ARCHIVES OF ACOUSTICS
30, 4, 473–482 (2005)

UNCERTAINTY IN STRUCTURE DYNAMICS RESULTING FROM MATRIX ILL-CONDITIONING

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(*received April 30, 2005; accepted October 23, 2005*)

In the paper there are discussed certain issues concerning ill-posed problems that frequently appear in inverse problems, modal analysis, acoustics and other methods making use of matrix algebra. There is presented the mathematical definition, application of the singular value decomposition method to ill-posed problems detecting as well as a new method of improving such problems conditioning by the use of the Tikhonov regularization method. In the paper are presented some results of solution estimation of the Fredholm integral equation of the first kind that is the classical ill-posed problem. Analysis was carried out in the Matlab environment by means of the least squares and Tikhonov regularization methods for both the noiseless and noisy cases.

Key words: ill-posed problem, ill-conditioned matrix, Tikhonov regularization method.

1. Introduction

Structure dynamic properties stand for the main quality indicator in design and condition monitoring processes [4, 5]. High accuracy of modal parameters is required if model-based methods are applied. Due to complexity of tested structures it is necessary to use advanced numerical methods for parameters identification as well as reduction of the measurement and processing errors. Measured characteristics are usually used as the input data in the process of model parameters estimation. In most cases these procedures are based on matrix algebra. Significant numerical errors can result from processing of ill-conditioned matrices (i.e. ill-posed problems), which frequently appear in inverse problems, modal analysis and other methods making use of matrix algebra. The problem of matrix ill-conditioning can stem from:

1. Physical properties of the tested system.
2. Properties of characteristics measured on real objects.

3. Mathematical operations required by the algorithm of the assumed method of analysis.

Uncertainty related to matrix ill-conditioning results from the fact that commercial software applications make use of the standard least squares method. Determinant of an ill-conditioned matrix $[A]$ is close to zero while the $[A]$ matrix is almost rank-deficient. In such a case, operation of matrix inverting required by the least squares method leads to gross numerical errors. Estimation of a correct solution is impossible without earlier improvement of the problem formulation (matrix conditioning [4]). Therefore regularization, as a method that makes it possible to solve ill-defined problems effectively, holds great interest.

2. Mathematical definition of ill-posed problems

According to the Hadamard definition, the equation:

$$[A]\{x\} = \{y\}, \qquad [A] : X \to Y \tag{1}$$

is well-posed provided thet the following conditions are satisfied:

1. Solution existence for each $\{y\} \in Y$, $\{x\} \in X$ such that $[A]\{x\} = \{y\}$,
2. Uniqueness: $[A]\{x_1\} = [A]\{x_2\} \Rightarrow \{x_1\} = \{x_2\}$,
3. Stability: $[A]^{-1}$ is continuous.

Equation (1) is ill-posed if one of the above conditions is not satisfied.

3. Identification of ill-posed problems

Identification of ill-posed problems can be performed by analysis of features of system matrix decomposition into singular values. Singular values resulting from the SVD decomposition of the system matrix $[A] \in R^{m\times n}$ $(m \geq n)$ are described by the equation:

$$[A] = [U]\,[\Sigma]\,[V]^T = \sum_{i=1}^{n} \{u_i\}\sigma_i\{v_i\}^T, \tag{2}$$

where

$[U]$, $[V]$ – orthonormal matrices of singular vectors: $[U]^T[U] = [V]^T[V] = [I]_n$,

$[\Sigma] = \begin{bmatrix} \sigma_1 & 0 & 0 \\ 0 & \ddots & 0 \\ 0 & 0 & \sigma_n \end{bmatrix}$ – diagonal matrix,

$\sigma_1 \geq \ldots \geq \sigma_n \geq 0$, σ_i – singular value of the $[A]$ matrix,

$\{v_i\}$, $\{u_i\}$ – right and left singular vectors of the $[A]$ matrix.

In case of a discrete ill-posed problem, the system matrix $[A]$ is always ill-conditioned, which means that determinant of the $[A]$ matrix is close to zero and the $[A]$ matrix is almost rank-deficient. The SVD decomposition of such an ill-conditioned matrix has the following properties [2]:

- singular values σ_i gradually decay to zero,
- with the increase in the i index, in the $\{v_i\}$, $\{u_i\}$ vectors, more changes in signs of elements of the $\{v_i\}$ and $\{u_i\}$ vectors are observed,
- $[A]$ matrix condition number is high (the highest to smallest singular value ratio $> 10^{14}$).

4. Tikhonov regularization method

Measured response of a real system (1) can be described by the equation:

$$[A]\{x\} = \{y_{sz}\} \;\Leftrightarrow\; [A]\{x\} = \{y_{\text{ideal}}\} + \{\eta\}, \tag{3}$$

where $\{y_{sz}\} \in R^{n\times 1}$ – measured noisy system response; $\{\eta\} \in R^{n\times 1}$ – noise; $[A] \in R^{n\times m}$ – system matrix; $\{x\} \in R^{m\times 1}$ – unknown solution; n, m – integers.

Numerical solution of the least squares method, which is commonly used for solving algebraical equations, is unique and unbiased only when the $[A]$ matrix rank equals m. Therefore an ill-posed problem solution obtained by the use of the least squares method:

$$\{x_{ls}\} = \arg\min_x \|\{y_{sz}\} - [A]\{x\}\|_2^2 \tag{4}$$

is unstable – the more noisy is the measurement data, the more obtained solution differs from the correct one. Modification of the equation of interest by replacing the $[A]$ matrix with a well-conditioned matrix as well as introducing additional constraints, do not guarantee obtaining correct solutions. Determining a correct solution by means of an inverse method is usually impossible without earlier improvement of the problem formulation (system matrix conditioning). In case of the Tikhonov regularization method, the unknown solution has the following form [4]:

$$\{x_\alpha\} = \arg\min_x \left\{\|\{y_{sz}\} - [A]\{x\}\|_2^2 + \alpha^2\|[L]\{x\}\|_2^2\right\}, \tag{5}$$

where α is the regularization parameter describing a compromise between an accurate fitting and smoothness of the obtained curve; $[L]$ is usually a unit matrix.

The L-curve is the most popular method for determining an optimal regularization parameter α [1].

The L-curve method [1, 2] consists in determining a graphical dependence between $\|\{y_{sz}\} - [A]\{x_\alpha\}\|_2^2$ and $\|[L]\{x_\alpha\}\|_2^2$ for all the possible α values in the logarithmic scale (Fig. 1). The optimal value of the regularization parameter α_{opt} corresponds to the coordinates of the L-curve corner. If $\alpha < \alpha_{\text{opt}}$ then the solution is close to the solution obtained by means of the least squares method. Assumption of $\alpha > \alpha_{\text{opt}}$ leads to a solution of an equation that differs significantly from the original one.

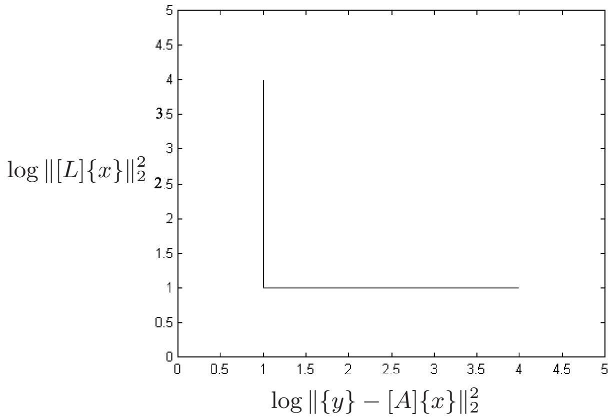

Fig. 1. L-curve method.

4.1. Tikhonov regularization as a filtration method

On the basis of the Eq. (2), an inverse operator value R_α can be determined according to the formula:

$$[R_\alpha] = \big([A]^T[A] + \alpha[I]\big)^{-1}[A]^T[U]^T \tag{6}$$

so that

$$[R_\alpha] = \big([V]\,[\Sigma]^T[U]^T[U]\,[\Sigma]\,[V]^T + \alpha[V]\,[I]\,[V]^T\big)^{-1}[V]\,[\Sigma]^T \tag{7}$$

therefore

$$\begin{aligned} [R_\alpha] \ &= \ [V]\big([\Sigma]^T[\Sigma] + \alpha[I]\big)^{-1}[\Sigma]^T[U]^T \qquad \text{or} \\ [R_\alpha] \ &= \ [V] \cdot \operatorname{diag}\left(\frac{\sigma_i^2}{\sigma_i^2 + \alpha} \cdot \frac{1}{\sigma_i}\right)[U]^T. \end{aligned} \tag{8}$$

Expression $w_\alpha(s_i^2) = \dfrac{\sigma_i^2}{\sigma_i^2 + \alpha}$ for $[L] = [I]_n$ is called a Tikhonov filter function. If $\alpha \to 0$ then $w_a(\sigma_i^2) \to 1$ so $[R_\alpha] \to 0$.

The Tikhonov filter function performance consists in filtering out small singular values of σ_i $(\sigma_i < \alpha)$.

5. Solution estimation of the Fredholm integral equation of the first kind by means of the least squares and Tikhonov regularization methods

Fredholm integral equation of the first kind is the classical example of an ill-posed problem [4]:

$$\int\limits_c^d K(s,t) \cdot f(t)\,dt = g(s), \qquad c \le s \le d, \tag{9}$$

where $K(s)$ – kernel, known square integrand; $g(s)$ – equation right side, known function; $f(t)$ – unknown solution; c, d – limits of integration.

Fredholm equation of the first kind belongs to the class of functional equations, in which the integrand is unknown. In acoustics, theory of elasticity and fluid mechanics, integral equations are used for describing physical phenomena with given boundary or initial conditions. Numerical methods of solving integral equations are widely used in analysis of continuous mechanical systems.

For Eq. (9) the following data were assumed [6]:

$$K(s,t) = (\cos(s) + \cos(t))^2 \left(\frac{\sin(u)}{u}\right)^2, \tag{10}$$

$$g(s,t) = \pi\left(\sin(s) + \sin(t)\right), \tag{11}$$

$$f(t) = a_1 e^{-c_1(t-t_1)^2} + a_2 e^{-c_2(t-t_2)^2}, \tag{12}$$

where $a_1 = 2$, $a_2 = 1$ are constants responsible for the solution form; $c_1 = 6$, $c_2 = 2$; $t_1 = 0.8$, $t_2 = -0.5$; $a = -0.5\pi$, $b = 0.5\pi$ – limits of integration; $n = 72$ is the assumed number of points belonging to the interval of integration.

Computations were carried out in the Matlab environment by means of the created software, making use of functions introduced in the Regularization Tools. Equation (9) was transformed to the following form:

$$[A]\{x\} = \{b\}. \tag{13}$$

Two cases were considered: noiseless, described by Eq. (13) and noisy, described by the following equation:

$$[A]\{x\} = \{\check{b}\}, \qquad \{\check{b}\} = \{b\} + e^{-3*\{q\}}, \tag{14}$$

where $\{q\}$ is the vector of random values ($q \in \langle 0, 1\rangle$) of the same length as the $\{b\}$ vector.

Solution was estimated applying two methods: the least squares method used by commercial applications and the Tikhonov regularization method implemented in the created software.

In case of Tikhonov regularization, the next step of the algorithm consisted in decomposition of the matrix $[A]$ into singular values:

$$[A] = [U] \cdot [S] \cdot [V]^T \tag{15}$$

and checking whether the right-hand side of the Eq. (13) describing noiseless case meets the discrete Picard condition. If the right-hand side $\{b\}$ of the equation describing noiseless case meets the Picard condition, then it is possible to determine solution $\{x_{\mathrm{reg}}\}$ for noisy case (14) by the use of the regularization method in such a way that $\{x_{\mathrm{reg}}\}$ approximates the exact solution $\{x\}$.

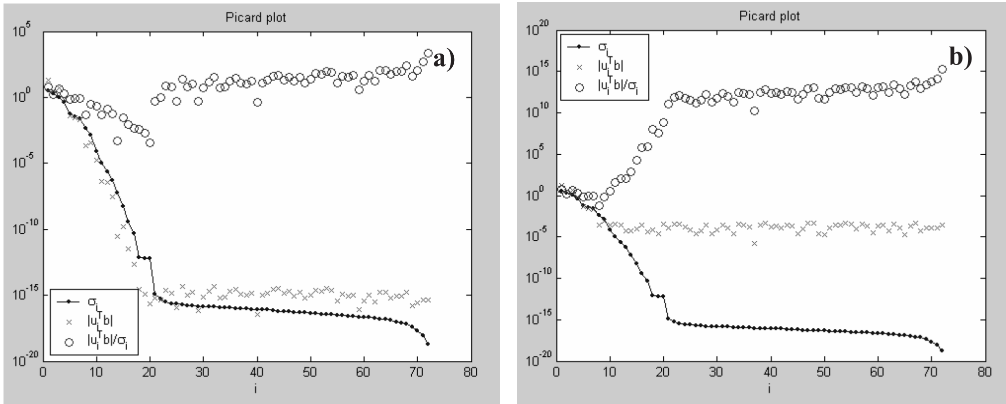

Fig. 2. Discrete Picard condition for noiseless (a) and noisy case (b).

In the Fig. 2 is presented a graphical interpretation of the discrete Picard condition for the noiseless (a) as well as the noisy (b) case.

In the noiseless case, for $i \leq 20$, Fourier coefficients meet the discrete Picard condition – they decrease more quickly than singular values σ_i. In the noisy case, for $i \leq 10$, Fourier coefficients decrease more quickly than the singular values, which means that the right-hand side of the Eq. (13) describing noiseless case meets discrete Picard condition. Therefore regularization aims at filtering out the singular values $\sigma > \sigma_{10}$ and leaving the rest of singular values unchanged.

In the next step, by the use of the L-curve method, the optimal value of the regularization parameter α_{opt} was determined. Solution estimation was carried out according to the following formula:

$$\{x_\alpha\} = \sum_{i=1}^{n} \frac{\sigma_i^2}{(\sigma_i^2 + \alpha_{\mathrm{opt}})} \cdot \sigma_i^{-1} \cdot \left(\{u_i\}^T \{b\}\right), \tag{16}$$

where σ_i are singular values; $\{u_i\}$ – left vector of singular values; α_{opt} – optimal regularization parameter.

5.1. Solution obtained by means of the least squares method

Solution estimation was carried out by the use of standard procedure introduced in Matlab. Maximal and mean values of percentage relative errors for noiseless data were calculated according to the equations (Figs. 3, 1):

$$\begin{aligned} e_{ls\ \mathrm{max}} &= \max\left(\left|\frac{\{x\} - \{x_{ls}\}}{\{x\}}\right| \cdot 100\%\right), \\ e_{ls\ \mathrm{mean}} &= \mathrm{mean}\left(\left|\frac{\{x\} - \{x_{ls}\}}{\{x\}}\right| \cdot 100\%\right). \end{aligned} \tag{17}$$

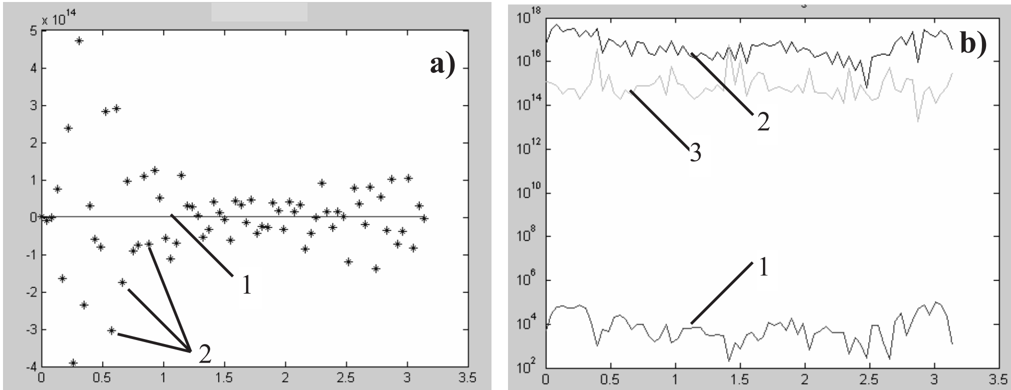

Fig. 3. a, b) Solution obtained by means of the least squares, a) noisy data (2), noiseless data (1); b) logarithm of the relative error: e_{ls} (1), $e_{ls\text{ noisy}}$ (2), $e_{ls\text{ stab}}$ (3).

The following values were obtained:

$$e_{ls\ \max} = 1.28 \times 10^5\ [\%], \qquad e_{ls\ \text{mean}} = 2.2 \times 10^4\ [\%]. \tag{18}$$

Matrix $[A]$ is ill-conditioned, its condition number: $n_{\text{cond}} = 1.011675 \times 10^{19}$. Therefore, in case of noiseless as well as noisy data, numerical algorithm of the least squares method doesn't work correctly. Maximal and mean values of relative percentage errors for noisy data were calculated on the basis of equations:

$$\begin{aligned} e_{ls\ \max}^{\text{noisy}} &= \max\left(\left|\frac{x - x_{ls}^{\text{noisy}}}{x}\right| \cdot 100\%\right), \\ e_{ls\ \text{mean}}^{\text{noisy}} &= \text{mean}\left(\left|\frac{x - x_{ls}^{\text{noisy}}}{x}\right| \cdot 100\%\right) \end{aligned} \tag{19}$$

and equal

$$e_{ls\ \max}^{\text{noisy}} = 6.12 \times 10^{17}\ [\%], \qquad e_{ls\ \text{mean}}^{\text{noisy}} = 4.5 \times 10^{16} [\%]. \tag{20}$$

Stability of the solution estimated by means of the least squares method can be assessed on the basis of the equations:

$$\begin{aligned} e_{ls\ \text{stab}\ \max} &= \max\left(\left|\frac{x_{ls} - x_{ls}^{\text{noisy}}}{x_{ls}}\right| \cdot 100\%\right), \\ e_{ls\ \text{stab mean}} &= \text{mean}\left(\left|\frac{x_{ls} - x_{ls}^{\text{noisy}}}{x_{ls}}\right|\right). \end{aligned} \tag{21}$$

Error values equal:

$$e_{ls\ \mathrm{stab\ max}} = 4.28 \times 10^{15}\ [\%], \qquad e_{ls\ \mathrm{stab\ mean}} = 2.4 \times 10^{14}\ [\%]. \tag{22}$$

Results obtained by means of the least squares method for noisy ill-posed problems are unstable and burdened with unacceptably big errors. Therefore, the least squares method cannot be used for solving ill-posed problems.

5.2. Solution obtained by means of the Tikhonov regularization method

Calculations were carried out in the Matlab environment. Optimal parameters of regularization obtained by the use of the L-curve method for noiseless (Fig. 4a) and noisy (Fig. 4b) case equal: $\alpha_{\mathrm{noiseless}} = 1.137 \times 10^{-14}$, $\alpha_{\mathrm{noisy}} = 7.39 \times 10^{-4}$.

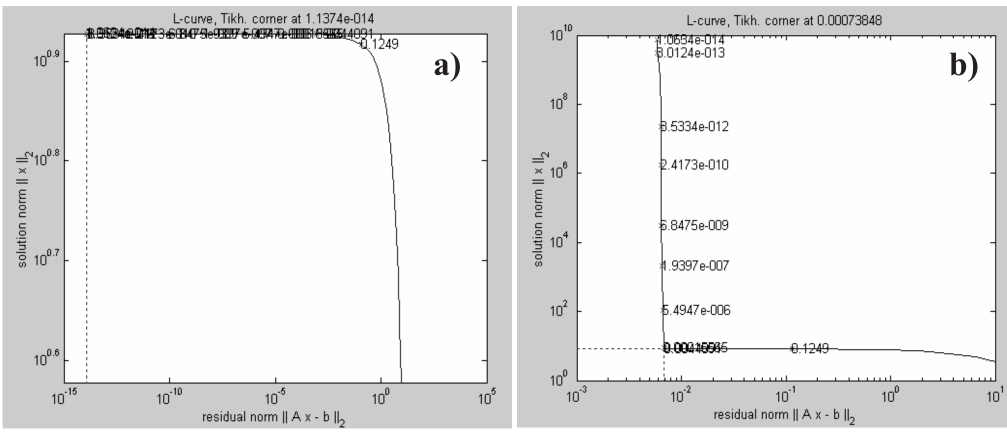

Fig. 4. Parameters of the L-curve corner corresponding to optimal parameter of regularization α_{opt} for noiseless (a) and noisy (b) case.

Solution obtained for noiseless data is presented in the Fig. 5a (***). Maximal and mean values of solution relative errors are described by the equations:

$$\begin{aligned} e_{\mathrm{Tikh\ max}} &= \max\left(\left|\frac{\{x\} - \{x_{\mathrm{Tikh}}\}}{\{x\}}\right| \cdot 100\%\right), \\ e_{\mathrm{Tikh\ mean}} &= \mathrm{mean}\left(\left|\frac{\{x\} - \{x_{\mathrm{Tikh}}\}}{\{x\}}\right| \cdot 100\%\right). \end{aligned} \tag{23}$$

The following values were obtained:

$$e_{\mathrm{Tikh\ max}} = 8.44\ [\%], \qquad e_{\mathrm{Tikh\ mean}} = 0.76\ [\%]. \tag{24}$$

Solution obtained by means of the Tikhonov regularization method for noisy case (Fig. 5a, - - -) is burdened with maximal and mean relative errors described by the

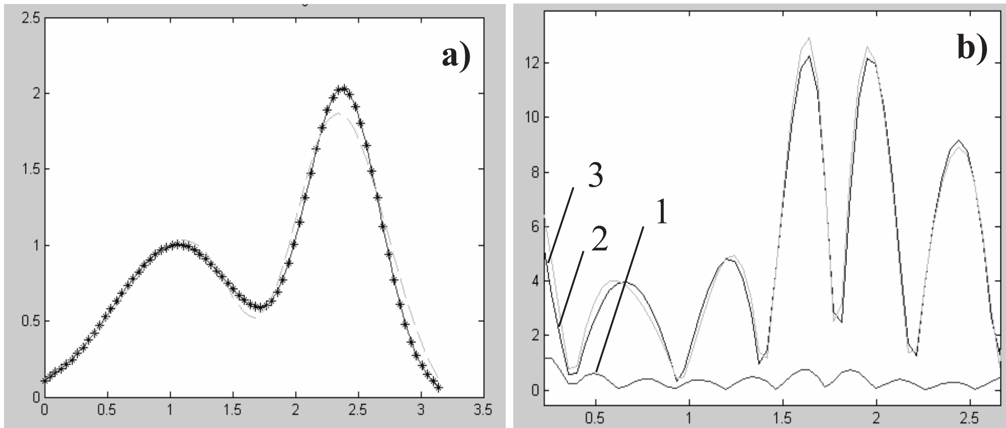

Fig. 5. a) Solution obtained by means of Tikhonov regularization method for noiseless case (***), noisy case (- - -) exact solution (—); b) solution percentage relative error: e_{Tikh} (1), $e_{\text{Tikh noisy}}$ (2), $e_{\text{Tikh stab}}$ (3).

equations:

$$e^{\text{noisy}}_{\text{Tikh max}} = \max\left(\left|\frac{x - x^{\text{noisy}}_{\text{Tikh}}}{x}\right| \cdot 100\%\right),$$
$$e^{\text{noisy}}_{\text{Tikh mean}} = \text{mean}\left(\left|\frac{x - x^{\text{noisy}}_{\text{Tikh}}}{x}\right| \cdot 100\%\right). \quad (25)$$

The following values were obtained:

$$e^{\text{noisy}}_{\text{Tikh max}} = 13\ [\%], \qquad e^{\text{noisy}}_{\text{Tikh mean}} = 11.82\ [\%]. \quad (26)$$

Stability of the solution obtained by means of the Tikhonov regularization can be assessed on the basis of equations:

$$e_{\text{Tikh stab max}} = \max\left(\left|\frac{x_{\text{Tikh}} - x^{\text{noisy}}_{\text{Tikh}}}{x_{\text{Tikh}}}\right| \cdot 100\%\right),$$
$$e_{\text{Tikh stab mean}} = \text{mean}\left(\left|\frac{x_{\text{Tikh}} - x^{\text{noisy}}_{\text{Tikh}}}{x_{\text{Tikh}}}\right| \cdot 100\%\right). \quad (27)$$

Error values obtained for estimated solution are as follows:

$$e_{\text{Tikh stab max}} = 14\ [\%], \qquad e_{\text{Tikh stab mean}} = 11.93\ [\%]. \quad (28)$$

On the basis of the obtained results it can be stated that the Tikhonov regularization method is an effective tool for solving noiseless as well as noisy ill-posed problems.

6. Conclusions

In the paper the author proposed a new software for solving ill-posed problems with the use of the Tikhonov regularization method implemented in the Matlab environment. The proposed software was used for solving the classical ill-posed problem – Fredholm integral equation of the first kind. Results obtained by means of the proposed software were compared with the results estimated on the basis of numerical least squares method. Maximal percentage relative errors of solutions estimated by means of the least squares method (e^{LS}) and the Tikhonov regularization method (e^{Tikh}) for the considered Fredholm integral equation of the first kind equal respectively:

- $e^{LS} = 6.12 \times 10^{17}\%$,
- $e^{\text{Tikh}} = 13\%$.

The research carried out proved that the least squares method cannot be used for solving ill-posed problems because of unacceptably big errors of the estimated solutions, while the Tikhonov regularization method is a stable and effective tool for solving the ill-posed problems.

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