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Regularized inversion of microphysical atmospheric particle parameters: Theory and application

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ABSTRACT

Retrieving the distribution of aerosols in the atmosphere via remote sensing techniques is a highly complex task that requires dealing with a wide range of different problems stemming both from Physics and Mathematics. We focus on retrieving this distribution from multi-wavelength lidar data for aerosol ensembles consisting of spherical particles via an iterative regularization technique. The optical efficiencies for spherical scatterers are examined to account for the behavior of the underlying integral equation. The ill-posedness of the problem and the conditioning of the discretized problem are analyzed. Some critical points in the model, like the assumed wavelength-independence of the refractive index and the fixed grid of investigated refractive indices, are studied with regard to their expected impact on the regularized solution. A new Monte-Carlo type method is proposed for retrieval of the refractive index. To validate the results, the developed algorithm is applied to two measurement cases of burning biomass gained from multi-wavelength Raman lidar.

1. Introduction

Qualifying and quantifying climate change, and researching its effects not only on nature, but also on human society as a whole, is one of the most pressing issues, science is facing at the start of the 21st century. While the global climate fluctuates on different scales, the influence that humans are having is one of the most important issues here. Human behavior and human society impact global and regional climate in very different ways. In this work, we will deal with atmospheric aerosols.

In the last 15 years research was already done in this area of solving the underlying inverse integral equation system to obtain microphysical parameters of aerosol particles from their optical properties. For instance, the first algorithms developed for the EARLINET (European AeRosol LIdar NETwork) community [1] are described in [2,3]. The solution is usually restricted to spherical particles, as the optical efficiencies for spheres are much easier calculable (via Lorenz-Mie theory) than for particles of other shapes, where Lorenz-Mie theory is not applicable anymore. One approach that was followed in [3,4] makes use of spline collocation and truncated singular decomposition. To solve the nonlinear problem with an unknown refractive index, the retrieval of the refractive index is handled by calculating solutions on a predefined grid and manually picking out solutions from that grid according to criteria like the residual error. This is also done in the algorithm from [5], except that a Tikhonov method is used for regularization here. Moreover, [5] employs a regularization approach which reduces extensive data postprocessing procedures. There is lots of research into the question how special a priori information on the solution can be used to improve results. In [6], for instance, the algorithm from [7] is extended to the special case of bi-modal distributions. Another example can be found in [8], which takes special care to incorporate a priori information on

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the solution in the form of a nonnegativity constraint. Additionally, new mathematical methods were considered, like for instance the maximum entropy method in [9] or Runge–Kutta type iteration methods in [10].

LIDARs (LIght Detection And Ranging) are laser based systems which detects diffusers (0.1 up to tens of microns diameter) along the beam, with a very good precision and in a very short time (seconds).The magnitude of the received signal is proportional to the number density of the atmospheric diffusers (molecules or aerosols), their intrinsic properties (i.e. probability of interaction with the electromagnetic radiation at the laser wavelengths, called cross-section value) and with the laser incident energy. To analyze the return signal P of a LIDAR means to find solutions for the equation which relates the characteristics of the received and emitted signal, and the propagation medium. The form of the equation depends of the interaction type, but for the purpose of this study is sufficient to use a simplified form of the equation, obtained for LIDARs without any high-spectral resolution components, such as elastic backscatter (Mie) LIDARs

$$P(z,\lambda_L) = C_S(z,\lambda_L)\beta(z,\lambda_L)\exp\left(-2\int_0^z \alpha(z',\lambda_L)\mathrm{d}z'\right). \tag{1}$$

where λ_L is the laser emitted – detected wavelength (usually λ_L = 355, 532 and 1064 nm), C_S is the system function, β is the total backscatter coefficient, α is the total extinction coefficient and z is the range. The system function C_S depends on the system efficiency, the transmitted and detected wavelengths, and decreases with the square of the range z. Due to the non-determination of the equation, supplementary assumptions have to made to relate the backscatter and the extinction coefficient in order to obtain a solution, see e.g. [11]. As consequence, only the backscatter coefficient can be derived with appropriate accuracy from elastic backscatter LIDAR. A similar equation can be written for vibrational Raman LIDARs

$$P(z,\lambda_L,\lambda_R) = C_S(z,\lambda_L,\lambda_R)\beta_m(z,\lambda_L)\exp\left(-\int_0^z \alpha(z',\lambda_L)+\alpha(z',\lambda_R)\mathrm{d}z'\right). \tag{2}$$

where the subscript "R" denotes the Raman shifted wavelength. In this case, the parameter which can be calculated directly is the extinction coefficient since β_m is only the molecular backscatter coefficient, see [12]. Advanced LIDAR systems with elastic and vibrational Raman channels deliver in the same time both backscatter and extinction coefficients, with sufficient accuracy for microphysical inversion to be applied. Therefore, we used in this study data coming from a multi-wavelength LIDAR system (elastic backscatter and Raman detection at several wavelengths). The laser radiation is emitted at 1064, 532 and 355 nm and collected at 1064, 532p (parallel), 532s (cross), 355, 607, 387 and 408 nm. In order to increase the dynamic range, almost all channels have both analog and photon counting detection. With this configuration, we can compute 3 backscatter (bsca) (1064, 532 and 355 nm) and 2 extinction (ext) (532 and 355 nm) profiles.

The question remains how to characterize the microphysical properties of the aerosols from the retrieved extinction and backscatter coefficient profiles gained from the measured LIDAR signals. Let $\Gamma_j(\lambda)$ be the function of aerosol optical coefficients, where j can take the values bsca for backscatter coefficients and ext for extinction coefficients.

Consider, we have a number size distribution of the particles denoted by $n(r)$, and that the particles form a homogeneous scattering medium. Furthermore, we will assume that all particles have a spherical shape. The relation between the optical data and the microphysical properties can be related to each other via a Fredholm integral equation of first kind [13]

$$\Gamma_j(\lambda) = \int_{r_{\min}}^{r_{\max}} k_j(r,\lambda,m)n(r)\mathrm{d}r. \tag{3}$$

The quantities $r_{\min}$ and $r_{\max}$ describe sensible lower and upper bounds for the size of the particles. They are usually chosen in such a way that we can expect resonant backscatter responses for the emitted wavelengths, see [14]. Let us take a closer look at the kernel function k. It can be shown [13] that the kernel function k for this integral equation is defined by

$$k_j(r,\lambda,m) = C_j(r,\lambda,m) = \pi r^2 Q_j(r,\lambda,m), \tag{4}$$

where $j \in \{\mathrm{ext},\mathrm{bsca}\}$. Here, the C functions are just the extinction and backscatter cross-sections. The functions Q are defined by $Q_j = C_j/G$, where G denotes the geometrical cross-section of the particle, which is, in the spherical case we are examining here, equal to πr^2. Knowing the number size distribution of the particles $n(r)$ and the refractive index m, all other important microphysical properties can be derived, e.g., the total surface-area concentration a_t, which can be calculated via

$$a_t = 4\pi\int_{r_{\min}}^{r_{\max}} r^2 n(r)\mathrm{d}r = 3\int_{r_{\min}}^{r_{\max}} r^{-1} v(r)\mathrm{d}r, \tag{5}$$

the total volume concentration v_t,

$$v_t = \frac{4\pi}{3}\int_{r_{\min}}^{r_{\max}} r^3 n(r)\mathrm{d}r = \int_{r_{\min}}^{r_{\max}} v(r)\mathrm{d}r, \tag{6}$$

and the effective radius $r_{\mathrm{eff}} = 3v_t/a_t$, where the volume distribution is given by $v(r) = \frac{4\pi}{3}r^3 n(r)$ or $\mathrm{d}v/\mathrm{d}\ln r = r v(r)$, respectively, see [15], resulting in the equation

$$\Gamma_j(\lambda) = \int_{r_{\min}}^{r_{\max}} \frac{3}{4r} Q_j(r,\lambda,m)v(r)\mathrm{d}r. \tag{7}$$