Information content of the kernel matrix for the phase function retrieval problem

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We investigate the information content of the radiation measurements to be used in the retrieval of the scattering properties of the atmosphere with the perturbation technique that we previously introduced. Applying this technique to different sets of data, we obtained solutions with varying accuracy. An analysis of these solutions shows that selecting linearly independent data in directions corresponding to small values of the scattering angle increases the number of pieces of information. (This result is in accord with conclusions reached by other researchers, based on a variety of criteria.) This information content should be largely independent of the method or methods employed to perform the inversion procedure. © 1999 Optical Society of America

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1. Introduction

In a companion paper[1] we used radiative perturbation theory to develop a retrieval technique to determine the scattering properties of an atmosphere. We have shown that it is possible to establish a system of equations represented by a kernel matrix, the inversion of which leads to a stable solution. In that paper we focused our attention on the determination of the characteristics of the kernel matrix (L dimension and γ) that lead to an accurate solution, addressing the data selection problem by using a set of uniformly distributed data. However, because the Sun position determines the position of the pattern of the scattering phase function and hence the scattering probability, we expect each of the data points to contain different information.[2,3]

Our aim in this paper is to determine a criterion for the selection of a good quality data set. We need to identify those data that contain the greatest amount of information: In other words, which is the best data set that allows us to retrieve the largest number of parameters. We already know[1] that the interdependence between data, and hence the interdependence between the different rows of the kernel matrix, restricts the number of coefficients we are able to retrieve. But we do not know how the quality of the aerosol scattering coefficients extracted from measured data depends on the chosen scattering angles. To study the influence of these two important factors on the information content of the observations, we analyze the quality of the retrieved coefficients under different observational conditions, including an examination of the spatial distribution and position (with respect to the Sun) of the different data sets. We point out at this stage that, although the focus of our present studies is the perturbation inversion technique, the estimates of information content should be equally valid for any inversion procedure.

In Section 2 we describe the characteristics of the measurements at the top of the atmosphere based on the range and the value of the scattering angles. We show the scattering coefficients retrieved from different groups of data, including those corresponding to potential satellite observational angles. In Section 3 we analyze the different solutions, correlating their accuracy, the degree of interdependence between data, and angles of scattering for each case.

2. Inversion of Synthetic Data

In our companion paper we have shown that radiative perturbation theory offers a suitable platform to solve the problem of retrieving the single-scattering albedo and the Legendre phase function coefficients from measurements of scattered radiation. We showed that it is possible to establish a system of equations represented by a kernel matrix, the inversion of which leads to a stable solution. That same

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Table 1. Observational Directions (θ_{obs}, φ_{obs}) and Corresponding Scattering Angles Θ_{scatt} for the Different Data Sets

Case	θ_{obs} (deg)	φ_{obs} (deg)	Θ_{scatt} (deg)
1	4	0, 30, 60, 90, 120, 150, 180	124, 123, 121, 120, 118, 117, 116
2	87	0, 30, 60, 90, 120, 150, 180	153, 140, 117, 91, 66, 44, 33
3	4, 32, 59, 87	0, 30	124, 152, 180, 153, 123, 145, 154, 141
4	4, 32, 59, 87	0, 90	124, 152, 180, 153, 120, 115, 104, 91
5	4, 32, 59, 87	90, 180	120, 115, 104, 91, 116, 88, 59, 33
6	4, 32, 59, 87	0, 180	124, 152, 180, 153, 116, 88, 59, 33
7	4, 32, 59, 87	150, 180	116, 91, 66, 44, 116, 88, 59, 33
8	4, 32, 59, 87	60, 240	121, 130, 128, 117, 117, 101, 83, 66
9	4, 32, 59, 87 (at the bottom)	60, 240	62, 79, 97, 113, 58, 49, 51, 62
10	70 (at the bottom)	2, 5, 10, 20, 30, 60, 90	178, 176, 171, 162, 152, 124, 97

approach, including the criteria for selection of γ and the L dimension, is used in this paper to obtain retrievals from different sets of data.

In this study we consider the Sun position fixed at $\theta_{sol} = 59.5°$ and the same perturbation in all cases. (Here perturbation refers to the difference between the true atmospheric model and the first guess.) The measured intensities were simulated using the Lenoble Haze-L phase function expansion coefficients[4] and a scattering albedo of $\omega_0^{pc} = 0.9$. The first guess and the kernel matrix were computed using the Henyey–Greenstein model[5] with $g = 0.75$ and a scattering albedo of $\omega_0^{bc} = 1.0$. The total optical thickness, which we assume known, was set to 0.2. (This value was chosen as indicative of the aerosol optical depth in the near-infrared wavelengths employed by a number of spaceborne instruments.) We did not incorporate random noise, as this was not the aim of the present study. In our companion paper, noise was included in our results.[1]

We considered a total of ten cases (data sets), of which eight correspond to observations at the top of the atmosphere and two to observations at the bottom. The reason for this imbalance is that ground-based instruments usually have the freedom to make any observations that may be considered relevant, whereas the observations of space-based instruments are largely preset by orbital parameters. Nevertheless, there is usually some flexibility in the design of the instrument and the measurement protocol.

Keeping in mind that the azimuth variable φ_{obs} is measured from the plane where the Sun is located, and the zenith observational angle θ_{obs} is measured from the vertical axis, Table 1 shows the pairs of coordinates (φ_{obs}, θ_{obs}) and the range of the angle of scattering for the data points corresponding to each study case. The selection of the different groups or cases was chosen in such a way that allows us to study the effects of the interdependence among the data and of the scattering direction on the quality of the solution. (We note here that the observational directions considered for cases 6 and 8 correspond to possible satellite sensor observational angles.)

Applying the radiative perturbation formalism to each data set, we retrieve the phase function expansion coefficients and the single-scattering albedo from[1]

$$\eta^{retr} = \mathbf{B}\Delta\mathbf{E} + \eta^{bc}.$$

Here $\mathbf{B}$ is the pseudoinverse of the kernel matrix $\mathbf{A}$, where $\Delta\mathbf{E} = \mathbf{A}\Delta\eta$. η^{bc} (η^{retr}) is a vector of dimension L, where each component η_l^{bc} (η_l^{retr}) is defined by $\eta_l^{bc} = \omega_0^{bc}\,\chi_l^{bc}$ ($\eta_l^{retr} = \omega_0^{retr}\,\chi_l^{retr}$) with ω_0^{bc} (ω_0^{retr}) the first guess (retrieved) single-scattering albedo and χ_l^{bc} (χ_l^{retr}) is the Legendre expansion coefficient of order l for the first guess (retrieved) phase function. $\Delta\mathbf{E}$ is a vector of dimension K, where each component is the difference between the measured and the base case intensity exiting in the direction $\Omega_k = (\theta_k, \phi_k)$.

The results of the inversions are shown in Table 2, where we indicate in parentheses for each retrieved

Table 2. Retrieved Coefficients from Different Data Distributions

Order	ω_0	1	2	3	4	5	6
True	0.90	2.41	3.23	3.37	3.23	2.89	2.49
Case 1	0.85	2.37	3.19	3.39			
	(5.5)	(1.4)	(1.1)	(0.5)			
Case 2	0.91	2.54	3.19	3.27	3.29	2.94	
	(1.1)	(5.5)	(1.1)	(3.1)	(1.8)	(1.7)	
Case 3	0.80	2.99	3.15	4.18			
	(10)	(24)	(2.3)	(24)			
Case 4	0.93	2.25	3.24	3.16	3.20	2.80	
	(3.5)	(6.6)	(0.3)	(6.1)	(0.7)	(2.9)	
Case 5	0.86	2.37	3.18	3.33	3.25	2.93	
	(4.3)	(1.7)	(1.8)	(1.3)	(0.7)	(1.6)	
Case 6	0.90	2.40	3.21	3.36	3.22	2.85	2.51
	(0.4)	(0.3)	(0.3)	(0.2)	(0.2)	(1.3)	(0.8)
Case 7	0.91	2.40	3.04	2.67	2.44		
	(1.2)	(0.4)	(5.6)	(21)	(24)		
Case 8	0.88	2.39	3.19	3.35	3.24	2.96	2.60
	(2.2)	(0.6)	(1.1)	(0.4)	(0.4)	(2.4)	(4.5)
Case 9	0.89	2.46	3.21	3.45	3.29	2.97	2.63
	(0.9)	(2.3)	(0.5)	(2.5)	(1.8)	(2.9)	(5.8)
Case 10	0.89	2.48	3.17	3.35	3.22		
	(0.9)	(2.8)	(1.6)	(0.4)	(0.3)		

Table 3. Singular Values for the Normalized Kernel Matrix Computed for Different Observational Data Sets

Case	k_1	k_2	k_3	k_4	k_5	k_6	k_7	k_8
1	1.000	0.305	0.083	0.017	0.001			
2	1.000	0.623	0.333	0.270	0.234	0.221		
3	1.000	0.329	0.169	0.102	0.069	0.061	0.023	0.003
4	1.000	0.554	0.132	0.115	0.076	0.025	0.026	0.002
5	1.000	0.536	0.443	0.120	0.070	0.047	0.024	0.009
6	1.000	0.736	0.443	0.143	0.092	0.060	0.042	0.012
7	1.000	0.398	0.331	0.079	0.052	0.029		
8	1.000	0.472	0.096	0.074	0.008	0.006		
9	1.000	0.455	0.097	0.070	0.009	0.007		
10	1.000	0.312	0.120	0.031	0.001			

coefficient the corresponding percentage error. The best L dimension of the kernel matrix, and hence the number of coefficients we are able to retrieve, is determined by the lowest acceptable singular value associated with the kernel matrix[1]: in our case 0.01. These (normalized) singular values are presented in Table 3. Therefore, because the kernel matrix depends on the observational directions, we expect to retrieve, as shown in Table 2, different numbers of coefficients according to the data interdependence found in each group of data. In this way we can explain, as mentioned in our companion paper, the correlation between the number of coefficients we are able to retrieve and the singular values associated with each kernel matrix (see Tables 2 and 3). However, the decay of the singular values clearly does not tell the whole story, as different cases with apparently the same number of pieces of information are seen to yield retrievals of different quality. Hence we infer that there must be more information content in the measured data sets that is not related directly to the mathematical problem of the interdependence between data. To investigate this extra information associated with the physics of the problem, we perform a more detailed analysis of the different solutions and their dependence on the different angles of scattering considered in each case.

3. Analysis

The analysis of the singular values associated with the kernel matrix allows us to evaluate the number of independent data found among the measurements considered in each case. Cases 1 and 2 correspond to observation cones, but with very different zenith angles. (Only half of the cone is actually considered, as the other half would provide no new information.) In case 1 we can see that the very small zenith angle leads to all data points being separated by just 1° or 2° (in terms of the angle of the scattering), whereas in case 2 the much larger zenith angle leads to an angular separation between the data of around 20°. This difference is clearly responsible for the faster decay of the singular values for case 1 (Table 3) and the associated fact that six coefficients were retrieved for case 2 and just four for case 1. However, the accuracy of the solution for both cases is similar, indicating that the interdependence between data present in case 1 does not completely negate the information content of these measurements. Because of the fact that for case 1 we are able to retrieve four coefficients with a percentage error lower than 6% (see Table 2), we conclude that this data set must have a useful information content, despite the data interdependence.

Cases 3, 4, 5, and 7 represent wedges of one form or another. Cases 3 and 7 are narrow wedges, but on opposite sides of the Sun, whereas cases 4 and 5 are quadrants. The decay of the singular values (Table 3) suggests that we should be able to obtain six or seven coefficients, with case 7 clearly the worst of this group. This is not entirely borne out by the retrievals (Table 2), which show that, in fact, case 3 is the worst. What is shown consistently by the results in both Tables 2 and 3, however, is that the broader wedges contain more information than the narrow wedges, as would be expected. In fact the best of these data sets is case 5, which has the widest range of scattering angles, plus the best singular values, consistent with the best retrievals.

Cases 6 and 8 represent observation planes and are thus more likely to correspond to the type of observations made by instruments such as the polarization and directionality of the Earth's reflectances[6] and the multiangle imaging spectroradiometer.[7] Case 6, in fact, has the widest range of scattering angles, and the slowest decay of its singular values, of all our ten cases, and it is not surprising that we are able to retrieve seven parameters with errors of order 1%. This shows that the best situation occurs when the measurements are in the solar plane. A data set taken at right angles to the solar plane would, of course, contain redundant measurements and so must be assumed to be the worst possible (planar) arrangement. We did not actually examine this situation, but case 8 is close, with the observation and solar planes being at 60°. We can see from Tables 1 and 3 that both the range of scattering angles and the decay of the singular values are inferior to case 6. Table 2 shows that we are still able to obtain seven parameters, but this time with errors approaching 5%.

Cases 9 and 10 are our only ground-based cases: one is a partial cone and the other a planar scan. Both are relatively restricted in their range of scattering angles and neither has a particularly good set of singular values. Nevertheless, the retrievals of seven and five parameters, respectively, are quite good. Protocols for ground-based radiometers can easily be tailored to obtain a wide range of information, so that there are fewer pressures to get it right before launch and deployment. (We are currently investigating the application of our technique to ground-based observations, and we will present those results at an appropriate time.)

The correlation between the magnitudes of the singular values and the quality of the corresponding retrievals is quite good, so that we can safely say that, before a measurement protocol is decided on, an analysis such as this would be worthwhile, regardless of what inversion technique is intended. A singular-value analysis cannot tell the entire story, of course. It provides an accurate picture of the amount of information that is contained within a given data set, but it does not tell us exactly which particular pieces of information can be most readily obtained.

The range of scattering angles within the data set is clearly a good guide as to which parts of the phase function are most likely to be obtained, at least in low optical thickness cases. (Note that perturbation theory is not a single-scattering approximation, but rather should be thought of as a single-scattering deviation from an initial state.) It is not surprising, of course, that data sets with a broader range of scattering angles almost always have a better set of singular values, as the kernels are clearly less similar to one another.

Measurements at the top and bottom of the atmosphere invariably sample different parts of the phase function, so it is not valid to compare these two situations too closely. However, we comment here that measurements at the bottom will almost always include some quite small scattering angles. As most of the energy is contained in the forward peak (in the case of aerosols or larger scatterers), these data sets are more likely to yield good values of the single-scattering albedo, as this is tied directly to a knowledge of the total scattering. We note that cases 9 and 10 yield good values for the retrieved albedo.

4. Conclusion

The analysis of the singular values of the kernel matrix is a common tool used to infer the quality of an obtained solution. Full justification of the correspondence between singular values and solutions can be found when both the kernel matrix and the solution are expanded in singular function bases.[8] Even though this is not our case (we are not expanding in singular function bases), we use the relationship between the singular values associated with the kernel matrix and the number of pieces of information to select an experimental set of data or to plan an experiment in such a way that the measurements contain the largest number of pieces of information. However, the actual information carried by the data will depend on the way the specific group of independent data describes the physics of the problem.[9] This is why we need to evaluate the role of the different groups of data in our specific inversion method.

Our results show that, as a first approximation, a set of observations will have more information if it covers a wide range of scattering angles. This, of course, is exactly what would be expected in the single-scattering regime where this angle may be related directly to the phase function. What is probably less expected is that our radiative perturbation technique can so often retrieve accurate values of the single-scattering albedo and asymmetry factor (especially cases 6 and 8), parameters which clearly depend on a knowledge of the forward part of the phase function, knowledge that is sparse in the case of top-of-atmosphere measurements. We believe that this can be explained by the interrelation of all the Legendre expansion coefficients to the overall phase function and to the general properties of the matrix inversion process (including regularization). Clearly, of course, a combined top and bottom of the atmosphere data set, when available, would contain the most complete set of information from which to attempt to extract the aerosol phase function.

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