**Atmospheric
Chemistry
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Discussions**

Interactive comment on "Towards inverse modeling of cloud-aerosol interactions – Part 1: A detailed response surface analysis" *by* D. G. Partridge et al.

Anonymous Referee #2

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Review of "Towards inverse modeling of cloud-aerosol interactions - Part 1: A detailed response surface analysis" by D. G. Partridge, J. A. Vrugt, P. Tunved, A. M. L. Ekman, D. Gorea, and A. Sorooshian Atmos. Chem. Phys. Discuss., 11, 4749-4806, 2011.

General comments

The article shows how, by using two dimensional response surface sensitivity plots, the feasibility of inverse modeling can be studied. Nine parameters of an adiabatic cloud parcel model are selected and the sensitivity plots of an objective function are studied in detail. Tuning of the objective function is performed based on sensitivity studies and model calibration is performed by numerical optimization and simple Monte Carlo. Only

synthetic data is used.

It is not fully clear for what purpose this article is written. In general, model sensitivity analysis should be the first step in any modelling application. In that sense, the text would make a good material for a textbook on aerosol modelling. Almost every modelling exercise in any applied field contains numerous iterations and reformulations. Many times by trial and error, sometimes by using some well established methodological recipes. It is not necessary to report these steps towards the final model formulation unless the methods used are of interest by novelty, for example. The lack of any real life observations makes the exposition to be more of a pedagogic nature, also.

The authors emphasize the choice of the objective function (OF). In general, OF includes the parametrization of the unknowns (e.g. the transformations used) the choice of parameters to estimate, the observations (i.e. the design of the measurement processes), the forward model formulation, and also the statistical distribution of the error term and the prior distributions for the parameters. Again, the formulation of all these is important in any inverse modelling. To my mind, the authors do not clearly distinguish between these different elements. Everything seems to be studied only in connection with the difficulties there will be in using a numerical optimization algorithm. The questions that are more interesting would be of the following type. What observation can and should be collected? What is the information content of these measurements? How should the model be parametrized with respected to the unknowns. What kind of prior information is available and needed to make the unknowns identifiable? Are we aiming to design a new measuring instruments? Are we trying use existing instruments and to perform experiments with maximum amount of information about a given model?

The authors give a hint of a more comprehensive modelling approach in a forthcoming "part 2" of the paper. For studying parameter uncertainty and identifiability in non-linear models the methods offered by Bayesian statistical analysis and MCMC simulation algorithms are superior in many ways to standard classical sensitivity analyses. Using

MCMC method, the multi-dimensional cost function surface (the posterior distribution of the model unknowns) can be explored fully. Non-identifiability can be diagnosed by MCMC, and by using suitable efficient and adaptive MCMC methods, it is usually possible to gather information even if some of the parameters have very wide marginal posterior distributions. The Bayesian approach allows for "fixing" the non identified parameters by a prior distribution instead of fixing them to a single value. Instead of two dimensional surfaces that are conditioned on some given values of all the other unknowns, one or two (or higher if needed) dimensional marginal posterior densities can be easily constructed from the MCMC chain.

As also noted by the authors, the sensitivity analysis obtained by varying two parameters while keeping other unknowns fixed can be misleading by revealing only parts of the cost function surface.

Without seeing the "part 2" of the article, I would suspect that some actually interesting geophysical results could be acquired by the MCMC analyses. So, to conclude, I'm looking forward for the part 2 that would describe full statistical uncertainty analysis by MCMC or related methods. Also, applying the methods to real observations would make the methodology more interesting for the typical readers of ACP.

My suggestion is to write the planned "part 2" using statistical inversion methodology and with real data in addition to simulated data. Consider including the most important lessons learnt from the sensitivity analyses of "part 1" as one section in the new article.

Specific comments

About terminology

In statistics the term "response surface" has been traditionally used for analyses where one is interested in the optimal value of some process model response and a set of designed experiments is used to form an approximate (usually quadratic or surrogate) model near the optimum response. These analyses are usually graphically aided with

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two dimensional plots of the "response surfaces". Here the term "response" is used for the value of the objective function. I must admit, that by looking at the title of the article, I was expecting to find a different kind of response surface analysis.

These plots used in the article could simply be called parameter sensitivity plots or conditional log likelihood surfaces, for example.

Section 2

It is not explicitly stated, whether exactly the same forward model is used both to simulate the synthetic data and to perform the inversion. Even if only studying or developing an inverse method it is advisable to generate the data with more a comprehensive model (with a higher resolution, for example), to avoid so called inverse crime [Kaipio & Somersalo, 2004].

Section 3

The main message seems to be that the inverse problem presented is difficult to solve, and care must be taken when defining the objective function, choosing the optimization method and selection the measurements. The information content studies show that: "the inclusion of the right type of information, not necessarily more information that is most important". Not very strong or helpful result to offer for anyone trying to solve similar problems.

Section 3.3: "an optimisation algorithm has not previously been applied to a cloud parcel model". This sounds a very strong statement. I can not give any evidence on the opposite, however.

Section 4

A simple Monte Carlo analysis is compared to one specific deterministic optimization method. Again, the conclusion is not very surprising. "A brute force MC approach is not only inefficient, but potentially also misleading", but optimization method can find "true" optimum that was used in generating of the synthetic data.

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Reference: J. Kaipio and E. Somersalo, Computational and Statistical Methods for Inverse Problems, Springer, 2004.

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