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Atmospheric Chemistry and Physics Discussions

Interactive comment on "Aerosol model selection and uncertainty modelling by adaptive MCMC technique" *by* M. Laine and J. Tamminen

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We warmly thank the 3 referees for the careful reading of our article and for the criticism and corrections offered.

The purpose of the article is to introduce and demonstrate a new method suitable for model selection problems. We would like to make the method available for the scientific community represented by ACP readers. The method is demonstrated by an example on GOMOS data, for which we have successfully used the methodology. We have already conducted some new computer experiments to study the geophysical implications of aerosol model selection. We feel that thorough validation with external data belongs to a larger follow-up article, and the current article serves as an introduction to the methods.

The helpful comments on the language and style of all the referees have been taken into account in the new revision. Some special questions raised by the referees are discussed below.

For referee #1:

Major comments

A large scale comparison on the use of different aerosol models and their effect on the GOMOS retrievals would surely be needed before any definite could be said about the merit of the approach on this particular case and whether the operational algorithm could be enhanced by the use of different aerosol model, or even a set of models depending on the altitude and location. This was not however the target of our paper. This has been clarified more in the text.

In our opinion, the estimated shape of the aerosol extinction transmission spectra could be used to infer the aerosol type, or the size distribution of the aerosols, however this is a subject of further study.

Minor comments

We have corrected and reformulated the abstract.

With regards to the use of convergence diagnostic measures for MCMC convergence. We are aware of these and our software calculates several of such numbers. However, a matter not directly linked to the present article or the AARJ method, we have still found the visual inspection of the chains to be the most reliable check when developing new methods and testing them with real applications. The statistical power of these tests to recognize that the chain has really converged is not known, especially for samplers utilizing reversible jump methodology and adaptation.

For the separate initial runs for each model the problem is a nonlinear estimation problem with 5-7 parameters. For this a chain of length 10 000 to 50 000 is typically sufficient. With good starting values, and with the aid of adaptive MCMC, a chain of length

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5000 can even suffice as a starting point for the AARJ.

For the RJMCMC run of the AARJ algorithm the needed length of the chain is no longer so easily seen beforehand and we are still lacking a common criteria on how to determine the chain length. Chains of length 50 000 in the AARJ step were performed to do the analysis in this article.

As for initial values, for the present problem those can be easily obtained by an initial least squares fit of the parameters. Together with an estimate of the uncertainty of these initial values they provide a good starting point for the chain and for the proposal covariance used by the MCMC methods. The visual (or a test statistic based) investigation is still needed to ensure that we have obtained the initial values right.

We have modified the introductory sentences on model selection in page 10794.

The technical corrections offered are taken into account in the new revision.

For referee #2:

Major comments

1. Does the method provide more accurate retrievals?

In fact, we expect that taking into account the modelling error increases the uncertainty in the results. But the uncertainty estimates are more realistic as we take the uncertainty in the modelling in to account.

2. What can be said about the type of aerosols based on the modelling?

The estimated shape of the aerosol extinction transmission spectra can be used to infer the size distribution of the aerosols, however this is a subject of further study.

Minor comments

1) We have reformulated and expanded the abstract.

2) The amount of aerosols above 30 km is typically very low, even not statistically

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distinguishable from zero with any model, and the choice of the aerosol cross-section model does not affect the retrieval of other constituents. This is clarified in the text.

3) Some of the terms of statistical or computational importance are not fully expanded in the article, partly due to the intended nature of the text being an introduction to a new computational method. Some clarification are now included in the text.

In Bayesian settings, when estimating both the model parameters and the noise level of the observations, some prior information must be put on the error variance. A standard choice is a Gamma distribution on the reciprocal variance. The distribution is chosen to be wide enough for the corresponding posterior to be determined mostly by the likelihood information.

The factor 2.4ˆ2 in the definition of the proposal covariance adaptation is one particular choice given in the literature for making the Monte Carlo errors of the estimates calculated from the chain as small as possible. The significance of this particular number is hard to determine, because it depends on the problem, the dimension of the unknown, and how "non-Gaussian" the posteriors will turn out to be.

4) 5)

A reference to the GOMOS instrument is given in the introduction of the article. A more thorough description of the instrument and the physics involved could be included to make the text more accessible to a general reader, on the expense of length of the article. As stated in the beginning, we would like to follow up this article with one with more comprehensive results on comparison over the operational results.

6)

You are correct that for the models 1 and 3 the reference wavelength is 500 nm. As for the models 2 and 4 we have used reference wavelengths 300 nm, 500 nm and 600 nm. This is stated in the caption of fig. 2. A second degree polynomial can be parametrized by giving the value of the polynomial at distinct "x" coordinates. This can

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be done, for example, by using suitable Lagrange polynomials as polynomial basis, or by reparametrising the standard monomial based polynomial coefficients using the so called Vandermonde matrix of the reference wavelengths.

The technical comments have been taken into account.

For referee #3:

Some more text concerning the implementation and application issues has been written, but we have tried not to expand the article too much from its original form.

An extension to time dependent model parameters is surely possible. Depending on how we model the time dependency, however, will make the number of parameter to grow. The model selection itself does not necessary increase the number of parameters. The method, in such form we have used it here, i.e. updating all the unknowns of one model in one block, and with current computers, can have up to 200 parameters. Using component wise update of the chain allows for, say, 1000 parameters, with the expense of longer computations. Using hierarchical models parameters and Gibbs type MCMC sampler for some of the unknowns, would allow for even larger number of unknowns.

1)

We have reformulated the abstract.

The aim is here to provide tools for a study of choosing the best model for given situation. The question of the ultimate right model for aerosol retrieval is not yet solved.

About the discussion on the implementation. We have given a more detailed pseudo code. However the actual implementation of the algorithm would still require some background information on implementing MCMC type of algorithms, and consulting the references given in the text.

2)-5) corrected

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6) The algorithm can be applied efficiently even when the competing models are more complex that the ones used in the example. More complex model, of course, increases the computational burden. If the computations become too heavy, AARJ can be used to validate more simpler model selection criteria, such as the Deviance Information Criteria (DIC). For the GOMOS problem, for example, we have seen that the AARJ results agree reasonable well with DIC, that can be calculated directly from separate individual MCMC runs

7) In geophysical inverse problem literature the forward model, or sometimes the model in short, stands for the mathematical or physical equations that are used to derive the noise free observations given the assumed state of nature. Statistical model adds the description on the observational error (noise) and possible a priori information on, for example, the smoothness structure of the solution. The use of the phrases "model" and "forward model" was checked and corrected.

8) corrected

9) The AARJ algorithm in itself does not add much to the computational burden. The extra calculations involve only some matrix vector products. The forward model calculations needed to calculate the model likelihoods are the ones that take the most CPU cycles. As several models are tried, some of which possibly do not fit the data, the overall chain will have larger rejection rate than the individual chains would have, and it will, thus, need to be run longer. That is one reason why the adaptivity is needed to make the sampler as efficient as possible.

10) Positivity prior can be set by MCMC, by just rejecting those proposed values which are not positive.

11) For the chain length, see our response to referee #1. A new section on computational considerations has been added to address these issues.

Interactive comment on Atmos. Chem. Phys. Discuss., 8, 10791, 2008.