Atmos. Chem. Phys. Discuss., 13, C12601–C12608, 2014
www.atmos-chem-phys-discuss.net/13/C12601/2014/

Atmospheric Chemistry and Physics Discussions

ACPD
13, C12601–C12608, 2014

Interactive comment on “Characterization of uncertainties in atmospheric trace gas inversions using hierarchical Bayesian methods” *by* A. L. Ganesan et al.

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Received and published: 27 February 2014

Response to Referee # 2

We thank the reviewer for his/her comments and provide responses below. Reviewer comments are provided with the author’s response following each comment.

1. Even though some correlation length scales and variances are not fixed from "expert knowledge" in this work, the functional form of the a priori covariance according to Eq (6) is still as simplistic as in most "traditional" studies. Of course, these simplistic forms are generally chosen because the full complexity of the "true" covariance is difficult

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to handle, but choosing a simple form means that it cannot actually be expected to become substantially closer to reality, thus heavily limiting the achievable gain from varying hyper-parameters.

Author's response: The functional form of the model-measurement uncertainty correlations was an exponential decay process in this application. However, the method that is presented is not limited to this particular form but could be any function (e.g., Matern covariance function, higher-order autoregressive process, etc). Furthermore, more complex covariance structures could be constructed that are functions of auxiliary variables relating to expected errors in the transport model. This manuscript presents a methodology and one application of it, but could be easily reformulated with other functional forms. We have modified the text to clarify that our chosen case study represents one of an infinite number of possible applications in the HB framework. Beginning on p33410, line 6, we have added, "The functional forms used in this application of the hierarchical Bayesian framework represent only one of many possible applications and can be reformulated to represent different assumptions."

2. If I understand correctly, the MCMC run of Sect 2.1 comprises 50000 calls of H*x, which is a computational demand more than 2 orders of magnitude higher than in most published atmospheric trace gas inversions studies. For many (if not most) regional or global applications, this will be prohibitive.

Author's response: With a relatively straightforward implementation of MCMC routines in a compiled programming language, we have found that problems with a parameter and/or observations space of order N$\sim$10ˆ4 are feasible on a reasonably powerful workstation. In practice, we would argue that, assuming even moderate decomposition of, for example, the parameter space, this order of magnitude would be appropriate for very many inverse problems. The main computational expense is in computing the inverse of covariance matrix R and the determinant of R, which are each O(Nˆ3) operations. The multiplication of H*x will scale with the number of observations and state vector elements.

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We note that various well-known methods can also be employed, which can dramatically increase the efficiency of MCMC routines for high-dimensional applications, should they be required. For example, measurement covariance matrices can be assumed to be "separable" in, for example, space and time, exploiting properties of the "Kronecker product" to convert the inverse of R into the inverse of smaller matrices (thus reducing the limiting "bottleneck" in our particular problem). Furthermore, dimensionality reduction can be used to reduce the number of elements in x or y into a smaller set of basis functions while retaining the majority of information in the system (e.g., principal components analysis). There are many existing methods that can be employed within this framework to extend the work into larger applications.

The text has been refined to state (beginning on p 33410, line 6 that, "In this particular application of hierarchical Bayesian modeling and MCMC, the main computational cost is in computing the inverse and determinant of the covariance matrix, R. Several methods exist to reduce the computational cost of inverting large (covariance) matrices, if required for higher-dimensional applications (see for example, Sun et al., 2012)."

3. Though I agree that missing information about the a priori PDF represents a major problem in atmospheric trace gas inversions, there are further problems with potentally larger impact, in particular errors in the modelled transport, and undersampling by the available data. I feel that potential improvements through the presented method need to be set into the context of these remaining problems. For example, biases in transport cannot possibly be detected by any hyper-parameter, and therefore represent an additional and potentially limiting error in the results.

Author's response: We agree with the reviewer that biases will not be fully captured in the formulation presented in the manuscript. The method, as formulated in this particular case, will attempt to represent any differences between the model and observations as "random" uncertainties in the system. Investigation of the influence of model biases will be the subject of further work. We have included a note in on p 33410, line 6 that, "Model parametric uncertainties have not been explicitly considered here but have to

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the potential to lead to biases in the outcome of the inversion."

We also note that the improvements made with this hierarchical method move toward better (if not complete) uncertainty quantification, but as we show in the pseudo-data experiment in section 2.2, the method still has some influence from the choice of a priori values and uncertainties of the hyper-parameters.

4. While I still think that this is a worthwhile study and should be published in ACP, given these caveats I do feel that the text substatially overrates the gain of the proposed method. The revised version should openly discuss these caveats, and already clearly name them in the abstract.

Author's response: The text has been reflected to discuss how this method can be extended into higher-dimensional applications (see comment 2), along with our comments regarding parametric model uncertainty (comment 3). The main feature of this manuscript is in presenting a new method and its advances in characterizing uncertainties. As such, we feel that the caveats associated with the choices of functional forms, which can be changed for different applications, do not need to be discussed in the abstract.

Minor comments:

5. Eq(1): All symbols should be riefly explained. Also mention that x,y etc are vectors.

Author's response: We have stated on p 33409, beginning line 4 that, "Fluxes and hyper-parameters could vary in space and time and are shown in this framework as vectors that could be estimated with spatial and temporal resolution." We have also added additional descriptive terms in the text (see below). For further clarity, the symbols are specified in the ACP format designating vectors (bold, italic), matrices (bold, roman) or scalars (normal, roman).

We have noted one correction – the autocorrelation timescale, tau, should have been represented as a scalar (rather than a vector) in this application and we have corrected

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the text throughout.

We feel that in general, the symbols have been well explained. For example, describing Equations 1 and 2, the text states that “The deviations between the vector of measurements, y, and model-simulated mole fractions, Hx, where H is a matrix that contains the sensitivities of atmospheric mole fractions to changes in emissions sources and x is a vector containing the emission sources, are weighted by uncertainty covariance, R. Similarly, deviations between emissions and their a priori values, xprior, are weighted by uncertainty covariance, P.” For equation 7, the text states, “We apply the hierarchical Bayesian model to use data, y, to estimate x, a vector of emissions and boundary conditions to the inversion domain, as well as a set of hyper-parameters that govern the a priori emissions and model-measurement uncertainty PDFs. The hyper-parameters include vectors mu_x and sigma_x, which describe the log mean and log standard deviation of a lognormal a priori emissions PDF, the vector sigma_y, which describes the standard deviation of a Gaussian model-measurement uncertainty PDF and scalar tau, which is a model-measurement autocorrelation timescale.”

6. p33406 line 15: Even if the "NHB" calculations are much less costly than "HB", many applications are certainly not of "low computational expense" depending on number of data and unknowns (see caveat above).

Author’s response: The text has been modified from “low computation expense” to “lower computational expense.”

7. p33406 line 18: The statement "the derived fluxes . . . strongly depend on these parameters" is true in many applications where data are sparse, but is not true in well-constrained situations. This means it is not a feature of Eq(2) per se.

Author’s response: We do not fully agree with this comment. In situations where data density is high and the model-measurement covariance matrix is not properly structured (including, critically, model representation covariances in space or time), there is the well-known danger of over-weighting the data and its model representation, result-

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ing in posterior emissions uncertainties that are significantly smaller than those that exist in the “true” system. In any situation, regardless of data density, these covariance matrices needs to be accounted for properly, and we feel that the HB framework, takes us in the right direction.

8. p 33410 line 5: Similarly to the comment above, the assumption of Gaussian model errors is certainly a great simplification of reality.

Author’s response: Similarly to our response to comment 1, we stress that we have presented only one application of the methodology, in which we assume Gaussian model errors. However, the form of this function is not fixed and can be assumed to be any distribution based on the user’s knowledge of the system. We have chosen Gaussian errors to be consistent with other inversions for our comparisons.

9. p 33411 line 19: I may have misunderstood, but isn’t rho(x | mu*, sigma*) the "true distribution" and not rho(x|y)?

Author’s response: To make it more clear, we have changed the text to state “. . .consistent with the marginal distribution rho(x|y).” and removed the word “true.”

10. p 33412 line 8: Formulation "shown trough Eq" is unclear.

Author’s response: We have reworded to state that “For each inversion, with parameter and hyper-parameter PDFs shown by Eq. 16. . .”

11. Sect 2.2: How did the actual emission estimates (as the primary result) compare to the truth?

Author’s response: The median of the posterior PDF is consistent in both cases with the “truth” (as shown by both HB and NHB passing through the 0.5, 0.5 point on the quantile-quantile plot). In this example, we fixed the median of the PDF to be the “truth” and data were generated from that PDF, so this result is expected.

12. p 33413 line 11: Formulation "monthly diurnal" is unclear.

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Author's response: The text has been revised to state, "....monthly model-measurement uncertainties , monthly means and..." 'Diurnal' has been removed as we go onto to state that it is diurnal in the same paragraph.

13. p 33415 lines 19-22: This sentence is not fully clear to me.

Author's response: The text has been moved to the end of section 2.2 and been revised to state "An important feature of the HB framework is that the posterior emissions PDF is less sensitive to assumptions about the hyper-parameters governing the a priori emissions PDF than if direct assumptions were made about this PDF, as is the case in a NHB framework. This is because, in a HB framework, the parameters governing the a priori emissions PDF are themselves informed by the data."

14. The assumption of constant SF6 fluxes is a potentially problematic one - if real SF6 fluxes vary within the month, estimates will have biases not accounted for in the error estimate (aggregation error).

Author's response: SF6 fluxes can be derived using this method at any resolution. In our application of the method, we chose to estimate constant monthly fluxes, but daily or hourly could be estimated through this method, if desired. This was a choice made in this application, but an investigation of the influence of this type of aggregation error on this particular problem is not thought to be central to the paper.

15. Fig 4: The inset should be described if present, but I rather feel the figure would win clarity (and not loose information) if the inset would be removed.

Author's response: The inset is important to be able to clearly see the values at the low-end of the scale. The caption has been change to include a description of the inset. It now states at the end of the caption, "For clarity, the inset shows a magnified view for countries with relatively small emissions."

16. Typos:- p 33413 line 23: due to

Author's response: Thank you for catching the typo. The text has been corrected.

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