Response to Interactive comment on

"A sensitivity study on the retrieval of aerosol vertical profiles using the oxygen A-band" by Colosimo et al.

We would like to thank the reviewer for the valuable comments. In the following response we will address each comment specifically (in blue italic). As a result of the comments we added additional calculations to our manuscript, which will be fully shown in the final manuscript and its supplement.

General comment

Colosimo et al. conduct a retrieval simulation study on how well the aerosol extinction vertical profile can be retrieved from solar backscatter satellite measurements of the O2A-band. The study in particular addresses the sensitivity of information content to instrument design parameters such as spectral resolution and signal-to-noise ratio. As acknowledged by the manuscript, previous assessments have covered the topic already to some extent. Nevertheless, the paper can make a genuine contribution since the findings are presented in a systematic and generically applicable way. The manuscript is generally well written and the methods appear robust. Overall, the main comment I have is that it would be timely to assess this question with real (not just simulated) data given that solar backscatter measurements of the O2A- band are available from various satellites (SCIAMACHY, GOSAT, OCO-2, GOME-2,...) covering a range of design parameters. Such studies are sparse and, mostly available for the low-resolution sensors indicating only limited information content for the aerosol vertical profile.

While I acknowledge that such work would be beyond the scope of the current manuscript, I would recommend considering the comments below which mostly center on a better discussion of potential real-world problems and real-world relevance.

Specific comments

1. As far as I can trace the methodology, the information content analysis is based on a "1-step" retrieval in the linear regime around the true state: the RTM is fed by the assumed atmospheric state, then it calculates the Jacobian matrix from which the averaging kernel and the DOFs are derived. This is a benign approach in several ways:

We thank the reviewer for the comments and suggestions about the methodology description.

We acknowledge that the simplicity of the model and the strong assumptions and constraints of this method, make such approach definitely not suitable for any kind of real world analysis, where the non linearity of the phenomenon and the imperfect knowledge of the parameters involved, require other techniques for the content of information evaluation.

The aim of our study however, as acknowledged by the reviewer, is an evaluation of the degrees of freedom of aerosol extinction retrieval, for different scenarios and instruments specifications from a theoretical point of view, where no real measurements are involved (no specific mission, instrument or location is considered).

According to the reviewer comment we added new text (page 12, line 21-25, page 13 and page 14 line 1-10), to cover a better explanation of the approach used:

*"An atmospheric state vector **x**, containing the parameters of interest, is related to a measurements vector **y**, through a forward model **F(x,b)**, which is a function of **x** and other model parameters not retrieved (vector **b**):*

$$\mathbf{y} = \mathbf{F}(\mathbf{x},\mathbf{b}) + \boldsymbol{\varepsilon}$$

where $\boldsymbol{\varepsilon}$ *is the measurements error vector (e.g., instrument noise).*
*For atmospheric remote sensing retrievals, **F(x,b)** is normally a radiative transfer model. The solution to the inverse problem is then to use the forward model and the information from the measurement vector **y** to construct an estimate of the atmospheric state. For an inverse problem, the a priori state vector **xa** is often used as an initial estimate. **xa** is ideally chosen to be close to the true state **x**, based on existing knowledge of the atmosphere.*
*Because of the nonlinear nature of the dependence of the model on the true state vector (and the real measurements), the solution for a full retrieval of the retrieved state vector, **x** ˆ, has to be found using an iterative process, which ends when an optimal agreement between the model **F(x,b)** and the real measurements vector **y** is reached. Such an approach, however, requires a good knowledge of the properties of the parameters involved in the measurements (aerosol micro-physical and optical properties, spectroscopic parameters, model uncertainties, surface properties) and the relative errors for every measurement (instrument noise).*
*Here we are interested in a theoretical and more general quantification of the aerosol retrieval information content for different scenarios, with no reference to any specific mission, instrument or location, we perform a one-step retrieval instead, assuming the a priori parameters to be known and a linear dependence of the forward model **F(x,b)** on the state vector **x**. The forward model is directly applied to our first guess (linear regime), assumed to be the true state, for which we define an a priori uncertainty. We then derive the corresponding information content, calculated using the optimal estimation method. We remark that this methodology is not applicable for retrieval with real data, where the high non-linearity of the physical process and the imperfect knowledge of the a priori parameters requires the use of an iterative approach.*
According to the Bayesian formalism, the linearisation of the forward model about the state vector can be expressed as:

$$\mathbf{y} = \mathbf{K}\mathbf{x} + \boldsymbol{\varepsilon}$$

*where **K** is the functional derivative matrix, also called Jacobian, which represents the change in the measurement for a unit change in the retrieved parameter.*
*For this study, the vertical aerosol extinction profile represents the retrieved parameter, **x**, and the elements of **K** represent the derivative of the radiance with respect to the aerosol extinction coefficients, for every single layer and every single wavenumber. VLIDORT provides analytic derivatives of the Stokes vector field with respect to any atmospheric or surface property (Spurr, 2006). The Jacobians required in Eq. (9) can be calculated from these weighting functions by the application of the chain rule. For every scenario, we fix the model parameters, calculating the radiance and the Jacobian with a single run of the code, before using these quantities for the estimation analysis.*

a) For the real-world problem, the retrieval would generally be initialized at a state that is not the truth and an iterative retrieval would be required. Since the forward model is probably quite non-linear, it is not a trivial task to make the algorithm converge at the true state.

An improved explanation of this point has been added to the text as outlined in the response to the previous question.

b) For the real-world problem, (non-retrieved) forward model parameters such as the shape, size, composition of the aerosols, such as spectroscopic parameters (line- mixing, collision induced absorption), or such as instrument parameters (radiometric calibration) would be imperfect inducing forward model errors. In particular, imperfect knowledge of spectroscopic parameters might preclude exploiting the theoretically available DOFs for the high spectral resolution cases.

We agree with the reviewer that there are multiple sources of error that could potentially influence the accuracy of real-world retrievals. Our study was aimed at finding the maximum information that can be retrieve in a case where the accuracy is dominated by photon noise and to investigate the impact of spectral resolution. The noise sensitivity section of the manuscript provides some idea on how the retrieval quality changes if additional errors, which we can assume to increase the noise, are added. Many of the errors listed by the reviewer will not lead to random errors and are notoriously difficult to assess. It is beyond the scope of this study to perform a detailed analysis of all the potential error sources associated with the measurement.

c) Is albedo part of the state vector or is at assumed known? If it is assumed known, I would consider this a particularly optimistic case of comment 1b) above since albedo is highly variable in time and space at the required level of knowledge. Thus, assuming albedo known will induce a large forward model error. Albedo has a large effect on the lightpath e.g. by mediating the importance of single-scattering versus multiple scattering radiances. Therefore, I would expect DOFs to be quite sensitive to whether albedo is a retrieval parameter or not.

We did not include albedo in the state vector, but rather used a sensitivity study, which was expanded to the vegetation case in the revised manuscript, to investigate its impact. Interestingly the sensitivity to albedo is much reduced at high spectral resolution and one can thus argue that it may not be necessary or desired to include albedo in the state vector at high spectral resolution. We believe that this one of the more interesting outcomes of our study.

The manuscript should be clearer in what methodology is exactly used. If the above concerns turn out to be relevant, they should be either addressed by sensitivity studies or, at least, be thoroughly discussed as potential hurdles on the way toward the realworld problem.

Please see expanded explanation given above.

2. Concerning the aerosol scenarios, it would help quoting the vertically integrated aerosol optical depth (AOD) in addition to extinction for all scenarios.

Looking at figure 1, AOD seems actually quite large (Is it >0.5 at 765 nm?) for all except the Marine-Arctic scenario. How representative are the chosen AODs for the global scale and, importantly, how do DOFs depend on AOD?

We agree with the reviewer.

The extinction values used for the urban and highly polluted were quite large (AOD = 1 for the urban case and AOD > 4 for the highly polluted).

Due to the theoretical nature of this study and our interest in exploring the maximum amount of information available for aerosol extinction retrieval, the choice of such high value of extinction was made to evaluate the limits of information availability, constraining the relative DoF.

While we acknowledge that such values are well above an average real world scenario, we remark that similar total AODs have been measured in specific locations, at particular times of the day or year, thus representing *rare, but not unseen, values for the columnar aerosol extinction.*

However, in order to evaluate DoF with more common values of AOD (still representing an upper limit for the optical depth) for both urban and highly polluted case, we replaced the highly polluted aerosol profile with the urban profile (AOD=1), and used a smaller aerosol extinction profile for the urban case with a total of AOD=0.5. We calculating the new DoF for this revised urban scenario and remove the previous highly polluted case from the manuscript.

The new results (AOD=0.5 for urban and AOD=1 for highly polluted) are now more in line with AODs measured worldwide in polluted urban areas.

We also added the corresponding AOD values in the text at pag. 8 line 24: "with a total aerosol optical depth AOD = 0.5."; pag. 9 line 2: "(AOD = 1)"; page 9 line 8: "(AOD = 0.44)", page 9 line 21: (AOD = 0.12); page 9 line 26: "They only represent a plausible parameterization of the upper extinction limit for the different scenarios"

The AOD value for every single aerosol profile was added in Fig.1.

Further, the choice of albedo does not seem representative for land surfaces. Albedo is assumed either 0.05, 0.1, or 0.9. Scientifically very interesting and large regions such as the tropics or mid-latitudes are covered by vegetation surfaces with albedo 0.2-0.4 (at 765 nm). The manuscript occasionally quotes results for albedo 0.3. I would recommend extending the discussion of these cases.

Following the reviewers suggestion, we extended the evaluation of the information content for a new scenario with albedo 0.3, typical of vegetated areas. We added new text in the manuscript at pag. 18 line 22-29;

"As expected, DoF in the vegetation, marine and arctic scenario are lower than in the previous cases, due to the generally lower aerosol extinction. At 5 cm−1 resolution, only the marine scenario allows the retrieval of pieces of information greater than unity, where for both vegetation and arctic case no information is available at this resolution. At 0.05 cm−1 , 3.84 pieces of information can be retrieved for the marine scenario and 3.43 for both vegetation and arctic case. Again, the low-to-high resolution change leads to an improvement in the DoF of a factor of 3.2 (marine), 4.7 (vegetation) and 10 (arctic)."

pag.19 line 5-8;

"However, higher spectral resolutions lead to a DoF improvement of a factor of ten, and the DoF at a resolution of 0.05 cm−1 is only 10 % lower than in the marine case. Similarly, the vegetation case shows the number of pieces of information is below 1 at 5 cm−1 and improves to 3.43 at higher resolution."

pag. 19 line 11-14;

"The retrieval results are thus independent of albedos above 0.3. The likely explanation is that above a certain threshold, backscattered radiation from the surface dominates over that from the aerosol and all the information comes from the O2 absorption rather than the intensity contrast between surface and aerosol."

pag. 19 line 21;

"The vegetation scenario allows the same retrieval with a DoF = 1 at 1 cm−1 resolution."

pag. 21 line 7-12.

“The vegetation, marine and arctic scenario results (panel (d), (e) and (f) respectively) agree with the previous tests. A resolution of FWHM = 0.05 cm−1 is needed to achieve DoF greater than 1 in the lower and mid-troposphere. The total number of DoF for the tropospheric levels (sum of Regions I and II) at FWHM = 0.05 cm−1 resolution is 2.72 (79 % of the total) for the vegetation case, 2.54 (66 % of the total) for the marine case and 2.49 (73 % of the total) for the arctic scenario. “

3. Why is only a narrow micro-window of the O2A-band used? Current algorithms exploiting real O2A-band measurements (e.g. applied to GOSAT, OCO-2) cover the entire band. As noted by the manuscript, a larger micro-window could help increase DOFs (and – covering the shortwave and longwave sides of the band – support an albedo retrieval).

While we agree that an analysis carried out over the entire Oxygen A-band would have been more exhaustive of the topic, we did not investigate the DoF for the entire (12950–13200 cm−1) for two reasons.

The range we use (from 13122 cm-1, where weak or small absorption occur, to the main absorption frequencies around 13140 cm-1), is able to account for almost the entire content of information available in the main absorption band (13122–13170 cm−1). This is because of the strong dynamics of the absorption process of the oxygen in that range.

In fact, an initial test with a wider spectral range (nor described or shown in the manuscript), covering not the entire A-band but the main absorption band (13122–13170 cm−1), showed that the DoF were similar (few percent higher) when compared with the range used in this work.

The second reason is related to computational time.

The DoF evaluation requires the simulation of high resolution radiance spectra (and relative Jacobian matrices) at 0.002 cm-1, and the convolution at different resolution for every single geometry and every single scenarios (7 in total, plus other tests as the geometry test and the different single scattering albedo test). The computational time needed for all the simulations required in this study, is quite substantial.

In the end, the chosen spectral range represents a good compromise between the computational time and the marginal loss of information. The general conclusions, i.e. that there is an advantage to use higher spectral resolution, is not impacted by the choice of a smaller spectral window.

4. Are the results dependent on the assumed scattering phase function, ie. is the assumed asymmetry parameter g=0.7 a critical choice?

No, it is not a critical choice.

In order to minimize the free parameters in the DoF evaluation, we kept the asymmetry factor fixed. The value of g=0.7 only represents a reasonable value for all of the scenarios considered.

5. The discussion of the multi-angle paper by Frankenberg et al., 2012, (P11874,L20) does not seem too applicable. Multi-angle geometry predominantly yields information on the scattering phase function and thus, on aerosol microphysical properties with only some marginal benefits for the aerosol height retrieval.

We agree that the multi-angle analysis from Frankenberg et al., 2012 is more oriented to exploring aerosol properties than aerosol vertical information. However, we cited the paper anyway because we were interested in citing it for its presentation of the principles of the retrieval and its applicability, despite the different purpose of the paper.

6. Figure 7 could be misleading or too simplistic since only downward propagating lightpaths are shown. The role of albedo does not become clear. Lightpath enhancement e.g. due to multiple scattering between the aerosol layer and the surface cannot be illustrated by the current figure.

We replaced the figure (now Fig. 9), adding the vegetation scenario and adding a better visual explanation of the physical processes occurring between surface and aerosol layers.