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INVERSION OF ELASTIC LIGHT SCATTERING MEASUREMENTS TO DETERMINE REFRACTIVE INDEX AND PARTICLE SIZE DISTRIBUTION OF POLYMERIC EMULSIONS

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Polymeric emulsions are well characterized by the knowledge of their particle size distributions (PSD). Elastic-light-scattering (ELS) measurements can be inverted to estimate the PSD in the range from 50 nm up to several micrometers. The relative refractive index of the particles is required in computation procedures to obtain the PSD. Small differences in the assumed refractive index may cause significant differences in the resulting PSD. From the scattering data, the refractive index can be determined. In this article we present the corresponding technique. We consider polymeric emulsions where the nonabsorption assumption is reasonable.

We propose a methodology based on Tikhonov regularization applied only to the distribution. However, we solve the minimization problem simultaneously with respect to the distribution and the refractive index. To select the regularization parameter, we include the Generalized Cross Validation (GCV) technique. From simulated ELS measurements we show that the problem is solved successfully.

Keywords: Elastic light scattering; Generalized cross validation; Tikhonov regularization

INTRODUCTION

Emulsion polymerization systems are typically composed by three coexisting phases: a continuous (usually aqueous) phase, monomer droplets, and polymer particles. In particular, the size of the polymer particles greatly affects the properties of the final material. So, the knowledge of the emulsion particle size distribution (PSD) is important to fully characterize the material.

The most popular technique for the determination of PSDs is elastic light scattering (ELS), since it is an easy to perform and nondestructive experimental technique. The emulsion sample is illuminated by a monochromatic beam and the scattered light, averaged over time, is measured as a function of the scattering angle. This angular intensity, having the same wavelength as the incident beam, is influenced by the

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size, the shape and the optical contrast of the particles (Mie theory [1]). The difficulty associated with this technique is related to the inversion of the measurements to extract the desired information form the data. Size, shape, and optical contrast can be described by a large number of parameters, which cannot completely be extracted from the intensity spectrum stem from a light scattering experiment. The reasons of this fact are: the ill-posed nature of the problem, the statistical noise of experimental data, and the existence of singularities.

The determination of the PSD from ELS measurements, assuming that all parameters in the model are known exactly has been studied by several authors [2–4]. Since the inverse problem can be stated as linear, several regularization methods can be applied [5,6]. A large variety of inversion techniques for light scattering data exist [7,8]. In general, these techniques are classified as either analytical or empirical. Analytical techniques involve formal solutions of integral equations that describe the light scattering process, and require the use of *a priori* information regarding the distribution function because of the ill-posed nature of the inverse problem. Empirical inversion techniques generally require that a parametric model of the light scattering process be developed. The parameters are then adjusted within physically realistic bounds so that a least squares fit of the measured data is obtained.

We are interested in the problem of determining PSD and relative refractive index of polydisperse colloidal particles. In this case the inverse problem is nonlinear. Some previous publications have considered this problem. Schnablegger and Glatter [9], reported a methodology to retrieve PSD and refractive index from ELS in the presence of scattered light reflected from the walls of the sample holder. They represented the sought distribution by a series of β-spline functions and imposed to the solution smoothing and positive constraints, and determined the regularization parameter by means of a sensitivity plot constructed from the residuals. Jones *et al.* [10] combined analytical and empirical inversion techniques to obtain optical parameters and PSD. They chose an orthonormal base to expand the solution and followed a procedure consisting in sequential steps: first, the retrieval of the refractive index through the use of the unconstraint solution, then, the retrieval of the PSD through the use of the constraint solution, and finally the retrieval of the absorption index by matching the measured and calculated scattering patterns. They concluded from simulated experiments that this procedure gives the best results for narrow distributions.

Our goal is to develop a more general and analytical methodology to estimate simultaneously PSD and refractive index from ELS measurements. Our approach involves techniques for the automatic determination of the regularization parameter, and yields good results with fewer empirical considerations.

THE DIRECT PROBLEM

Consider a given particle of a particular shape, size and composition, which is illuminated by a light beam of a specific wavelength, intensity and polarization. The determination of the resulting electromagnetic field from the scattering process, based on the solution of Maxwell equations is called the 'direct problem'. The most important exactly soluble problem in the theory of absorption and scattering by small particles is that by a sphere of arbitrary radius and refractive index, derived by Mie [11] and other authors [12]. The angular scattered intensity due to a polydisperse system can be regarded as a linear combination of Lorenz–Mie form factors $S(\theta, D, m)$, where θ is the scattered angle, D is the particle diameter, and m is the relative complex refractive index of the particles in the solvent. If we proceed and regard the coefficients of the linear combination as a continuous function $f(D)$ that represents the emulsion PSD, we obtain the integral expression that has to be evaluated to find the angular-dependent scattering curve of the polydisperse system, as

$$I(\theta, m) = \int_{D_{\min}}^{D_{\max}} S(\theta, D, m) f(D) dD \tag{1}$$

For the calculations of the direct problem we use the computer programs reported in the literature [13]. A similar program is also given in [14].

The complex relative refractive index m is defined as the ratio of the complex refractive index of the particle n_1 to that of the solvent n_2. Because of the small value of the imaginary part of the refractive index (i.e. absorption coefficient), m is approximated by its real value (i.e. scattering coefficient). Scattering and absorption coefficients are usually refer as optical constants. We use this approximation since for the range of wavelengths of the incident beam commonly used in the experimental equipments, the absorbed light by the polymer particles can be neglected for the materials we are considering.

As a concluding remark, it can be said that the availability of reliable optical constants is critical for the use of Mie theory.

THE INVERSE PROBLEM

In practice, it often occurs that the particles responsible for the scattering cannot be analyzed directly. From a study of the scattered field, we then have to determine the characteristics of the particles.

In this article, we consider that the particle characteristics to be determined from the scattered intensity spectrum, $I(\theta, m)$, are $f(D)$ and m. All other parameters are assumed known. It is obvious from Eq. (1) that the relation between $I(\theta, m)$ and $f(D)$ is linear. Contrarily, m is in the kernel of the integral equation, so its relation with respect to $I(\theta, m)$ is nonlinear. Thus, the determination of all the unknowns needs the solution of a nonlinear inverse problem.

There are two aspects to be taken into account to solve this class of nonlinear inverse problem. The first one, the relations described in last paragraph, will allow us to derive a quasi-analytical solution. The second is that the problem ill posedness is only with respect to $f(D)$. This property can be described by the fact that small perturbations on m produces large differences in $I(\theta, m)$ when one evaluates the direct problem, behavior opposite to that observed for ill posedness. On the other hand, the decay rate of the singular values of the kernel of the integral equation, which can be used as a measure of the degree of ill posedness [5], is practically not affected by the value of m.

Regularization of the Inverse Problem

The general formulation of the inverse problem addressed in last paragraphs is the following.

Consider the integral equation

$$T(m)[f] = \int_{-\infty}^{\infty} S(\theta, D, m) f(D) dD = I(\theta, m) \tag{2}$$

where the distribution $f(D)$ and the parameter m are the unknowns. Noisy measurements $g(\theta)$ are available, with experimental error $\varepsilon(\theta)$, i.e.

$$g(\theta) = I(\theta, m) + \varepsilon(\theta). \tag{3}$$

We propose to find the solution of the problem optimizing the following functional

$$\text{Min } J(m,f) = \| T(m)[f] - g(\theta) \|^2 + \gamma = \| L(f) \|^2 . \tag{4}$$

Equation (4) shows that we apply Tikhonov [15] regularization only to $f(D)$. $L(f)$ is the smoothing restriction included as the *a priori* information about the sought distribution and γ the regularization parameter which weighs this inclusion.

The possible local minima are found solving the equations:

$$\frac{\partial}{\partial m} J(m,f) = 0, \quad \frac{\partial}{\partial f} J(m,f) = 0,$$

which result in:

$$\left(\frac{\partial}{\partial m} T(m)[f]\right)^* \left(T(m)[f] - g\right) = 0 \tag{5}$$

$$f = \left(T(m)^* T(m) + \gamma L\right)^{-1} T(m)^* g \tag{6}$$

Substitution of Eq. (6) into Eq. (5) yields:

$$\left(\frac{\partial}{\partial m} T(m)[(T(m)^* T(m) + \gamma L)^{-1} T(m) \times g]\right)^* \times (T(m)[(T(m)^* T(m) + \gamma L)^{-1} T(m)^* g] - g) = 0. \tag{7}$$

In fact, the solution of this single equation (Eq. (7)) in terms of m, for a specific value of the regularization parameter γ, gives an estimation of the sought parameter, i.e., $\tilde{m}$. The evaluation of Eq. (6) using $\tilde{m}$ gives the estimation of the PSD, $\tilde{f}$.

Although γ, m, and f must be determined to solve the problem, *a prior* selection of the regularization parameter must be performed, since γ is constant in the minimization problem (Eq. 4)), as usual in Tikhonov regularization. The relation between the selection of the regularization parameter and the quality of the estimations is analyzed in the next section.

Selection of the Regularization Parameter

We follow two different approaches for the selection of the regularization parameter. The first one can be applied in any situation since no estimation on noise level is needed. It involves an iterative procedure whose behavior is robust and gives good estimations of the problem unknowns. The second approach is more analytical and needs no iterations. However, it needs one to assume bounds on the perturbation of the sought parameter and on the measurement noise which greatly affects the quality of the solution. Thus, its application in real experiments may be more difficult.

Iterative Method

For any γ Eq. (7) can be solved and the value of m determined. It has been noticed that regardless the γ value, the solution $\tilde{m}$ is nearly the same. In fact, this is true as long as γ is in a range where multiple solutions in Eq. (7) are avoided. Contrarily, the estimated distribution $\tilde{f}(D)$ obtained evaluating Eq. (6) for each γ may differ greatly. It is necessary to obtain the optimal value of the regularization parameter to retrieve the correct distribution. The Generalized Cross Validation (GCV) technique developed by Wahba [16] for the selection of the regularization parameter for linear inverse problems could be used. This is possible since once m is determined, the inverse problem stated by Eq. (2) becomes linear.

We propose an iterative procedure for the selection of the regularization parameter, γ, to find the estimation of the unknown parameter in the kernel, $\tilde{m}$, and the unknown distribution $\tilde{f}$, that can be summarized as follows

1. Select an initial value of the regularization parameter, γ_0.
2. Find $\tilde{m}_1$ such that Eq. (7) is fulfilled.
3. Find a new value of the regularization parameter γ_{GCV_1} applying the GCV technique, for the linear problem stated using $\tilde{m}_1$.
4. Repeat Steps 2 and 3 finding $\tilde{m}_i$ and γ_{GCV_i} for $i = 1, 2, \ldots$ until the parameters values stay invariant. Call $\tilde{m}$ and γ the final values.
5. Find $\tilde{f}$ evaluating Eq. (6).

The application of this iterative process gives, in few steps, good estimations of the solution of the inverse problem.

One Step Method

We analyzed an alternative method based on Neubauer's technique [17] to select the optimal regularization parameter that can be used when good estimations of the modeling error and the noise level present in the measurement are known.

Let m^o be the exact value of parameter m. As a consequence of the uncertain value of parameter m in the kernel, there is an error h that can be considered as a modeling error, given by

$$\| T(m) - T(m^o) \| = h(m) \leq \tilde{h}. \tag{8}$$

Let also $\delta = \| \varepsilon \|$ be the noise level present in the measurement. Neubauer [17] derived a method for choosing the regularization parameter that takes into account this situation (see the appendix). The constant value of γ in Eqs. (4), (6) and (7) should be changed by $\gamma(m)$, the optimal regularization parameter that corresponds to the problem defined to each value of m. Notice that an additional term containing $d\gamma(m)/dm$ will appear in Eqs. (5) and (7). The simultaneous solution of Eqs. (7) and (A-3) gives, in one step, the values of $\tilde{m}$ and of the regularization parameter $\gamma_{\text{Neub}} = \gamma(\tilde{m})$. Finally, as before, $\tilde{f}$ is found from Eq. (6). It should be said that Neubauer's method is derived for $\| L(f) \|^2 = \| f \|^2$ in Eq. (4).

In practice, $h(m)$ can never be known exactly, since $T(m^o)$ is unknown, then a superior bound $\tilde{h}$ should be estimated. In this case the obtained solution may differ greatly form the optimal.

COMPUTATIONS AND RESULTS

To illustrate the validity of the regularization method to obtain the refractive index and the PSD of a polymeric emulsion from the knowledge of the scattered intensity spectrum, we consider two examples.

In order to compare the results for situations involving random measurement errors, we assume normally distributed uncorrelated errors with zero mean and constant standard deviation. The simulated noisy measurements can be expressed, in the discrete domain, as

$$g_{\varepsilon i} = g_i + \varepsilon_i \tag{9}$$

where $g_i = I(\theta_I)$ is the exact solution of the direct problem for the exact value of the parameter m^o and the exact distribution **f**, corresponding to a particular scattered angle θ_i, and ε_i the noise added at that angle. Let us write the discrete version of the inverse problem stated by Eq. (4) as

$$\min_{\mathbf{f}, m} \mathbf{J} = \| g_\varepsilon - \mathbf{A}(m)\mathbf{f} \|^2 + \gamma\, \mathbf{f}^{\mathrm{T}}\mathbf{H}\mathbf{f} \tag{10}$$

where vector g_ε represents the scattered intensity for all measured angles, matrix $\mathbf{A}(m)$ the discrete form of the operator $T(m)$, $\mathbf{H} = \mathbf{K}^{\mathrm{T}}\mathbf{K}$ and $\mathbf{Kf}$ is the discrete form of $L(f)$. We consider in all cases $L(f)$ as the second derivative of f.

The first example corresponds to a polystyrene emulsion in water ($m^o = 1.1867$) having spherical particles with diameters in the range of 50–2550 nm distributed as a broad number PSD, as the one shown in Fig. 1. The simulated spectrum g_ε (Fig. 2) corresponds to 70 equally spaced scattered angles from 12° to 150°, where the noise standard deviation σ_ε is equal to 1% of the mean value of the measurements. We use this data to retrieve m^o and **f**, the solution of the inverse problem.

The results obtained following the iterative method are $\tilde{m} = 1.1867$ and $\tilde{\mathbf{f}}$ as in Fig. 1 (solid line), for $\gamma = 4.0\text{E}5$. The first stage of this method requires to minimize J in Eq. (4), or **J** in Eq. (10), for a given value of the regularization parameter γ. We explored the solutions obtained for different values of γ, some of them transcribed in Table I, and we visualized the evolution of the functional plotting $J_\gamma(m)$ *vs* m in Fig. 3 by introducing Eq. (6) into Eq. (4). The results of performing the iterative process

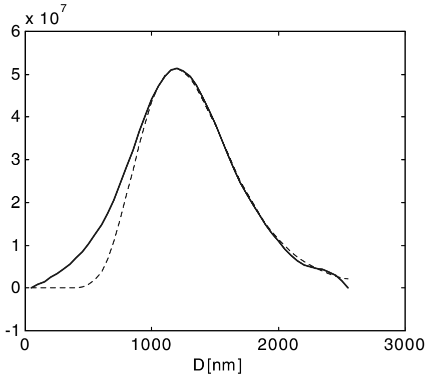

FIGURE 1 Real (- - -) and estimated (—) PSD for Example I.

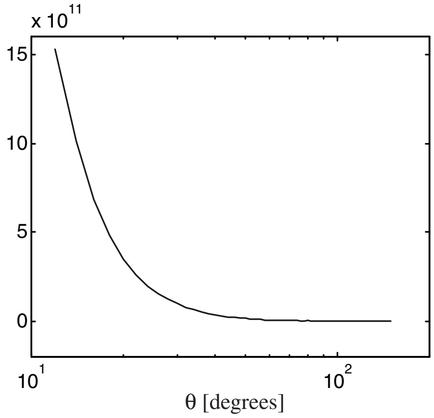

FIGURE 2 Light scattering spectrum for Example I.

TABLE I Results of the iterative method for Example I

γ_0	$\tilde{m}_1$	γ_{GCV_1}	$\tilde{m}_2$	γ_{GCV_2}	$\tilde{m}_3$	γ	$\tilde{m}$
1.0E 1	undetermined						
1.0E 0	1.1895	1.0E 5	1.1875	3.2E5	1.1869	4.0E5	1.1867
1.0E 1	1.1890	1.6 E	1.1875	3.2E5	1.1869	4.0E5	1.1867
1.0E 2	1.1885	2.0E 5	1.1870	4.0E5	1.1867	4.0E5	1.1867
1.0E 3	1.1885	2.0E 5	1.1870	4.0E5	1.1867	4.0E5	1.1867
1.0E 4	1.1850	3.2E 5	1.1870	4.0E5	1.1867	4.0E5	1.1867
1.0E 5	1.1875	3.2E 5	1.1870	4.0E5	1.1867	4.0E5	1.1867
1.0E 6	1.1860	5.0E 5	1.1865	5.0E5	1.1866	5.0E5	1.1866
1.0E 7	1.1845	1.0E 4	1.1850	3.2E5	1.1869	4.0E5	1.1867
1.0E 8	1.1830	5.0E 3	1.1885	2.0E5	1.1872	4.0E5	1.1867
1.0E 9	1.1805	2.5E 3	1.1870	4.0E5	1.1867	4.0E5	1.1867
1.0E 10	1.1745	8.0E 2	1.1885	2.0E5	1.1872	4.0E5	1.1867

are shown in the other columns of Table I. For each value of $\tilde{m}$ we applied the GCV technique and obtained a new value of the regularization parameter, γ_{GCV}. The last two columns show that the convergence of the method is achieved from any initial value.

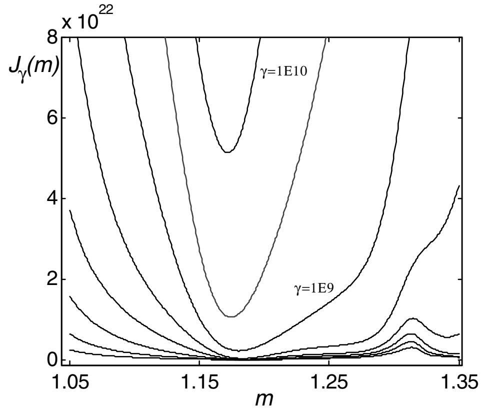

FIGURE 3 Evolution of the functional for Example I.

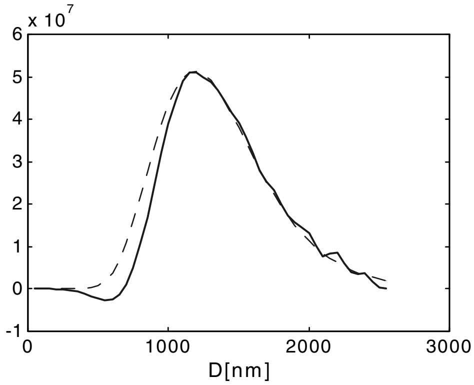

FIGURE 4 Real (- - -) and estimated (—) PSD for Example I obtained by the one step method.

The results obtained applying the one step method are $\tilde{m} = 1.1867$ and $\tilde{\mathbf{f}}$ as in Fig. 4, obtained for $\gamma_{\mathrm{Neub}} = 1.1\mathrm{E}4$. This solution was obtained using the exact norm of the modeling error $h(m)$, not available in real experiments. We tried for several values of $\tilde{h}$ with no success, showing that the one step method is not appropriate for this case. The difference between the retrieved PSDs in Figs. 1 and 4 is due to the fact that in the one step method $\| L(f) \|^2 = \| f \|^2$, as we said in the previous section.

The second example was taken from the literature [9]: a bimodal gaussian distribution shown in Fig. 6 represents the volume distribution of an emulsion. Its exact relative refractive index is m^o=1.25. The simulated measurements, shown in Fig. 7, were generated with additive noise with statistical parameters as in the first example.

For this case we show the results obtained using the iterative procedure. The result for the steps found for two different starting points are shown in Table II. Figure 8 shows the functional behavior for some specific values of the regularization parameters.

Thus, the solution obtained is $\tilde{m} = 1.252$, $\gamma = 3.1\mathrm{E}5$ and the estimated PSD as in Fig. 6 in solid line.

1

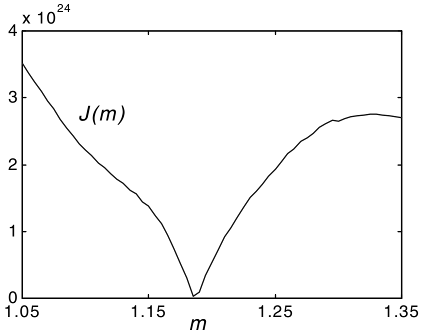

FIGURE 5 Evolution of the functional for Example I obtained by the one step method.

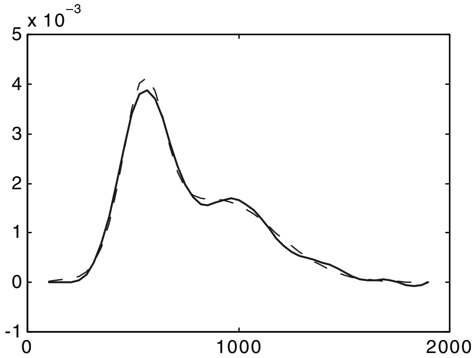

FIGURE 6 Real (- - -) and estimated (—) volume PSD for Example II obtained by the iterative method.

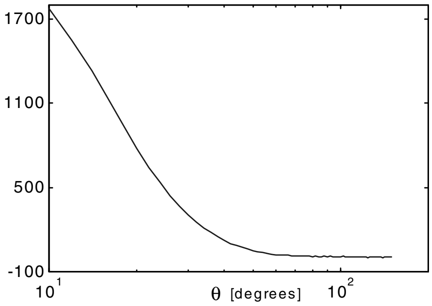

FIGURE 7 Light scattering spectrum for Example II.

TABLE II Results of the iterative method for Example II

γ_0	$\tilde{m}_1$	γ_{GCV_1}	$\tilde{m}_2$	γ_{GCV_2}	$\tilde{m}_3$	γ	$\tilde{m}$
1.0E6	1.242	2.5E7	1.250	3.1E5	1.252	3.1E5	1.252
1.0E11	1.278	5.6E7	1.254	3.5E5	1.252	3.1E5	1.252

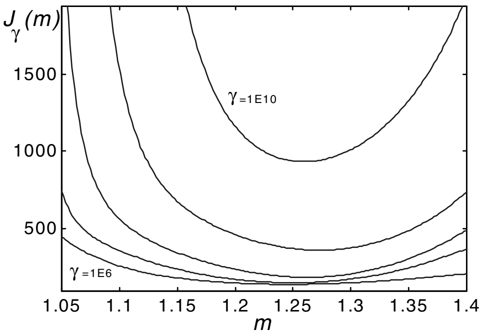

FIGURE 8 Evolution of the functional for Example II.

CONCLUSIONS

An inversion technique that retrieves the particle size distribution and the relative refractive index of nonabsorbing spherical particles from simulated measurements of ELS has been developed. The general formulation of the problem takes the form of a nonlinear inverse problem since the Fredholm equation representing the light scattered has an unknown parameter in its kernel.

The solution is obtained by means of an iterative procedure that improves the values of the refractive index and the regularization parameter, based on the generalized cross validation technique. Attempts to use a noniterative method based on Neubauer's approach [17] were less successful.

Because of the ill-posed nature of the inverse light scattering problem, *a priori* information regarding the PSD was used as in Tikhonov regularization. No *a priori* information about the refractive index was necessary. High accuracy of the resulting refractive index for scattering data with typical error level was observed.

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NOMENCLATURE

$\mathbf{A}$ = matrix form of operator T
D = particle diameter
f = particle size distribution (PSD)
$\mathbf{f}$ = vector form of PSD
g = noisy ELS measurement
$\mathbf{H}$ = matrix form of L
I = light scattering intensity
J = functional
L = smoothing restriction on f

m = relative particle refractive index
n_1 = particle refractive index
n_2 = solvent refractive index
S = Lorentz–Mie scattering function
T = operator that represents the integral equation

Greeks

ε = experimental error
γ = regularization parameter
λ = wavelength of the incident beam
θ = scattering angle

Superscript

$\sim$ = estimated values
$*$ = adjoint

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APPENDIX

Generalized Cross Validation (GCV)

One of the most popular methods for the determination of the regularization parameter is the GCV due to Golub and Wahba [16].

For the regularized linear inverse problem in discrete form given by

$$\underset{\mathbf{f}}{\mathrm{Min}} \parallel \mathbf{Af} - g_\varepsilon \parallel^2 + \gamma \mathbf{f}^{\,T}\mathbf{Hf}, \tag{A-1}$$

the GCV criterion for the selection of the regularization parameter γ is to minimize the function $V(\gamma)$

$$\underset{\gamma}{\mathrm{Min}}\, V(\gamma) = n\frac{\parallel \mathbf{Af} - g \parallel^2}{(\mathrm{traza}(\mathbf{I} - \tilde{\mathbf{A}}(\gamma)))^2} = n\frac{\sum_{i=1}^{n} (\gamma/(\lambda_i + \gamma))^2 z_i^2}{\left(\sum_{i=1}^{p} \gamma/(\lambda_i + \gamma) + n - p\right)^2} \tag{A-2}$$

where, $[z_1 z_2 \cdots z_n]^{\mathrm{T}} = \mathbf{U}^{\mathrm{T}} g$, $\lambda_i (i = 1, \ldots, p)$ are the eigenvalues of $\mathbf{X}^{\mathrm{T}}\mathbf{X}$, $\lambda_i = 0$, $i > p$. $\mathbf{U}$ is defined by the singular value decomposition (SVD) of $\mathbf{X} \rightarrow \mathbf{X} = \mathbf{UDV}^{\mathrm{T}}$ where $\mathbf{X} = \mathbf{AK}^{-1}$, $\mathbf{H} = \mathbf{K}^{\mathrm{T}}\mathbf{K}$, and $\tilde{\mathbf{A}}(\gamma) = \mathbf{A}(\mathbf{A}^{\mathrm{T}}\mathbf{A} + \gamma\mathbf{K}^{\mathrm{T}}\mathbf{K})^{-1}\mathbf{A}^{\mathrm{T}}$.

Neubauer's Method

For the regularized linear inverse problem in discrete form given by

$$\underset{\mathbf{f}}{\mathrm{Min}} \parallel \mathbf{A}(m)\mathbf{f} - g_\varepsilon \parallel^2 + \gamma \mathbf{f}^{\mathrm{T}}\mathbf{If},$$

where $\parallel \mathbf{A}(m) - \mathbf{A} \parallel \leq h$ and $\parallel g_\varepsilon - g \parallel \leq \delta$, the regularization parameter γ is selected as the value that satisfies:

$$N(\gamma, g_\varepsilon, \mathbf{A}(m)) = \gamma^3 \langle (\mathbf{A}(m)\mathbf{A}(m)^{\mathrm{T}} + \gamma\mathbf{I})^{-3} g_\varepsilon, g_\varepsilon \rangle == (Dh \parallel \mathbf{f}_\gamma \parallel + \delta)^2 \tag{A-3}$$

where $D = 1.1$ and $\mathbf{f}_\gamma = (\mathbf{A}(m)^{\mathrm{T}}\mathbf{A}(m) + \gamma\mathbf{I})^{-1}\mathbf{A}(m)^T g_\varepsilon$.

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