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Optimization of regularization parameter of inversion in particle sizing using light extinction method

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Abstract

In particle sizing by light extinction method, the regularization parameter plays an important role in applying regularization to find the solution to ill-posed inverse problems. We combine the generalized cross-validation (GCV) and L-curve criteria with the Twomey–NNLS algorithm in parameter optimization. Numerical simulation and experimental validation show that the resistance of the newly developed algorithms to measurement errors can be improved leading to stable inversion results for unimodal particle size distribution.

Keywords: Particle size analysis; Light extinction; Inversion algorithm; Regularization parameter

1. Introduction

Particle sizing by light extinction method (LEM) has advantages of speed and simple instrument. With known refractive index, particle diameter, ranging from $x = 0.1$ to $10\ \mu\text{m}$, and its concentration can be obtained simultaneously. The critical problem with LEM is the determination of particle size distribution (PSD) from measured extinction spectrum, caused mainly by the oscillation behavior of kernel function *versus* particle size, namely the extinction coefficient Q_{ext} *versus* the size parameter $\alpha = \pi x/\lambda$, so that ill-posed equations often arise (Su et al., 2004; Xu, Cai, Ren, & Grehan, 2004a; Xu, Cai, Su, Zhao, & Li, 2004b).

In optical particle sizing, inversion algorithm is one of the main interests of many researchers. Two types of such algorithms have been developed: dependent and independent. The dependent model algorithm assumes that the particle system to be measured conforms to a given size distribution, e.g. lognormal or Rosin–Rammler, which is characterized by two parameters to be decided by the dependent model algorithm. And the independent model algorithm does not assume any particle size distribution in advance, but solves directly the Fredholm integral equations of the first kind. As a critical problem of the independent model algorithm, optimization of the regularization parameter calls for discussion.

2. Inverse problem in multi-wavelength light extinction method

The multi-spectral light extinction method is based on the measurement and inversion of a series of extinction ratios corresponding to a set of wavelengths. When the incident light traverses a particle system, its original intensity is reduced due to scattering and absorption by the particles suspended in the medium. To quantify such a process, Lambert–Beer law is employed:

$$\frac{\ln(I_0/I)_j}{L} = \int_{x_{\min}}^{x_{\max}} N(x) C_{\text{ext}}(\lambda_j, x, m)\, \mathrm{d}x \tag{1}$$

where $x_{\min}$ and $x_{\max}$ are the lower and upper limits of the particle diameter range of PSD; $N(x)$ the number frequency distribution; C_{ext} is the extinction cross-section determined from the wavelength λ_j, diameter of the particles x as well as the refractive index of the particle m. Eq. (1) is the Fredholm integral equa-

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tion of the first kind, which can be numerically discretized into matrix form as follows:

$$\mathbf{Tq} = \mathbf{y} \tag{2}$$

where the element of the coefficient matrix **T** can be calculated by $T_{j,i} = C_{\text{ext}}(\lambda_j, m, x_i)$, where x_i is the effective diameter of each diameter interval, **y** the spectrum vector corresponding to the different wavelengths and **q** is the solution vector of frequency distribution (number frequency or volume frequency distribution).

More generally, some other optical particle sizing methods, e.g. laser forward diffraction and multi-wavelength forward light scattering flux method, can also bring about similar linear equation group as Eq. (2). The only difference is the kernel function in the integral.

Mathematically, once the rank of matrix **T** is full, the solution can be directly obtained by mathematical inversion, $\mathbf{q} = \mathbf{T}^{-1}$y. However, when the matrix is ill-posed, traditional mathematical operations as well as classical optimization methods are invalid for solving such a problem. In addition, solution to such an equation group has the constraint

$$\mathbf{q} \geq 0 \tag{3}$$

3. Inversion algorithms for PSD

3.1. Twomey (or Tikhonov) algorithm

Obviously, Eq. (2) can be solved by non-negative least-squares (NNLS) algorithm (Lawson & Hanson, 1974), namely

$$\min_q(||\mathbf{Tq} - \mathbf{y}||), \quad \mathbf{q} \geq 0 \tag{4}$$

However, such a method has the disadvantage that the PSD solution is very sensitive to the measurement error of **y** so that **q** presents an oscillating behavior. To overcome such a weakness, regularization method is introduced in order to give stable and real solution **q** to ill-posed problems (Tikhonov & Arsenin, 1977; Twomey, 1977). In such a method, matrix **L** and the regularization parameter γ (or "Lagrange multiplier" and "smoothing factor") are introduced to modify Eq. (4) to

$$\min_q(||\mathbf{Tq} - \mathbf{y}||^2 + \gamma||\mathbf{Lq}||^2) \tag{5}$$

Nevertheless, such an algorithm cannot ensure non-negative solution. Therefore, a further combination with the NNLS algorithm is introduced to form the Twomey–NNLS algorithm.

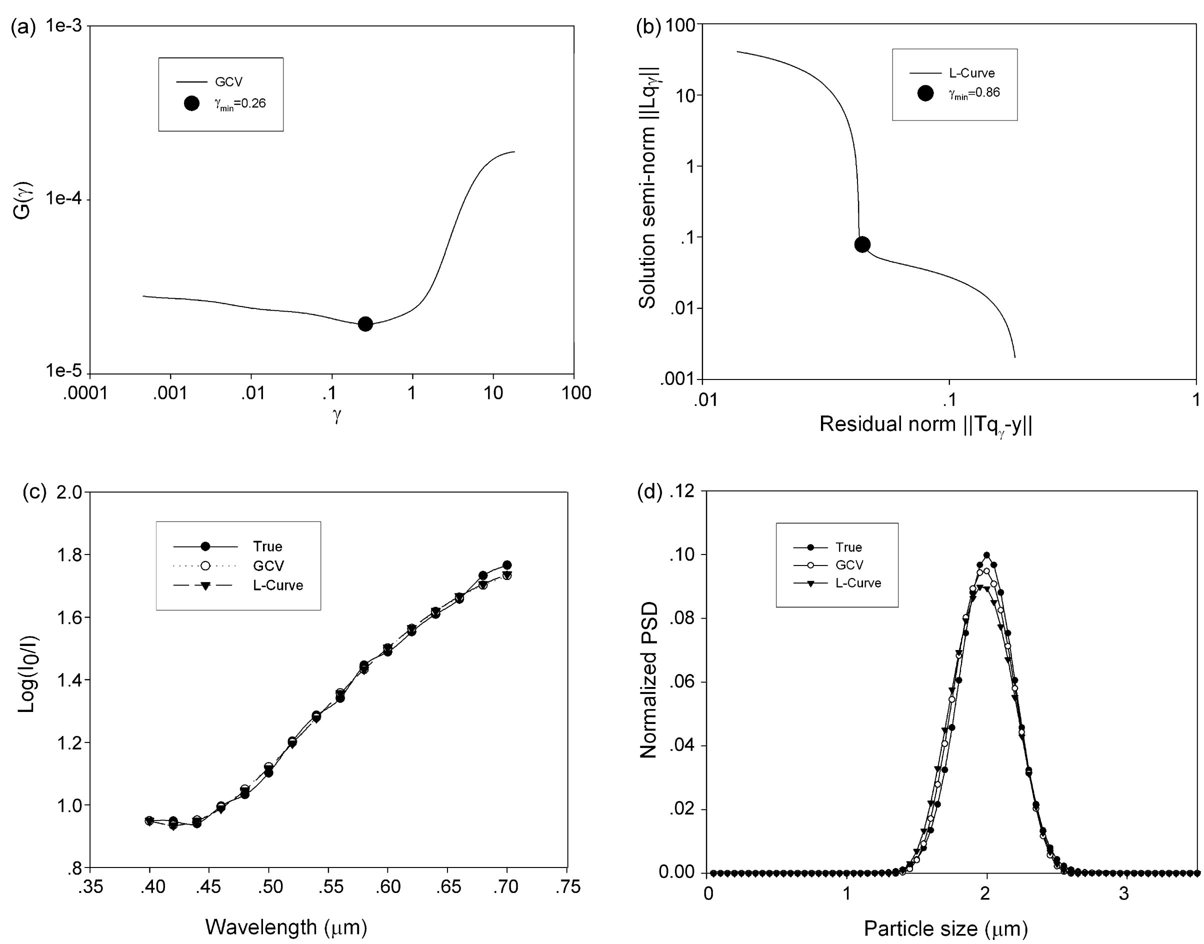

Fig. 1. (a–d) The regularization parameters and inversion results for particles with unimodal size distribution.