Atmos. Meas. Tech. Discuss., 6, C759–C762, 2013
www.atmos-meas-tech-discuss.net/6/C759/2013/

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

Anonymous Referee #1

Received and published: 3 May 2013

General comments

The manuscript by Hartl and Wenig describes a comprehensive model study on the regularisation of the least squares retrieval of vertical profile information from MAX-DOAS measurements. Currently, two approaches for the retrieval of information on trace gas and aerosol vertical profiles from MAX-DOAS measurements exist, namely the retrieval of the full vertical profile using optimal estimation methods and the least

squares retrieval of only a few parameters that describe the profile. Implementations of the latter approach are usually numerically less expensive and much faster, in particular if they are based on look-up tables. However, so far parameterised retrievals suffer from a thorough characterisation in terms of errors and numerical stability.

Hartl and Wenig investigate the behaviour of a parameterised aerosol retrieval using the methodological framework of regularisation theory and thereby bridge the gap between more complex retrievals of the full profile and more simple parameterised least squares algorithms which so far lack a comprehensive error analysis. The authors present a thorough characterisation of the errors and the stability of the retrieval. A main result is that a stable retrieval can only be achieved if a regularisation is performed, and it is shown that a dynamical choice of the regularisation parameter is necessary. It is furthermore shown by Hartl and Wenig how a weighting of the intensities should be performed if these are used as further measurement parameters. Both findings are also likely of importance for algorithms that retrieve the full profile using optimal estimation.

The paper is very well written and fits into the scope of AMT. I only have very few comments and recommend a publication of the manuscript after addressing some minor comments which are mainly of technical nature.

Specific comments

I suggest to remove '... and westward viewing direction' from the title. The viewing direction for which the case studies have been performed is only a very specific aspect, and simulations have also been performed for northward viewing directions. As far as I understand it, the conclusions drawn from the presented studies are valid for any viewing direction, and you state this explicitly in the introduction (P2587, L19).

I am a bit concerned about the way the regularisation has been performed. Actually, it is not valid to introduce a regularisation term in the form $\gamma^2(\mathbf{x}-\mathbf{x_a})^\mathbf{T}(\mathbf{x}-\mathbf{x_a})$ because the state vector $\mathbf{x}$ consists of elements with different physical units (extinction with unit of inverse length and dimensionless AOD). Thus, the effect of the regularisation would be very different if different units (e.g., cm^{-1} instead of km^{-1} for extinction). I wonder why you did not introduce a regularisation in the form $\gamma^2(\mathbf{x}-\mathbf{x_a})^\mathbf{T}\mathbf{L}^\mathbf{T}\mathbf{L}(\mathbf{x}-\mathbf{x_a})$ as proposed in the outlook. You should at least do so formally, with $\mathbf{L}$ being the identity matrix for this particular choice of units of the measurement vector.

The parameterisation error is potentially one of the main errors that can arise when using a parameterised approach instead of a retrieval of the full profile. This error has been discussed conceptually in section 2.4. However, it would have been very interesting to see how large this error can actually be, e.g. in cases of uplifted layers or multiple aerosol layers.

Technical comments

Eq. 8: The use of $\mathbf{y}$ as a vector in state space is a bit confusing since in most publications $\mathbf{y}$ represents the measurement vector. I suggest to replace $\mathbf{y}$ with $\mathbf{x}$.

P.2592, L5: Please define the regularisation norm explicitly. Is it not clear whether it is given by the sqare of $(\mathbf{x}-\mathbf{x_a})^\mathbf{T}(\mathbf{x}-\mathbf{x_a})$ or of $\gamma^2(\mathbf{x}-\mathbf{x_a})^\mathbf{T}(\mathbf{x}-\mathbf{x_a})$.

P2595, L9: Replace ‘least square’ with ‘least squares’.

P2597, L13: Replace ‘least square’ with ‘least squares’.

P2600, L23: Replace ‘orders’ with ‘orders of magnitude’.

P2601: ‘Top’ and ‘bottom’ of Fig. 3 are confused.

P2608, L2: Shouldn’t it be ‘with Φ_{rel} getting *smaller*’?

P2609, top: I don’t really get the point why the inclusion of intensities can be considered as an augmentation of the data vector rather than an additional contribution to the measurement vector.

P2610, L5: You mention that the information content decreases for small relative az-

imuth angles. But simultaneously, also the AOD increases. Might this also lead to the observed decrease in information content?

P2614, L6: I don’t see why Kalman filtering in two directions should only be applied if ‘these sequences are regarded as equally valid or good’. Usually, a Kalman filter combines forward and backward directions with the respective covariances as weight (e.g., Rodgers et al., 2000; Frieß et al., 2006) and thus accounts for the varying quality of both sequences.

P2615, L1: Not only problems with the underlying model assumptions can cause large residuals, but also systematic errors in the measurements.

Fig. 2 and 3: I suggest to bring the panels in both figures in the same order (i.e., West on top, East on bottom, low aerosol left, high aerosol right).

Fig. 3: Units for y-axis are missing (molec^2/cm^5).

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