 from which the origin of the problem to calculate **f** for an ill-conditioning matrix

Table 1
Singular values, $\sigma_i$, as a function of the index $i$, for $N = 8$.

| $i$ | $\sigma_i$ |
|---|---|
| 1 | 0.78400 |
| 2 | 4.3794(−2) |
| 3 | 1.7098(−3) |
| 4 | 5.2203(−5) |
| 5 | 1.1951(−6) |
| 6 | 1.9121(−8) |
| 7 | 1.8960(−10) |
| 8 | 8.7399(−13) |

or rank deficient matrix can be explained. The coefficients of the expansion of $\mathbf{f}$ in the basis $\{\mathbf{v}_i\}$ are inversely proportional to the singular values. Any small error in $\mathbf{g}$ will be amplified by the small values of $\sigma_i$. Therefore, not all values of the singular values should be taken into account when errors are included in $\mathbf{g}$.

The division of $\mathbb{R}^n$ and $\mathbb{R}^m$ into the four fundamental subspaces [11], the range of $\mathbf{K}^{\mathrm{T}}$, $\mathrm{R}(\mathbf{K}^{\mathrm{T}})$, the null space of $\mathbf{K}$, $\mathrm{N}(\mathbf{K})$, the range of $\mathbf{K}$, $\mathrm{R}(\mathbf{K})$, and the null space of $\mathbf{K}^{\mathrm{T}}$, $\mathrm{N}(\mathbf{K}^{\mathrm{T}})$, is very important at this point. Since $\mathbb{R}^n = \mathrm{R}(\mathbf{K}^{\mathrm{T}}) \oplus \mathrm{N}(\mathbf{K})$ and $\mathbb{R}^m = \mathrm{R}(\mathbf{K}) \oplus \mathrm{N}(\mathbf{K}^{\mathrm{T}})$, one can consider moving the boundary between the subspaces in $\mathbb{R}^n$ and $\mathbb{R}^m$. For $\mathbb{R}^n$ these will define another subspace for the solution $\mathbf{f}$, make part of the basis $\{\mathbf{v}_i\}$, with the undesired small singular value belonging to the nullspace of $\mathbf{K}$. For $\mathbb{R}^m$ this will represent which part of data can be conveniently treated in the inversion procedure.

Defining $\dim(R(\mathbf{K}^{\mathrm{T}})) = k$, the problem to find the solution using the singular value decomposition will be complete if the value of $k$ is established. It is important to say that $k$ is not necessary the rank of the matrix. For noise free systems and rank deficient problem that will be case, but for system with any error in $\mathbf{g}$, even the small experimental errors, the optimum value of $k$ has to be calculated.

Finding the optimum value of $k$ in the singular value decomposition method is analogous to find the optimum $\lambda$ parameter in the Tikhonov regularization. Here also one can use the $L$ curve analysis to choose the best value of $k$. The $L$ curve, for $N = 32$ and for the same error introduced in the Tikhonov regularization analysis, is presented in figure 5. Since $k$ is discrete it is easy to see its optimum value, the curvature calculation not being necessary. It is clear that this optimum value, from the above figure, is equal to 3. The computed solution, that is,

$$\mathbf{f}_3 = \sum_{j=1}^{3} \frac{\mathbf{u}_j^{\mathrm{T}}\mathbf{g}}{\sigma_j}\mathbf{v}_j \tag{13}$$

is presented in figure 6.

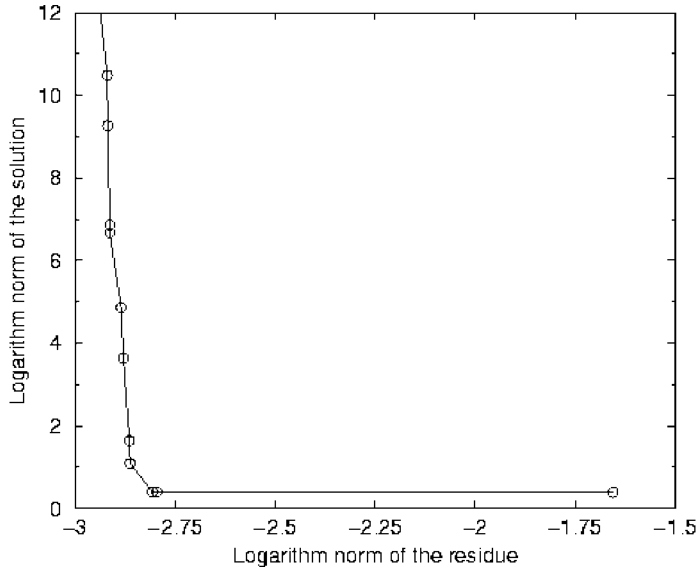


Figure 5. $L$-curve for the singular value decomposition method.

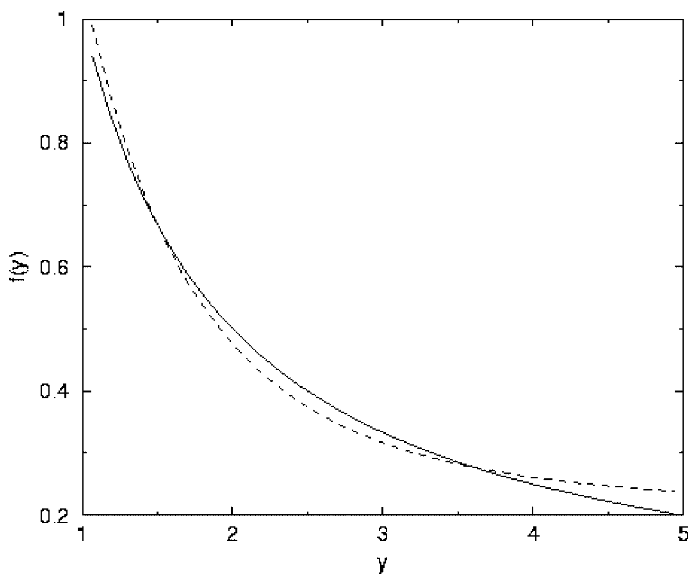


Figure 6. Exact value (solid line) and calculated value using singular value decomposition (dashed line) of the function $f(y)$.

The basis **v**, the vector column **u** and the singular values were calculated using the algorithm described in the previous section. The simplicity in which the solution was found, and its associated precision, makes the singular value decomposition method a better method to use when compared to the Tikhonov regularization.

## 6. Conclusions

The Tikhonov regularization and the singular value decomposition, two methods to treat linear ill-posed inverse problems, were presented and compared. The analysis was carried out on a model system and under the parametric $L$ criterion. The conclusion is very clear: the singular value decomposition should be used in the place of Tikhonov regularization for ill-posed problems.

The non-convergence aspect of the $L$ curve is not a new result [18] although no comparison between these two methods, using this criterion, has appeared. The nature of the comparison of these two methods can be further explored if one recall that Tikhonov regularization is in fact a constrained least square problem. The minimum of (2) is required with the restriction (3). The solution found satisfies these criteria.

On the other hand when using the singular value decomposition one seeks for a solution such that, $\mathbf{f} \in \mathrm{R}(\mathbf{K}^{\mathrm{T}})$. Therefore, if another solution, $\mathbf{x}$, has been found it has to be of the form $\mathbf{x} = \mathbf{f} + \mathbf{f}_{\mathrm{N}}$, where $\mathbf{f}_{\mathrm{N}} \in \mathrm{N}(\mathbf{K})$. Due to the orthogonality of these two subspaces, $\|\mathbf{x}\|_2^2 = \|\mathbf{f}\|_2^2 + \|\mathbf{f}_{\mathrm{N}}\|_2^2 > \|\mathbf{f}\|_2^2$ which shows the solution obtained is indeed the solution with minimum norm. No restriction has to be impossed when using the singular value decomposition. All that has to be done is to fix the dimension of $\mathrm{R}(\mathbf{K})$ using the $L$ curve.

Another important aspect when comparing these two approach is the filter factor, $w$, that each method uses. For the singular value decomposition this filter factor is equal to $w_1 = 1$ if $i \leqslant j$ and $w_i = 0$ if $i > k$. Manipulating equation (6), with $a_1 = a_2 = 0$, one obtains the filter factor for the Tikhonov regularization $w_i = \sigma_i^2/(\sigma_i^2 + \lambda)$. This shows another important diference between these two approaches. In the SVD method there is a sudden change in the filter factor whereas in the Tikhonov regularization the undesired small singular values are damped slowly. In the Tikhonov regularization all the singular values are taken into account and this will amplify the errors in the data. The filter factor in the SVD method is more effective.

For some problems, such as in the inverse of potential energy functions from second virial coefficient [4], some information about the solution can be available. In this case the Tikhonov regularization will give a very reliable solution since, instead of the norm of the solution one can use the norm of $\mathbf{f} - \widehat{\mathbf{f}}$ in the $L$-curve. This explains why the Tikhonov regularization has become so often used. Nevertheless if no information is available about the solution, then the singular value decomposition should be used. Together with that, not only the Tikhonov regularization, but also the singular value decomposition, can be investigated by other methods to choose the optimum parameter. One of these methods could be the generalized cross validation [19], but this has to be investigated further in the comparison of these methods.

## Acknowledgements

The author would like to thank Prof. H. Rabitz at Princeton University where this work has started. Acknowledgements goes also to CAPES, CNPq and FAPEMIG for financial support.

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