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Atmospheric Measurement Techniques Discussions

Interactive comment on "Regularisation model study for the least squares retrieval of aerosol extinction time series from UV/VIS MAX-DOAS observations for a ground layer profile parametrisation and westward viewing direction" *by* A. Hartl and M. O. Wenig

A. Hartl and M. O. Wenig

ahartl@cityu.edu.hk

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Response to referee #1
We thank the reviewer for the careful and kind review of our manuscript and apologise for careless mistakes we could have spotted ourselves.

Response to general comments

1) We removed the last part “and westward viewing direction" in the title.

2) We are particularly grateful for pointing out this negligence. The way the parameter vector $\mathbf{x}$ is defined in the paper (with different units) indeed does not allow to compute the norm of $\mathbf{x}$ or the regularisation term $\gamma^2(\mathbf{x}-\mathbf{x}_a)^T(\mathbf{x}-\mathbf{x}_a)$. We have corrected this by redefining $\mathbf{x}$ as $\mathbf{x} = (k_{\mathsf{L}_1} \cdot 1\,\mathrm{km}, k_{\mathsf{L}_2} \cdot 1\,\mathrm{km}, \tau_{\mathsf{L}}, \tau_{\mathsf{E}})^T$ and $\mathbf{x} = (k_{\mathsf{L}} \cdot 1\,\mathrm{km}, \tau_{\mathsf{L}}, \tau_{\mathsf{E}})^T$, respectively, so that all fit parameters have the same unit (none). Multiplying by 1 km is exactly what we did in all calculations. This definition amounts to fitting scaling factors for the extinction coefficients, but we prefer to express results in terms of extinction coefficients themselves. The correction entails changes ($k_L \rightarrow k_L \cdot 1km$) at the following places of the previous manuscript:
- Eq. (15), eq. (16) and text in between.
- P2604, L2.
- P2609, L16.
- P2610, L26.
- Fig. 1.
- In captions for figs. 6, 8, 9, 10 and 16.
- Labels in figs. 9 and 13 (top left)

Alternatively, one could keep the original definition $\mathbf{x} = (k_{\mathsf{L}_1}, k_{\mathsf{L}_2}, \tau_{\mathsf{L}}, \tau_{\mathsf{E}})^T$ and use a different scalar product/norm, e.g. of the form $||\mathbf{x}||_L = (\mathbf{x}^T L^T L \mathbf{x})^{1/2}$, as you suggested. We prefer vector components having the same unit.

3) We agree that for an uplifted layer, multiple layers etc., the representation error is probably the largest error contribution for most components of the retrieval vector (not necessarily the AOD). We haven’t looked at how well such profiles can be represented by our simple parametrisation, i.e. we haven’t made the fit for eq. (21) or calculated any numbers, mainly for the following reasons:
(i) We wanted to keep the focus on regularisation, not parametrisation and think the latter point deserves a wider discussion (maybe similar to [Vlemmix, T. et al.: Ability of the

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MAX-DOAS method to derive profile information for NO2: can the boundary layer and free troposphere be separated?, Atmos. Meas. Tech., 4, 2659-2684, 2011]) that compares boundary layer with full profile parametrisations to answer questions like: does the retrieval of typical (aerosol) profiles profit from the "over-determined" parametrisation or is the risk of failing to represent realistic profiles in practice too high?
(ii) Our rationale for using a boundary layer parametrisation leading to an "over-determined" inverse problem was, on the one hand, to address certain questions (like regularisation, the possibility to retrieve further aerosol optical parameters) using a simple model that avoids a priori information as much as possible. In this context we are not interested in profiles that cannot be represented well. For profile retrieval from measured data, on the other hand, we envisage a two step procedure, where this robust, simple retrieval will precede the full profile retrieval (i.e. as empirical a priori). In this case, we would discard first retrievals with a high residual (due to high representation errors).
For the sake of completeness, we would like to add that error estimates in eq. (22) are the result of various linearisations. We are not sure whether for our model the one for the representation error would hold, e.g., for arbitrary, multiple layers etc.

Response to technical comments
Eq.(8): The vector $\mathbf{y}$ was changed to $\mathbf{x}$.
P2592, L5: In this sentence we mean the norm of $\mathbf{x} - \mathbf{x}_a$. We deleted "regularisation" to make this clear.
P2595, L9: "least square" → "least squares".
P2597, L13: dito.
P2600, L23: "orders" → "orders of magnitude".
P2601, L15: "top" ↔ "bottom".
P2608, L2: Correct, this is a mistake: "ϕ_{rel} getting larger" was changed to "ϕ_{rel} getting smaller".
P2609, top: A measurement (as component of the fit vector) which can be more or

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less directly expressed in terms of the fit parameters mathematically acts more or less like the a priori, the only difference being that the a priori represents an *assumed* measurement of the fit parameters. Taking this point of view can help to understand the effect and possible interference measurement and a priori/regularisation, especially in our case (fig. 14 in comparison to fig. 11), where the errors of the intensities are modified.

In this sense, the paragraph p. 2608, lines 27ff. was meant to give an interpretation for the fact that the retrievals in fig. 14 behave so differently for different solar positions and regularisation parameters. But since we do not substantiate the usefulness of this interpretation for our particular case and this comment confused more than it helped, we decided to delete this passage.

P2610, L5: Yes, of course. We refer to this in lines 2 & 3 as "... the fact that extinctions increase and the lengths of the light paths generally decrease ...". We used "extinctions" merely to avoid using of "AODs" all the time.

P2614, L6: We completely agree that varying quality of the retrieval for forward and backward direction is accounted for when combining them using a Kalman filter. The point we intended to make was that in cases, where a retrieval sequence evidently starts with a large impact of the a priori — and thus of its quality — a combination might not automatically improve the retrieval. On the other hand, one doesn't have to start the retrieval chain at an obviously bad place.

Since we haven't discussed this point in detail, nor quantified the effect of combining both directions for our examples or actually applied a Kalman filter, we changed this passage to "Results from different retrieval sequences (for example in forward/backward direction) can be combined and used to estimate the actual smoothing error.".

P2615, L1: The sentence was changed to: "Large values of the residual suggest a problem with assumptions on the underlying model or the (systematic) measurement errors.".

Fig. 2 and 3: Fig. 2 has been rearranged (Left: West, right: North). References in the

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text have been changed accordingly.
Fig. 3: Units added to y-axis.

Interactive comment on Atmos. Meas. Tech. Discuss., 6, 2583, 2013.