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Atmospheric Chemistry and Physics Discussions

Interactive comment on "Inverse modeling of cloud-aerosol interactions – Part 2: Sensitivity tests on liquid phase clouds using a Markov Chain Monte Carlo based simulation approach" *by* D. G. Partridge et al.

Anonymous Referee #2

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Review of acpd-11-20051-2011: "Inverse modeling of cloud-aerosol interactions - Part 2: Sensitivity tests on liquid phase clouds using a Markov Chain Monte Carlo based simulation approach"

Some general comments

The article aims:

1. To study sensitivity of a specific cloud parcel model to a set of aerosol size distribution parameters by using synthetic observations.

2. To test and demonstrate a specific DREAM MCMC sampling algorithm for performing sensitivity analysis and estimating the parameter posterior distributions.

While no analysis on real observations are performed, this methodological demonstration is still probably of interest to the aerosol modelling community.

As in the review of the first part of this two part paper, I would have liked to see some discussion on design of experiments: how the simulated observations relate to possible real observations. Are there measuring devices available for such observations? Some parameters are seen to be uninformative with respect to the simulated observation. Would some reparameterization or different observational setup solve the problem?

Although the authors do not seem to agree, the use of same forward model to generate the data and solve the inverse problem will only provide information on the formal algorithmic flawlessness of the procedure. For relevant study of the underlying inverse problem, discretization, modelling error and ill-posedness of the problem, more comprehensive model for simulation of the "truth" is needed.

The specific remarks below concern mainly about terminology and the description of the statistical framework employed.

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line 3: In the term Markov chain Monte Carlo the word "chain" is not usually capitalized. This applies to the whole paper.

line 8: "... modelling framework is shown to successfully converge to ...". Framework converges? Maybe: "is shown to successfully estimate the correct calibration parameters"

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line 10: "best values" is quite strong, and usually one refers to maximum a posteriori (MAP) instead of maximun likelihood when prior distribution is used explicitely.

line 12: P is capitalised in P(theta|Y), but in the next line it is not

line 14: P(theta|Y) should be p(theta)

line 15: Here you refer to the likelihood as objective function but later OF is defined as a function of model residuals.

line 17: Schoups and Vrugt (2009) is missing in the references.

line 25: "before any data is collected" is not correct. Prior can, without any problems, depend on independent observations. Modelling is always an iterative process, as also discussed here, so both model and priors can be changed after iteration.

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line 2: likelihood is (unnormalized) distribution of observations given the parameters. As the posterior is a product of prior and likelihood, the distributional form is important for the posterior. Least squares minimization corresponds to Gaussian likelihood, i.e. Gaussian observational error. From a statistical perspective, least squares is a consequence of Gaussian modelling of the errors.

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line 17: "powerful array of statistical measures" is not true in practice as convergence diagnostics can only diagnose non-convergence, not convergence (furthermore, their statistical power to detect that the chain has not converged can be low). I see no convergence diagnostics used in this paper.

line 27: "detailed balance" and "ergodicity" are terms specific to Markov chain and MCMC literature and are possibly not very well understood by the readers of ACPD

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line 8: strictly speaking, the chain either is in the stationary distribution or not. In MCMC, stationary distribution is the limiting distribution so it is never reached, at least

exactly.

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line 2: "OF is simple least squares estimator". I think estimators and objective functions are different entities, although closely related. You could say that OF is the weighted sum-of-squares function. Estimator is what you get when you minimize the OF with respect to the parameter. Least squares and maximum likelihood estimators are the same for Gaussian likelihood and can even be said to correspond to the same OF, even if defined differently.

line 10: The weights w_i which act as inverse variance of observational error are set to 1. But this value will certainly affect the size and shape of posteriors distributions as the more concentrated the posterior will be near the mode, the more Gaussian they tend to be, by simple linearization arguments. Later, observation error is set to be 10%. Do you then change the weights accordingly?

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line 11: The inclusion of Matlab command line is irrelevant here. You could just say that additive Gaussian noise is added to the observations with 10% standard deviation.

line 6: The word "corrupt" seems out of contents. Every measurement is bound to have some noise. If an observation is "corrupt", it typically is an outlier of some sort.

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line 20: Performance of MCMC algorithm

This section explains how DREAM works for error free observations and for observations with 10% error added.

The authors show that the algorithm is "performing" in the sense that is works correctly. For a real performance study, one would like to see comparisons to alternative methods, such as plain Metropolis-Hastings using numerical Jacobian for construction proposal distribution, for example, some timings, estimates of Monte Carlo errors of the chain estimates or estimate of the efficient number of simulations. There is mild nonlinearity in the pairwise correlation figures (e.g., Fig.9) but no sign of multi modality. Also, the number of parameters is only four. Would it be possible to solve this problem with more standard MCMC algorithms, even more efficiently?

In Figs 3 and 4 the MCMC chain plots show the upper/lower prior limits are reached for several of the parameters. Either the observations are not informative or prior specifications are too restricted. It is typical that experts, not accustomed to provide multi-dimensional priors, tend to think in terms of one dimensional conditional distributions instead of marginal distributions when defining limits, and thus give too limited bounds.

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line 18: Only 20% of the model simulations are used in analysis. This seems rather inefficient. Do you recommend this as a general rule for DREAM, or have you used some diagnostics to infer this percentage?

line 25: It is not clear from the text what is meant by relative sensitivity. Caption in Fig. 7 suggests that the prior range is used as scale. This is not stated in the text. This sensitivity, as said, depends solely on the relative choice of the prior bounds. And also, as discussed above, it depends on the weights w_i used in the likelihood "OF".

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line 18: maybe you should re-think the points given as advantages; are these really the main advantages. In the third item, problems are given as advantages. About the fourth item: are you running the code in parallel, or is this just a possible advantage.

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line 8: limitations of what? Why is the second item "a limitation"?

line 22: Why do you say that introducing more prior would produce more "confident"

sensitivity estimates? Confident in what sense? Wouldn't the posteriors then include more information from the prior and less from the observations.

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line 23 "the objective being ..." this sentence is very hard to understand. What model input parameters? Do you mean a priori parameter values? What is a "measurement estimate"? What are "associated observations"?

Interactive comment on Atmos. Chem. Phys. Discuss., 11, 20051, 2011.