The use of derivative spectrum of solution in regularization

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Abstract

The article is devoted to a new way of choosing the regularization parameters in the Tikhonov method as applied to inverse problems of light scattering. The derivative spectrum of the calculated solution is used as the selection criterion. The suggested method is compared with other well-known techniques such as the L-curve and the Generalized Cross Validation.

1. Introduction

The Fredholm equation of the first kind appears in many applied problems concerned with the determination of geometrical parameters of small particles:

$$\int_c^d K(\theta, a)\cdot\omega(a)\cdot da = I_S(\theta) \tag{1}$$

where $K(\theta,a)$ is the kernel of the integral equation, which characterizes light scattering by one particle with a characteristic dimension of a at an angle θ in the spherical coordinate system; $\omega(a)$ is the probability density function of particles sizes; $I_s(\theta)$ is the intensity of light scattered by the particle ensemble. It should be noted that Eq. (1) convolves the intensity of the light scattered by the particles with their sizes. The case of independent light scattering is considered.

The Tikhonov regularization method is one of the techniques widely used to solve this equation. According to the Tikhonov method, Eq. (1) has the following operator form [1, 2]:

$$\left(\alpha L + A^* A\right)\omega_\alpha = A^* I \tag{2}$$

where A is an operator that corresponds to the integral equation (1), A^* is the complex conjugate counterpart of A; ω_α is the required function corresponding to $\omega(a)$; I denotes $I_s(\theta)$, and the operator L is either the identity matrix or has the following form [1]:

$$L\omega = \omega - \frac{d^2\omega}{da^2} \tag{3}$$

The article deals with the presentation of the operator L in form of Eq. (3).

As the problem (1) is ill-posed, certain additional criteria [1, 2] should be applied in order to get acceptable results. The first derivative spectrum of the calculated $\omega(a)$ is suggested to be used as one of such criteria. It is known [3] that the higher harmonics of the solution of Eq. (1) converge to the exact solution slower than its lower harmonics. One should find the solution the first derivative spectrum of which contains the smallest number of the highesto-order harmonics. In the symbolic form this can be put in the following equation:

$$\min\left(\max\left(F_i\left(\omega_\alpha\right)\Big|_{\alpha_{\min} < \alpha < \alpha_{\max}}\right)\right) \tag{4}$$

where F_i is the magnitude of the i-th harmonic of spectrum F solution's derivative ω_α; $\alpha_{\min}$ and $\alpha_{\max}$ are the boundaries of the range of variation of the parameter α.

In Eq. (4), the regularization parameter α varies within certain boundaries. The boundaries are determined by the application of some additional requirements. The model investigation of the functional given by Eq. (5) below, as described in [4], is used in order to constrain these boundaries:

$$\frac{\left\|\omega_\alpha - \omega\right\|_{L_2}}{\left\|\omega\right\|_{L_2}} \tag{5}$$

where ω_α is the solution of Eq. (1) corresponding to a certain value of the parameter α; ω is the exact solution of Eq. (1).

In [4] it is shown that the functional (5) has one minimum. Since the mentioned functional is in fact the analog of relative error in the L_2 space, the minimum of the function will be reached when ω_α is the closest to the exact solution in the L_2 space. The optimal regularization parameter value will correspond to that ω_α. One can state that the value of the optimal regularization parameter and the corresponding solution is the best among all possible solutions for a given second term of Eq. (1). The results of a model investigation, shown in the next section, are used to determine the variational boundaries of the parameter α.

2. Simulations

The conventional Mie theory was used in order to compute the kernel of the integral equation (1).

From the physics point of view, there are some requirements to $\omega(a)$: this function should be defined from 0 to ∞ and should have a finite number of extrema; the values of $\omega(a)$ are above zero; it is bounded from above by a given constant C and satisfies the following standardization condition:

$$\int_0^\infty \omega(x)dx = 1 \tag{6}$$

The distributions of Raileigh, χ^2, Nakagami, Gamma etc. satisfy the requirements. In this article the distribution of Raileigh and χ^2 are used as an approximation of the particle size distribution. These approximations are described in [5] and [6].

In order to make the analysis more realistic, families of Raileigh and χ^2 distributions were used instead of one fixed form of the probability density function (PDF). The used PDF families are shown in Fig. 1.

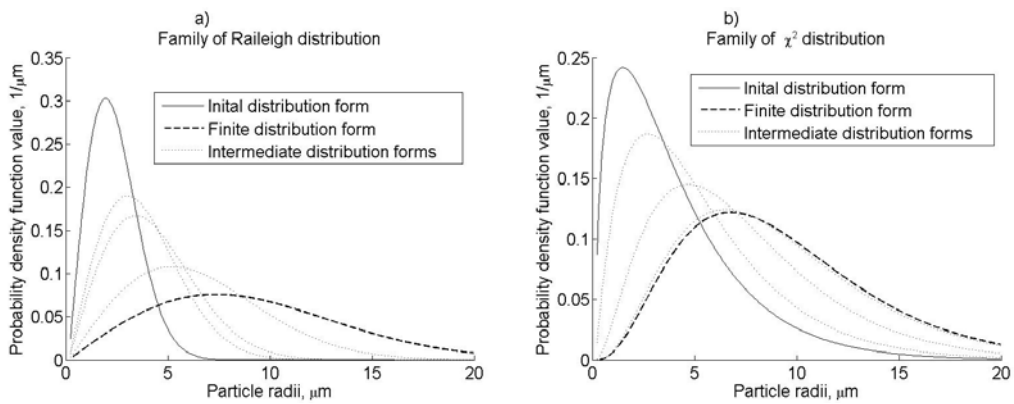

Figure 1: Families of Raileigh and χ^2 distributions

The following simulations were performed to determinate the boundaries of the “best” regularization parameter magnitudes, i.e., the parameter values that in each case, when the equation is solved, correspond to ω_α which is the closest to the exact solution. In the simulations such regularization parameter values, that minimize Eq. (5), were segregated.

The frequency diagrams of the regularization parameter values spread are presented in Fig. 2.

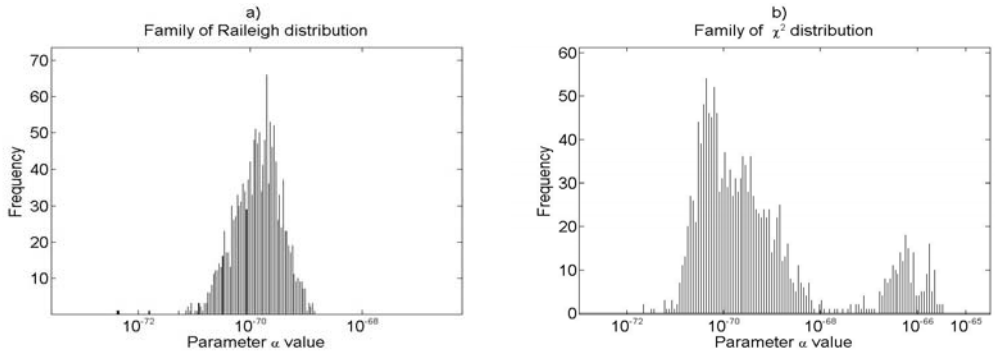

Figure 2: Spread of optimal regularization parameter values.

Figure 2 shows that α values are concentrated in certain limits for both families of distributions. In the case of the Raileigh distribution family the values of α parameter are within 10^{-69} – 10^{-71}, as for the χ^2 distribution family they are within 10^{-65} – 10^{-72}. These regularization parameter limits were used to calculate the solution of the Fredholm equation of the first kind by applying the criterion (4).

It is reasonable to present the solution of Eq. (1) for distribution families in the form of the errors described by Eq. (7):

$$\nu(a_j) = \frac{\bar{\varpi}(a_j) - \omega_\alpha(a_j)}{\max\left(\bar{\varpi}(a_j)\right)} \cdot 100\%, \tag{7}$$

where $\bar{\varpi}(a_j)$ is the exact solution at a_j, $\omega_\alpha(a_j)$ is the calculated solution at a_j.

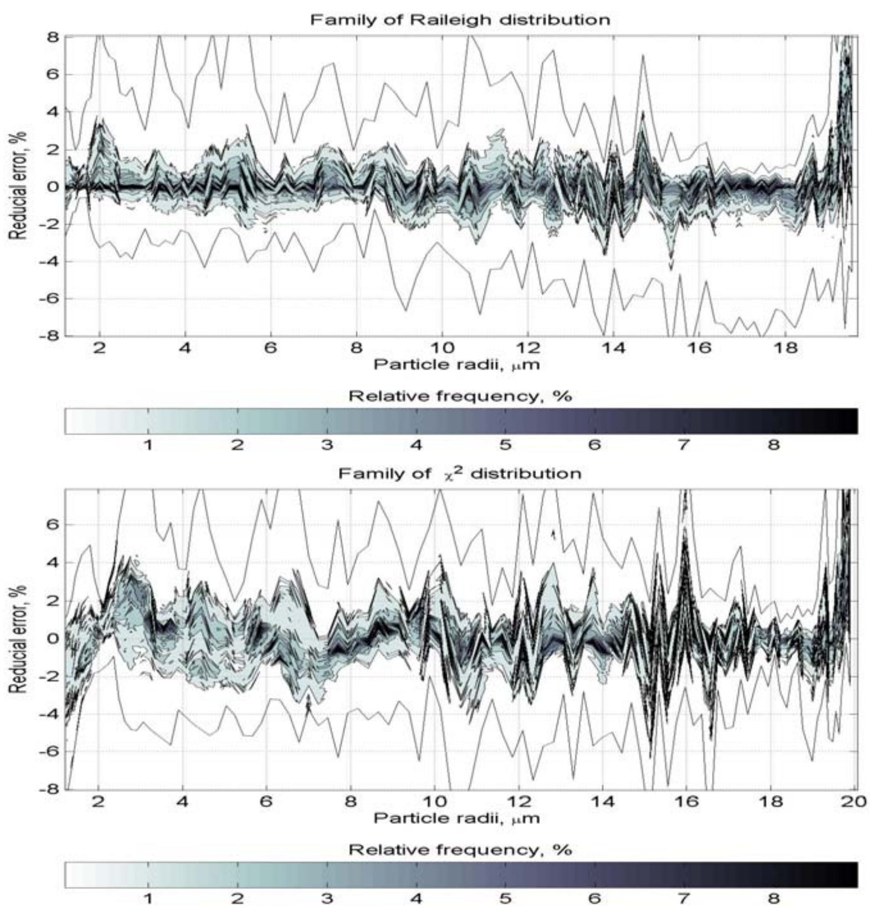

Figure 3: Results of $\omega(a)$ computatation for families of Raileigh and χ^2 distributions.

In Fig. 3 the results of $\omega(a)$ computations for families of Raileigh and χ^2 distributions are shown. By fixing the particle size value a one can see the boundary values of $\omega(a_i)$ and relative frequency of calculated $\omega(a_i)$ on the y axis. In fact, having the fixed particle radius magnitude we deal with a histogram of the spread of $\omega(a_i)$ determination errors values. Instead of the usual histogram frequency, the relative frequency is used. The same colors correspond to the $\omega(a)$ values that occur with the same relative frequency.

Similar simulations were also performed for other methods of regularization parameter determination such as the *L*-curve [7, 8] and the Generalized Cross Validation [9]. Comparison of the derivative spectrum method with the *L*-curve and Generalized Cross Validation methods proved the advantages of the suggested method.

3. Conclusions

The new way of regularization parameter determination in Tikhonov regularization method is proposed. The advantages of the suggested method over the *L*-curve and Generalized Cross Validation techniques are demonstrated.

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