

ON THE DISCRETE LINEAR ILL-POSED PROBLEMS

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ABSTRACT

An inverse problem of photo-acoustic spectroscopy of semiconductors is investigated. The main problem is formulated as the integral equation of the first kind. Two different regularization methods are applied, the algorithms for defining regularization parameters are given.

1. THE STATEMENT OF THE PROBLEM

An inverse problem of photo-acoustic spectroscopy of semiconductors taking into account carrier diffusion and recombination consists of the recovering of real function $f(x)$, $x \in (-l, 0)$, $l > 0$, which is a part of the following boundary value problem [1]:

$$\frac{d^2 n(x)}{dx^2} - \left(\frac{1}{\tau} + i\omega\right)n(x) + f(x) = 0, \quad (1.1)$$

$$-Dn'(0) = v_s n(0), Dn'(-l) = v_s n(-l). \quad (1.2)$$

Values of $\Phi(0)$ are measured in the experiment for different values of frequencies $\omega_1, \omega_2, \dots, \omega_N$. Here the function $\Phi(x)$, $x \in (-(l_b + l), l_g)$, $l_b, l_g > 0$ is the solution of the boundary value problem

$$\frac{d^2 \Phi(x)}{dx^2} = \frac{i\omega}{\alpha(x)} \Phi(x) - V(x), \quad (1.3)$$

$$\Phi(-(l_b + l)) = 0, \quad \Phi(l_g) = 0. \quad (1.4)$$

Here $\alpha(x)$ is a known piecewise constant function and

$$V(x) = \begin{cases} i\omega n(x), & x \in [-l, 0], \\ 0, & x \notin [-l, 0]. \end{cases}$$

Using Green's functions for boundary value problems (1.1)-(1.2) and (1.3)-(1.4), the inverse problem (1.1), (1.2) is reduced to the solution of the Fredholm integral equation of the first kind [2]

$$\int_{-l}^0 K(\omega, x)f(x)dx = g(\omega) \quad (1.5)$$

with the kernel $K(\omega, x)$ of the exponential type. It is well known that such problem are ill-posed. Since the function $g(\omega)$ is measured only for finite discrete set of frequencies $\omega_1, \omega_2, \dots, \omega_N$, the problem (1.5) is discrete ill-posed. Furthermore, any measured data contain random errors $\epsilon_j, j = 1, 2, \dots, N$ bounded by the errors level

$$\left(N^{-1} \sum_{j=1}^N \epsilon_j^2 \right)^{1/2} \leq \delta$$

for some positive δ . Therefore, for the numerical solution of the inverse problem it is necessary to calculate the function $\bar{f}(x)$ on the basis of discrete data $g_j, j = 1, 2, \dots, N$ of the following form:

$$g_j = \bar{g}_j + \epsilon_j = (\varphi_j, \bar{f})_X + \epsilon_j, j = 1, 2, \dots, N, \quad (1.6)$$

where $\varphi_j(x) = K(\omega_j, x)$ are known linearly independent functions, $\bar{f}, \varphi_j \in X, X$ is a Hilbert space with the inner product

$$(\varphi_j, \bar{f})_X = \int_{-l}^0 \varphi_j(x)\bar{f}(x)dx.$$

A lot of problems in signal processing, geophysics can be formulated in the form (1.6), a good overview of discrete ill-posed problems is given in [3; 4].

Because of finite number of data, the solution of the inverse problem is nonunique, therefore, we look for the normal pseudo-solution $f^+(x)$ of the problem (1.6). It can be shown that $f^+(x)$ has the form

$$f^+(x) = \varphi(x)Q^{-1}\bar{g}, \quad (1.7)$$

where $\varphi(x) = (\varphi_1(x), \varphi_2(x), \dots, \varphi_N(x)), \bar{g} = (\bar{g}_1, \bar{g}_2, \dots, \bar{g}_N), Q$ is $N \times N$ Gram matrix with elements $q_{j,k} = (\varphi_j, \varphi_k), j, k = 1, 2, \dots, N$. See, for example, [5].

Since, the inverse problem (1.6) is ill-posed, the matrix Q^{-1} is ill-conditioned and for the numerical solution it is necessary to use a special regularization method. The Tikhonov's regularization method is very popular, which is convenient to use in semi-continuous form [6]. Accordingly to this scheme, the approximated solution is the function $f_\alpha(x)$ which minimizes on the space X the functional

$$\sum_{j=1}^N [(f, \varphi_j) - g_j]^2 + \alpha \|f\|_X^2, f \in X.$$

Here α is the regularization parameter which should be chosen. Although, during last thirty years the theory of regularization is quite well developed, the problem of finding parameter α is still important. See, for example, some recent papers [7; 8; 9; 10; 11; 12].

2. THE REGULARIZATION PARAMETER PROBLEM

All methods for determining the regularization parameter α can be divided into several types accordingly the used additional information. One group of methods uses *a priori* information concerning the error level δ . Usually one use the discrepancy principle [13]. It is noted that the discrepancy principle yields oversmoothed solution. It is shown in [14] that this method provides the smallest error propagation in the approximated solution but it gives the worst resolution. In reality, the error $\|f_\alpha - f^+\|$ can be reduced for some greater error propagation at the expense of improving the resolution. Such approach leads to the majorant principle [13], if an estimate of $\|f_\alpha - f^+\|$ is available [14]. Such approach was used also, for example, in [15; 16]. It should be noted that such estimate is not possible for entire X space and further assumption concerning the upper bound of the norm $\|f^+\|$ is necessary. In this case, the optimal choice of α is possible.

If *a priori* value $\|f^+\|$ is unknown, then one try to obtain it from the data, for instance, using the norm $\|f_\alpha\|$. Such approach is realized in [15]. We also use this idea in our paper.

Unfortunately, the sharp estimate of δ is desirable, since the accuracy of $\|f_\alpha - f^+\|$ is very sensitive to the change of δ . Therefore, we are interested in methods that do not use the error level δ . We mention *L*-curve method [7; 8], quasi-optimal choice [13], cross-validation method [6] (see also [9]). Unfortunately, all these methods are heuristic and they can not provide the convergence $f_\alpha \rightarrow \bar{f}$ as $\delta \rightarrow 0$, where \bar{f} is the solution of the integral equation

$$\int_{-l}^0 K(\omega, x) \bar{f}(x) dx = \bar{g}(\omega),$$

or of operator equation

$$T\bar{f} = \bar{g} \tag{2.1}$$

with a compact operator T in the Hilbert space X . Really, if for any $g \rightarrow \bar{g}$ the convergence $f_\alpha = R_{\alpha(\delta)}g \rightarrow \bar{f} = T^{-1}\bar{g}$ holds and $R_{\alpha(\delta)}g = Rg$, then simply $R \equiv T^{-1}$ and R is continuous, i.e. the inverse problem (2.1) is not ill-posed. So, for discrete ill-posed problems we should not expect that for $n \rightarrow \infty$ and $\delta \rightarrow 0$ we will get the convergence $f_\alpha \rightarrow f^+$. This means that any heuristic method of choosing the regularization parameter sometimes fail even for finite n . The non-convergence of the L -curve method is proved in [10].

3. THE METHOD OF THE REGULARIZATION FUNCTION

As it follows from [6], the regularized solution $f_\alpha(x)$ has the form

$$f_\alpha(x) = \varphi(x)(Q + \alpha E)^{-1}g, \quad (3.1)$$

where E is the unit $N \times N$ matrix. Our analysis is based on this formula and the estimate obtained earlier in [14]

$$|f_\alpha(x) - f^+(x)| \leq \Lambda(\alpha, x)(\delta + \alpha\|q\|_2), \quad (3.2)$$

where

$$q = Q^{-1}\bar{g},$$

$$\Lambda^2(\alpha, x) = \sum_{j=1}^N \frac{z_j^2(x)}{(d_j + \alpha)^2},$$

$$(z_1(x), z_2(x), \dots, z_N(x))^T = U\varphi(x),$$

UDU^T is the orthogonal decomposition of the matrix Q , $D = \text{diag}\{d_1, d_2, \dots, d_N\}$ is the diagonal $N \times N$ matrix of eigenvalues $d_j, j = 1, 2, \dots, N$.

If an estimate of $\|q\|$ is known, then the optimal choice of the regularization parameter α is that which provides minimal right-hand side of the inequality (3.2) (the majorant principle). We note that such regularization parameter depends on x , hence we have the regularization function $\alpha = \alpha(x), x \in (-l, 0)$.

Usually $\|q\|$ is unknown, in this situation we estimate $\|q\|$ from the data. The simplest way is to substitute the true vector q with the vector

$$q_\alpha = (Q + \alpha E)^{-1}g.$$

However, more precise approach can be used. From the definition of the q_α substituting $g = \bar{g} + \epsilon = Qq + \epsilon$ we deduce the equality

$$q = q_\alpha + \alpha(Q + \alpha E)^{-1}q - (Q + \alpha E)^{-1}\epsilon, \quad (3.3)$$

where $\epsilon = (\epsilon_1, \epsilon_2, \dots, \epsilon_N)^\top$. Substituting this formula for q into the right-hand side m times, we have

$$q = \sum_{j=1}^m \alpha^{j-1} (Q + \alpha E)^{-j} g - \sum_{j=1}^m \alpha^{j-1} (Q + \alpha E)^{-j} \epsilon + \alpha^m (Q + \alpha E)^{-m} q. \quad (3.4)$$

If m is quite large and $\alpha < 1$, then it is sufficient to use the first term. Substituting it into (3.2), we obtain the method for the choice of the regularization parameter. This method is not heuristic, since it uses the error level δ .

4. THE ANALYSIS OF SOME CLASSICAL METHODS

It is possible to use different values of the number m . Formula (3.4) allows us to analyze some well-known classical methods. For example, if $m = 2$ we obtain from (3.4) the quasi-optimal value of regularization parameter α , which can also be obtained from the relation criterion function. Really, for $m = 2$ we have

$$q \approx q_\alpha + \alpha(Q + \alpha E)^{-2} g = q_\alpha - \frac{\alpha}{2} \frac{dq_\alpha}{d\alpha}$$

and therefore

$$f^+ \approx f_\alpha - \frac{\alpha}{2} \frac{df_\alpha}{d\alpha}.$$

The best fitting is to find α providing minimum to the criterion function $\|\alpha \frac{df_\alpha}{d\alpha}\|$ (quasi-optimal value). In similar way the criterion function is formulated in [13].

If we use $m = 1$ and the formula (3.3), we obtain the inequality

$$\|q\|_2 \leq \|q_\alpha\|_2 + \|(Q + \alpha E)^{-1}\|_1 (\delta + \alpha \|q\|).$$

In order to find the best estimate of $\|q\|_2$ we need to minimize the right-hand side of the inequality. We may expect that the minimizer α of the criterion function

$$\frac{\|q_\alpha\|_2}{\|(Q + \alpha E)^{-1}\|_1} + \alpha \|q\|_2 + \delta$$

will be close to the optimal value. The constant δ does not change the position of the minimum and may be omitted. Neglecting the term $\alpha \|q\|_2$, we obtain the criterion function of the cross-validation method [6]. It can be seen that this method is not quite precise because it uses m equal only to 1. The cross-validation method was suggested for the case when errors $\epsilon_j, j = 1, 2, \dots, N$ are a white noise. This assumption is crucial for the application of the cross-validation method. Using our scheme and $m > 1$ we may use such criterion function without requiring the *a priori* distribution of measuring errors ϵ as well as in situations when the cross-validation method fails.

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DISKREČIŪJŲ BLOGAI SĄLYGOTŲ UŽDAVINIŲ KLAUSIMU

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Darbe nagrinėjamas foto-akustinės spektroskopijos puslaidininkiuose uždavinys, kuriame į vertinami nešėjų difuzijos ir rekombinacijos procesai. Reikia atstatyti šaltinio funkciją $f(x)$, jei žinoma antrosios eilės difuzijos lygtis ir atitinkamos kraštinės sąlygos. Naudojantis matavimų, atliktų įvairiuose dažniuose, rezultatais sprendžiamas atvirkštinis uždavinys, keli reguliarizacijos algoritmai, sprendžiamas reguliarizacijos parametrų parinkimo uždavinys. Naujieji metodai yra lyginami su klasikinais reguliarizavimo algoritmais.