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ON THE USE OF THE FOURIER TRANSFORM IN ILL-CONDITIONED PROBLEMS

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Abstract: Recently the new method using the Fourier transform for the solution of ill-conditioned matrix problems had been proposed [1]. Thorough analysis has shown that in opposite to the claim of authors the new method is not superior to the commonly used methods.

Keywords: Fredholm integral equation of the first kind, convolution equation, ill-conditioned matrices, singular value decomposition, discrete Fourier transform, QR algorithm.

1 Introduction

Inverse problems are among the most challenging computations in science and engineering because they involve determining the parameters of a system that is only observed indirectly. Typical are the tasks of the remote sensing, electromagnetic defectoscopy, ultrasonic detection and other methods of indirect diagnostics. Often the blurring of results due to imperfect measurements belong to this class of problems. If the quantity-to be-determined from measurement results is extremely sensitive to the measurement error, the problem is called ill-posed. Many of ill-posed problems of indirect sensing are described in terms of the Fredholm integral equation of the first kind

$$\int_a^b k(x,y)f(x)dx = g(y) \qquad (1)$$

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where the unknown quantity $f(x)$ is to be inferred from the results of measurement $g(x)$. The kernel $k(x,y)$ of integral equation (1) is the characteristics the measuring instrument of the method involved. A special case of (1) is the convolution equation

$$\int_{-\infty}^{\infty} k(y-x)f(x)dx = g(y) \tag{2}$$

where $k(x)$ is the impulse response of the measuring instrument. Discretisation of (1) leads to standard matrix equation

$$\boldsymbol{K}\cdot\boldsymbol{f} = \boldsymbol{g} \tag{3}$$

For the ill-posed problems the matrix of the discrretised model is usually ill-conditioned too. If the number of measurements M is equal to number of unknowns N (i.e. $\boldsymbol{K}$ is a square matrix) then $\boldsymbol{g}$ can be obtained by the inversion of $\boldsymbol{K}$

$$\boldsymbol{f} = \boldsymbol{K}^{-1}\cdot\boldsymbol{g} \tag{4}$$

If the number of measurements is larger than the number of unknowns, $M > N$, then the least squares solution is usually taken. i.e. the vector $\boldsymbol{f}$ minimising the norm

$$\min_{\boldsymbol{f}}\left\{\left\|\boldsymbol{g}-\boldsymbol{K}\cdot\boldsymbol{f}\right\|^2\right\} \tag{5}$$

which leads to the solution of the system of $N\times N$ equations with the square matrix $\boldsymbol{K}^T\cdot\boldsymbol{K}$

$$\boldsymbol{K}^T\cdot\boldsymbol{K}\cdot\boldsymbol{f} = \boldsymbol{K}^T\cdot\boldsymbol{g} \tag{6}$$

If $M < N$ the solution is not unique and usually the solution with the minimum norm $\|\boldsymbol{f}\|$ is accepted.

Since the right hand side $\boldsymbol{g}$ is never given exactly usually instead of $\boldsymbol{g}$ the vector $\boldsymbol{g}_E = \boldsymbol{g} + \varepsilon$ is on the left hand side of (3) or (6) where ε is the error vector. The error vector may represent not only the errors of measurement but also the round-off errors of the numerical inversion procedure itself and/or other processing of data as well. In consequence the result $\boldsymbol{f}$ is loaded by certain error too and one gets instead of exact $\boldsymbol{f}$ the vector $\boldsymbol{f}_E = \boldsymbol{f} + \eta$. The error amplification factor is defined as

$$\zeta = \frac{\|\eta\|\|\boldsymbol{g}\|}{\|\varepsilon\|\|\boldsymbol{f}\|} = \sqrt{\|\boldsymbol{K}\|\|\boldsymbol{K}^{-1}\|/N^2} = \sqrt{\sum_i|\lambda_i|^2\sum_i 1/|\lambda_i|^2\Big/N^2} \tag{7}$$

This factor is usually larger than one, usually if $\zeta >> 1$ the significant error amplification occurs and the matrix $\boldsymbol{K}$ is called ill-conditioned. It can be shown that

For the convolution equation using the Fourier transform (2) one obtains the simple product

$$\hat{k}(\omega)\hat{f}(\omega) = \hat{g}(\omega) \tag{8}$$

where $\hat{k}(\omega)$, $\hat{f}(\omega)$ and $\hat{g}(\omega)$ are Fourier spectra of $k(x)$, $f(x)$, and $g(x)$. Solution of (8) is straightforward

$$\hat{f}(\omega) = \hat{g}(\omega) / \hat{k}(\omega) \tag{9}$$

however, in case of the right side loaded by error equals

$$\hat{f}_E(\omega) = \hat{g}_E(\omega) / \hat{k}(\omega) \tag{10}$$

i.e.

$$\hat{f}_E(\omega) = \hat{f}(\omega) + \hat{\eta}(\omega) = \hat{g}(\omega) / \hat{k}(\omega) + \hat{\varepsilon}(\omega) / \hat{k}(\omega) \tag{11}$$

The nature of the error amplification can be easily revealed from (11). While the spectral components of physical signals decrease with frequency, the error terms having the character of white noise remain roughly constant. The transfer function $\hat{k}(\omega)$ decreases with frequency too, therefore the ratio of high frequency of noise components becomes relatively more pronounced. For zero points of transfer function the term $\hat{\eta}(\omega) = \hat{\varepsilon}(\omega) / \hat{k}(\omega)$ even grows to infinity. Therefore usually the results of inversion of ill-conditioned matrix oscillate wildly with high frequency. Numerically is (8) processed using the discrete Fourier transform, i.e. $\hat{k}(\omega)$, $\hat{f}(\omega)$, $\hat{g}(\omega)$ $\hat{\varepsilon}(\omega)$ and $\hat{\eta}(\omega)$ are represented by discrete vectors

$$\hat{\boldsymbol{k}} = \left[\hat{k}_0, \hat{k}_1, \ldots, \hat{k}_{N-1}\right] \tag{12}$$

in points $\omega_n = n\Omega$, $n = 0,1,\ldots N-1$ which are multiples of discretisation step Ω, and the same holds for the discrete vectors $\hat{\boldsymbol{f}} = \left[\hat{f}_0, \hat{f}_1, \ldots, \hat{f}_{N-1}\right]$, $\hat{\boldsymbol{g}} = \left[\hat{g}_0, \hat{g}_1, \ldots, \hat{g}_{N-1}\right]$ and similarly for $\hat{\boldsymbol{\varepsilon}}$ and $\hat{\boldsymbol{\eta}}$. The discrete version of (10), and (11) reads

$$\hat{f}_n = \hat{g}_n(\omega) / \hat{k}_n \,, \; n = 0,1,\ldots N-1 \tag{13}$$

$$\hat{f}_{En} = \hat{f}_n + \hat{\eta}_n = \hat{g}_n / \hat{k}_n + \hat{\varepsilon}_n / \hat{k}_n \,, \; n = 0,1,\ldots N-1 \tag{14}$$

The high frequency oscillations in $\hat{\boldsymbol{f}}_E$ can be in the spectral domain attenuated by the suitably chosen weighting function $\hat{w}(\omega)$, or in the discrete form by a weighting vector $\hat{\boldsymbol{w}} = \left[\hat{w}_0, \hat{w}_1, \ldots, \hat{w}_{N-1}\right]$

$$\hat{f}_{Rn} = \hat{w}_n \hat{g}_{En} / \hat{k}_n \tag{15}$$

i.e. the "regularised" solution (15) is taken instead of the "error" solution (14). In the extreme case when $\hat{k}_i$ is very small the corresponding frequency component in (15) are simply cut-off taking respective $\hat{w}_i = 0$.

The most often used method of damping the high frequency oscillations in solution vector of the ill-posed matrix problems is the Tichonov's method of "regularization" based on minimisation of the sum of squares of norms $\|\boldsymbol{g} - \boldsymbol{K} \cdot \boldsymbol{f}_R\|$ and $\|\boldsymbol{f}_R\|$, i.e.

$$\min_{\boldsymbol{f}}\left\{\left\|\boldsymbol{g}-\boldsymbol{K}\cdot\boldsymbol{f}_R\right\|^2+a\left\|\boldsymbol{f}_R\right\|^2\right\} \tag{16}$$

weighted by the "regularization parameter a, based on least squares solution of the matrix equation

$$\begin{bmatrix}\boldsymbol{K}\\ a\boldsymbol{I}\end{bmatrix}\cdot\boldsymbol{f}_R=\begin{bmatrix}\boldsymbol{g}_E\\ \boldsymbol{0}\end{bmatrix} \tag{17}$$

The method of cutting-off the higher spectral components can be used also for non-convolutional problems of type (1) written in the discrete matrix form (3). Independently of number of equations M and number of unknowns N there exist the unique singular value decomposition method factoring the matrix $\boldsymbol{K}$ with M rows and N columns into the form

$$\boldsymbol{K}=\boldsymbol{U}\cdot\Sigma\cdot\boldsymbol{V}^T \tag{18}$$

where $\boldsymbol{U}$ is the $M\times N$ column orthonormal matrix, Σ is the diagonal matrix with N nonnegative diagonal elements σ_n, $n=1,\ldots,N$, $\Sigma=\text{diag}[\sigma_n]$, and $\boldsymbol{V}$ is the $N\times N$ orthonormal matrix. The solution of (18) can then be written in the form

$$\boldsymbol{f}_s=\boldsymbol{V}\cdot\Sigma^{-1}\cdot\boldsymbol{U}^T\cdot\boldsymbol{g}=\sum_{i=1}^{N}\frac{\boldsymbol{u}_i^T\cdot\boldsymbol{g}}{\sigma_i}\boldsymbol{v}_i \tag{19}$$

where $\Sigma^{-1}=\text{diag}[1/\sigma_n]$, $\boldsymbol{u}_i^T$ are the rows of $\boldsymbol{U}^T$, and $\boldsymbol{v}_i$ columns of $\boldsymbol{V}$. This solution works independently of the fact if $M>N$, $M=N$, or $M<N$. In all cases the solution (19) minimises the norm

$$\min_{\boldsymbol{f}}\left\{\left\|\boldsymbol{g}-\boldsymbol{K}\cdot\boldsymbol{f}\right\|^2\right\} \tag{20}$$

Even for singular matrices when some $\sigma_n=0$ certain type of the solution can be found simply setting zero instead of $1/\sigma_n$ in Σ^{-1} in (19). This is equivalent to cutting-off unwanted spectral components in (15). If we do the same for the ill-conditioned matrix for those σ_n which are smaller than certain limit, then we are using in fact windowing with rectangular window in the sense analogous to (15)

2 Fourier transform inversion method

In the recently published work [1] the authors claim to reach better results in inversion of the ill-conditioned matrices with making use of the discrete Fourier transform of the matrix itself, of the unknown and of the right hand side as well. The elements of the discrete Fourier transform matrix $\boldsymbol{F}$ read

$$\{\boldsymbol{F}\}_{k,\ell\in(1,N)}=\left\{\tfrac{1}{\sqrt{N}}\,\mathrm{e}^{-2\pi(k-1)(\ell-1)/N}\right\}_{k,\ell\in(1,N)} \tag{21}$$

The Fourier transform matrix is a symmetric matrix with the property $\boldsymbol{F}^*\cdot\boldsymbol{F}=\boldsymbol{I}$, i.e. $\boldsymbol{F}^{-1}=\boldsymbol{F}^*$. One can easily write for (3)

$$\boldsymbol{F}\cdot\boldsymbol{K}\cdot\boldsymbol{F}^*\cdot\boldsymbol{F}\cdot\boldsymbol{f}=\boldsymbol{F}\cdot\boldsymbol{g} \tag{22}$$

or

$$\hat{\hat{\boldsymbol{K}}}\cdot\hat{\boldsymbol{f}}=\hat{\boldsymbol{g}} \tag{23}$$

where $\hat{\hat{\boldsymbol{K}}}=\boldsymbol{F}\cdot\boldsymbol{K}\cdot\boldsymbol{F}^*$ is row- and column-Fourier-transformed matrix $\boldsymbol{K}$ and $\hat{\boldsymbol{f}}$ and $\hat{\boldsymbol{g}}$ are the discrete Fourier spectra of $\boldsymbol{f}$ and $\boldsymbol{g}$. Instead of solving (3) one can solve (23) with subsequent inversion

$$\boldsymbol{F}^*\cdot\hat{\boldsymbol{f}}=\boldsymbol{F}^*\cdot\boldsymbol{F}\cdot\boldsymbol{f}=\boldsymbol{f} \tag{24}$$

Note that in case of convolutional problem (2) the matrix $\hat{\hat{\boldsymbol{K}}}$ must be diagonal with elements equal to $\hat{\boldsymbol{k}}=\left[\hat{k}_0,\hat{k}_1,...,\hat{k}_N\right]$ in (12).

3 Results and conclusions

The authors in [1] claim that the calculation using (23) and (24) leads to better results than the commonly used methods as e.g. Gauss-Jordan elimination method, QR method, or SVD method. As a testing device they use the matrix employed also in [2]

$$\begin{bmatrix}3 & 3 & 3 & 3\\ 5 & 5 & 5 & 5+\delta\\ 6 & 6 & 6+\delta & 6\\ 4 & 4+\delta & 4 & 4\end{bmatrix}\cdot\begin{bmatrix}x_1\\ x_2\\ x_3\\ x_4\end{bmatrix}=\begin{bmatrix}1.2\\ 1.3\\ 1\\ 0.5\end{bmatrix},\qquad \begin{bmatrix}x_1\\ x_2\\ x_3\\ x_4\end{bmatrix}=\begin{bmatrix}16/5\delta+0.4\\ -11/10\delta\\ -7/5\delta\\ -7/10\delta\end{bmatrix} \tag{25}$$

where the small disturbance δ is taken between $\delta\in(10^{-3}-10^{-14})$ and the exact solution (shown above) using the Cramer rule is easily obtained. Our results are shown in Tables 1 through 4.

Table 1. The solution using the Singular value decomposition

	x_1	x_2	x_3	x_4
δ = 1E-8	3.199997634233E+08	-1.099999308869E+08	-1.399999030618E+08	-6.999992907459E+07
δ = 1E-9	3.199971162495E+09	-1.099991261178E+09	-1.399987914113E+09	-6.999919868034E+08
δ = 1E-10	3.199724466667E+10	-1.099922764353E+10	-1.399885227223E+10	-6.999164750499E+09
δ = 1E-11	3.198856498745E+11	-1.099704419566E+11	-1.399459227526E+11	-6.996928516500E+10
δ = 1E-12	3.198596686178E+12	-1.099042649116E+12	-1.399042807803E+12	-7.005112292580E+11
δ = 1E-13	3.054973458180E+13	-1.056996915902E+13	-1.337075487763E+13	-6.609010545151E+12
δ = 1E-14	1.973866770514E+14	-8.386531412627E+13	-8.525580080273E+13	-2.826556212237E+13

Table 2. Singular values of the matrix

	σ_1	σ_2	σ_3	σ_4
δ = 1E-8	1,85472E+01	9,91000E-10	1,63220E-10	1,00000E-09
δ = 1E-9	1,85472E+01	9,90995E-11	1,63230E-11	1,00000E-10
δ = 1E-10	1,85472E+01	9,90995E-12	1,63284E-12	1,00003E-11
δ = 1E-11	1,85472E+01	9,90913E-13	1,63200E-13	1,00009E-12
δ = 1E-12	1,85472E+01	9,97066E-14	1,71425E-14	9,99405E-14
δ = 1E-13	2,66454E-15	1,85472E+01	9,76996E-15	9,76996E-15
δ = 1E-14	6,28037E-16	1,85472E+01	2,90881E-15	1,00249E-15

Table 3. Gauss-Jordan elimination

	x_1	x_2	x_3	x_4
δ = 1E-8	3.200000021115E+08	1.100000027409E+08	-1.400000006175E+08	-6.999999835301E+07
δ = 1E-9	3.199999735398E+09	1.099999908986E+09	-1.399999883930E+09	-6.999999420817E+08
δ = 1E-10	3.199999735248E+10	1.099999908986E+10	-1.399999884140E+10	-6.999999420817E+09
δ = 1E-11	3.199937562753E+11	1.099999908986E+11	-1.399999884161E+11	-6.999377696027E+10
δ = 1E-12	3.199093929060E+12	1.099695013264E+12	-1.399875550248E+12	-6.995233655474E+11
δ = 1E-13	3.188389116722E+13	1.098066163355E+13	-1.394920238566E+13	-6.954027148014E+12
δ = 1E-14	3.275345183542E+14	1.147611475294E+14	-1.432963517800E+14	-6.947701904483E+13

Table 4. Fourier method solution

	x_1	x_2	x_3	x_4
δ = 1E-8	3,199999943512E+08	1,099999926749E+08	-1,400000088445E+08	-6,999999243182E+07
δ = 1E-9	3,199999735631E+09	1,099999908986E+09	-1,399999884163E+09	-6,999999420817E+08
δ = 1E-10	3,199999735271E+10	1,099999908986E+10	-1,399999884163E+10	-6,999999420817E+09
δ= 1E-11	3,199919806289E+11	1,099919980040E+11	-1,400079813109E+11	-6,999200131363E+10
δ = 1E-12	3,199715543425E+12	1,099902218052E+12	-1,399875550248E+12	-6,999377751242E+11
δ = 1E-13	3,196395674214E+13	1,104015316365E+13	-1,386913681074E+13	-7,054666767748E+12
δ = 1E-14	3,198579280803E+14	1,049134004103E+14	-1,509729420539E+14	-6,397158561606E+13

It is to be pointed out that the matrix (25) is not a typical ill-conditioned matrix, it belongs to the class of the so called “numerically rank-deficient” matrices as seen from the Table 2. There is no substantial difference between the three methods. Slightly better results in last rows of Table 3 deserve more thorough investigation.

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