Optics Communications 366 (2016) 154–162

Contents lists available at ScienceDirect

Optics Communications

journal homepage: www.elsevier.com/locate/optcom

Application of the LSQR algorithm in non-parametric estimation of aerosol size distribution

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ARTICLE INFO

Article history:
Received 19 July 2015
Received in revised form
14 December 2015
Accepted 17 December 2015
Available online 28 December 2015

Keywords:
The least squares QR decomposition algorithm
Aerosol size distribution
Optimal wavelength set
Non-parametric estimation

ABSTRACT

Based on the Least Squares QR decomposition (LSQR) algorithm, the aerosol size distribution (ASD) is retrieved in non-parametric approach. The direct problem is solved by the Anomalous Diffraction Approximation (ADA) and the Lambert–Beer Law. An optimal wavelength selection method is developed to improve the retrieval accuracy of the ASD. The proposed optimal wavelength set is selected by the method which can make the measurement signals sensitive to wavelength and decrease the degree of the ill-condition of coefficient matrix of linear systems effectively to enhance the anti-interference ability of retrieval results. Two common kinds of monomodal and bimodal ASDs, log-normal (L-N) and Gamma distributions, are estimated, respectively. Numerical tests show that the LSQR algorithm can be successfully applied to retrieve the ASD with high stability in the presence of random noise and low susceptibility to the shape of distributions. Finally, the experimental measurement ASD over Harbin in China is recovered reasonably. All the results confirm that the LSQR algorithm combined with the optimal wavelength selection method is an effective and reliable technique in non-parametric estimation of ASD.

1. Introduction

Atmospheric aerosols usually play a crucial role in influencing the Earth's radiation balance and reducing the visibility [1,2]. The interest in the field of atmospheric aerosol properties has been sustained owing to the great number of engineering applications such as atmospheric science, astrophysics, and remote sensing, etc. For example, modeling the optical properties of aerosols is important for remote sensing applications as well as for estimating the direct climate forcing effect of particulate matter in the atmosphere [3]. Moreover, the aerosols cause significant negative influence on the human health and environment. Especially on the Earth's surface, where people live and the highest concentrations of aerosols are found, the aerosols present a serious health hazard. Nowadays, the particle matter (PM), regarded as a criteria pollutant, has been a hot research topic for numerous studies in the context of air pollutions [4,5]. A major obstacle to the reliable determination of the particle size distribution of PM is the lack of accurate measuring and modeling of the complex optical properties of various aerosols. In addition, in-situ measuring the properties of aerosols presented in the atmosphere is of great relevance to further understanding the influence of aerosols and their optical properties on human health and atmospheric environment [6,7]. Generally, there are three important properties of aerosols, i.e. aerosol size distributions (ASDs), aerosol optical depths (AODs), and Ångström exponents. Especially, accurate understanding and modeling of the optical properties of aerosols depend heavily on the knowledge of the particle size distribution. The ASD has a significant influence on radiative transfer and meteorological phenomena and plays an important role in determining the climatic trends [8,9]. The ASD is also regarded as a vital evaluation criterion of environmental quality, and the influence of atmospheric aerosols on human health depends heavily on the knowledge of aerosol size. Moreover, any uncertainty in the ASD can lead to an uncertainty in estimating the AOD, and then to an uncertainty in radiative forcing by the aerosols [8,10,11]. Thus, without accurate measurement of the ASD, AOD, and Ångström exponent, especially the ASD, the effects of the aerosols on the climate, meteorology, human health, and air quality, would remain highly uncertain. To date, although several global ground-based aerosol observation networks have been established to study the properties of the atmospheric aerosols, e.g. AERONET, MODIS [12], accurate determination of the ASD is still regarded as an unsolved problem and needs further research.

During the last two decades, various methods have been developed to determine the ASDs, i.e. the aerodynamic method, the optical measurement method, electrical mobility and condensation method, electrical sensing zone method, ultrasonic

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http://dx.doi.org/10.1016/j.optcom.2015.12.040
0030-4018/

Nomenclature

Cond[**A**]	the condition number of matrix **A**
D	the particle diameter, μm
$f(D)$	the volume frequency distribution
I	the intensity of the laser, $W/(m^2\ sr)$
I_0	the total intensity of the laser, $W/(m^2\ sr)$
L	the geometric thickness of the particle system, m
m	the complex refractive index
N_D	the total number concentration of the suspended particle system
N	the number of subintervals
Q_{ext}	the extinction efficiency
S	the number of the incident wavelengths

Greeks symbols

λ	the incident wavelength of the laser, μm
δ	the relative deviation of the particle size distribution
η	the sensitivity coefficient
τ	the transmittance of the particle system
χ	the size parameter of particles

Subscripts

est	the estimated value
ext	the extinction efficiency
L-N	the log-normal distribution
Gamma	the Gamma distribution
max	the maximum value
mea	the measurement value
min	the minimum value
true	the true value

measurement method, and the electron microscopy method [4,13]. For the aerosol particle properties can be derived by measuring a variety of scattering properties, such as extinction or scattering information at multiple wavelengths, scattering information at multiple angles, or multiple-scattering information, the optical measurement method coupled with inverse techniques has drawn much attention in the field of estimating ASD [14]. In addition, the optical measurement method also provides a sufficient size-measuring resolution over a broad range of sizes (from nanometer to millimeter), which covers the main size range of aerosols (between 0.001 and 10 μm) [5]. The optical measurement method usually contains the spectral extinction measurement, dynamic light scattering measurement, combined scattering, and extinction measurement, angular scattering measurement etc. [13]. Among these techniques, the spectral extinction technique is most viable, for it only requires a simple optical layout and can be realized by using the commercial spectrophotometer [15]. Usually, the spectral extinction technique is based on the Lambert–Beer law, and the general description of light absorption and scattering properties of particles is described by the Mie theory. Unfortunately, the calculation of the Mie theory can only be used to predict radiative properties of spherical particles, and the calculation is time-consuming [1,15]. To remedy this problem, the Anomalous Diffraction Approximation (ADA) was introduced by Van de Hulst [16] to study the optical properties of non-spherical particles. Lots of numerical simulation and experimental results showed that the ADA could be successfully applied to calculating the radiative properties of spherical and non-spherical particles [17,18]. Thus, the ADA is used to solve the direct problem in the present research.

Generally speaking, the methods for determining ASD can be classified into three different categories, the analytic inversion model, the dependent model, and the independent model [18]. Under the dependent model, the ASD is known beforehand to satisfy certain distribution and retrieved by inverse algorithms, which is widely used in various science and engineering applications recently [5,19,20]. However, under the independent model, the prior distribution information of ASD cannot be known in practice. To determine the ASD under the independent model, there are parametric and non-parametric estimation approaches. In the parametric estimation under the independent model, an assumed distribution function, e.g. Johnson's S_B (J-S_B) function and the modified beta (M-β) function, is employed to approximately estimate the ASD [18,19]. Due to the assumed distribution functions can only estimate the ASD approximately, the deviation between the actual distribution and estimated results is inevitable [21,22]. Different from the parametric estimation approach, there is no assumed distribution function in the non-parametric estimation approach, and the ASD is divided into many subintervals and recovered by measuring the spectral extinction data of multi-wavelengths. In other words, this approach is independent of any given a priori information of ASD. Consequently, the non-parametric estimation approach can avoid the inevitable discrepancy of the parametric estimation approach due to the deviation of assumed ASD function from the true distribution. The only obstacle in the non-parametric estimation approach is to solve the Fredholm integral equation of the first kind, a well-known ill-posed problem which leads to highly unstable solutions because even small noise components in the measured quantities can cause extremely large spurious oscillations in the solutions [21]. Fortunately, the Fredholm integral equation of the first kind could be discretized and solved by many inverse algorithms, e.g. the generalized eikonal approximation (GEA) method [23,24], the conjugate gradient algorithm (CGA) [25], and the generalized cross-validation (GCV) [26]. The Least Squares QR decomposition (LSQR) algorithm, one of the iterative regularization methods based on Lanczos bidiagonalization and QR factorization, was first developed by Paige and Saunders [27] in 1982 to solve the discrete optimization problems. This algorithm is demonstrated to be well suited for the simultaneous estimation of unknown functions or parameters with high numerical reliability as well as removing the numerical difficulty associated with the singularity of the adjoint equation in various circumstances [27,28]. However, to the best of our knowledge, few studies have investigated the application of LSQR algorithm to retrieve the ASD. The objective of present work is to apply the LSQR algorithm to estimate the spherical ASD theoretically and experimentally. The remainder of this research is organized as follows. First, an optimal wavelengths selection algorithm is studied. Then, the common monomodal and bimodal ASDs, i.e. the log-normal (L-N) and Gamma distributions are estimated by the LSQR. In the sequel, the effect of measurement errors on the accuracy of estimation is investigated. Meanwhile, the actual measurement ASD in Harbin of China is reconstructed experimentally. The main conclusions and prospects for further research are provided finally.

2. Direct problem

2.1. The principle of the spectral extinction method

The fundamental principle of the spectral extinction method is