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Interactive comment on "Objectified quantification of uncertainties in Bayesian atmospheric inversions" *by* A. Berchet et al.

Anonymous Referee #1

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This paper describes the potential of so-called "marginalized inversions" in the objective interpretation of inversion results. According to the authors, the method offers great potential compared to the classical inversions in which subjective choices are unavoidable. I think that the authors might have a good point here, and unfortunately the system has to be simplified quite dramatically to use the method. However, I found the paper very difficult to digest. The theoretical framework consists of many individual steps, which are all combined in a single paper. As further detailed below, the reduction of the state and observations (section 3) is not really vital for the paper. Also the authors employ a plume filtering technique, and present many other details of their method, including two models. All in all, this leads to a rather difficult paper to digest. I really did my best to fully understand the results, but had large difficulties. Specifically, the rather condensed presentation of the results (figures 5 and 6, table 1) does not do

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justice to the paper and is very difficult to understand. I would propose to remove a significant amount of theoretical concepts from the paper and to shorten the paper in that respect. Instead, a more detailed analysis of the results (more in a step-by-step fashion) would greatly enhance the readability. For instance, it would be very instructive for a reader to see what typical time series look like ('truth' versus "OSSEs"). I understand that this requires a substantial amount of rethinking the paper. However, I think this is needed to address a wider audience and to make a larger impact.

Major comments:

1. Language The paper contains many small mistakes and strange language constructions. A native speaker should correct the manuscript. In the minor comments list I have listed some, but not all the places where I encountered ill-formulated constructions.

2. Structure of the paper The paper addresses basically two separate methodological topics. First, the "marginalized inversion" paves the way for an objective choice of uncertainties of the prior fluxes and observations. Second, and required by the computer intensive nature of the marginalized inversion, the authors discuss the reduction of the state space and the observational space (section 3). This latter part seems to me a "paper in a paper" as it is not really vital for the problem. The only aim is to define a system with a size that is manageable. It would be my suggestion to remove the second part from the paper (i.e. most of section 3.1) and to summarize it in a few lines (e.g. just give the dimension of the state space and the number of observations). Now this part reads as a rather technical paper, which is not fully exploited ("In the following, only heuristic aggregation and sampling is chosen", see also last part of the section on page 4793). I think the work in section 3 is interesting, but should be presented in a separate paper. For the rest of the paper, I suggest some drastic re-arrangements and clarifications in the minor comments below.

Page 4778, line 11: computing → performing

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Page 4778, line 18: includes → calculates

Page 4778, line 24: "real observation sites". This is somewhat misleading, since the reader might think you also use real observations. I suggest: "with simulated observations on existing observation sites..."

Page 4778, line 26: gas → methane

Page 4779, line 11: reliably → reliable

Page 4779, line 11: understanding → understanding of

Page 4779, line 14: "inquire into the surface fluxes" → "obtain information about the surface fluxes"

Page 4779, line 16: the transport, the atmospheric chemistry, and the surface fluxes: "the" should be removed three times.

Page 4779, line 20: inferring back → inferring

Page 4779, line 27: on the vertical column → over the vertical column

»» from here on I mostly skip correcting small English grammar issues. Please use a native speaker to correct manuscript.

Page 4780, line 4: "The Bayesian....possible in order to....". Rewrite.

Page 4780, line 15: "of the errors the transport model makes, ". Rewrite, e.g. "transport model error statistics".

Page 4780, line 20: enlarge → enlarges

Page 4780, line 22 and on...to Page 4781, line 17: Most of this is the description of the method, and does not belong in the introduction. Refrain to a short description of Maximum Likelihood and maybe something about biases of non-continuous measurements.

Page 4781, line 14: do not prevent?? I think "do prevent".

Page 4782, line 11: cause a variability → cause variability

Page 4782, line 13: infer back → infer

Page 4782, line 21: please define that x refer to the fluxes.

Page 4783, line 2 and 3: Is assimilated really what you mean here? I think converted is better.

Page 4783, line 21: Kalmam→ Kalman Also, here it is probably wise to state that matrix R refers to the uncertainties in both the observation and the projection of the fluxes to the measurement space (Hx). So, model representation errors are in R.

Page 4784, line 2: purely→pure

Page 4784, line 19: said tuple?? What do you mean by said? The tuple mentioned above?

Page 4784, line 21: a local dependence? Unclear what is meant here. If I understand this well, it represents the posterior solution for a specific choice (R,B).

Page 4785, line 19: located to → located at. It is unclear here, what is meant with "dummy tuple". I understand that for each (R,B) you can calculate an x_a, P_a, but what do you mean by "dummy".

Page 4785, line 21: needed samples → required samples. Unclear what is a sample here: do you mean one particular (R,B)? Also, what is mean by "local" vectors x_a. Are there also non-local vectors? I see the symmetry with respect to x_a, but I do not see why the P_a drops out of the sampling procedure.

Page 4786. The pdf of (R,B). After equation (2) it is stated that "we assume no prior information of the uncertainty matrices". Here a chi-squared distribution is assumed. Please explain this better.

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Page 4786, line 6: This part of the paper becomes very messy. You are in the middle of a "theory" section, in which the Monte-Carlo method is explained. Here this is mixed up with a "method" section, in which a practical choice is motivated (only diagonal matrices (R,B)). A whole section is now devoted to the effect of diagonal matrices on the inversion ("too optimistic a reduction of uncertainties on the fluxes" → "a too optimistic reduction of the uncertainties on the fluxes"), and the reduction of the state space, with a reference to section 3. I suggest separating the "method" and "theory" in a better way, i.e. to move the particular setting to section 3. Given the more practical application that follows, it seems logical to stop section 2 here and start section 3 with the Maximum Likelihood (figure 1).

Page 4786, line 23: infered → inferred Here it is claimed that the Maximum Likelihood choice for (R,B) would overestimate the error reduction in the case of diagonal matrices (R,B). However, a valid question here is what is wrong with the Maximum Likelihood solution using full matrices (R,B), since this would provide a realistic solution to the inverse problem.

Page 4787, line 23: "each others" → "each other"

Page 4788, line 10: reduce → reduced; damp → dampen; shall→should The discussion here links nice to the part on diagonal (R,B) matrices in section 2.

Page 4788, line 15: "physical". I would remove this word.

Page 4788, line 17: straighter → straightforward

Page 4788, line 18: space → spaces

Page 4788, line 26: "a number of pieces of data" → "a number of data points"

Page 4789, line 20: "in order to inquire into the" → "in order to study"

Page 4789, line 26: said → processed

Page 4790, line 1: write → derive

Page 4790, eq. 5: The term E_w seems misprinted (or needs better introduction).

Page 4793, line 4: depicts → represents

Page 4797, line 24: the z_{abs} is not really clear to me. It will lead to an asymmetric distribution of errors, at least for positive emissions. This is also illustrated in figure 5, which shows large values of z_{abs} (all due to overestimates???).

Page 4798, line 10: But each inversion that provides a posterior error covariance matrix can be used to calculate these scales, am I right? So also the ML method without marginalization?

Page 4798, line 24: couple → couples

Page 4798, bottom: the role of BCs remains rather vague. What criteria are used to flag?

Page 4799, line 12: ays → days

Page 4799, line 14: oxydation → oxidation

Page 4780, line 24: punctual → localized Unclear also if wildfire emissions are included now or not. I assume they are not optimized. So why mention these emissions?

Page 4801: Here, it should be mentioned on which timescale the emissions are allowed to vary. I guess 10 days, like the LBCs, but I could not find it. The pseaudo-data or obtained using an inversion with real data. Now I wonder why (i) not to use real data in the framework (ii) in what respect the simulated data reflect already large biases in the system. Anyhow, this is one of the part of the paper that needs rethinking. It is hard to understand what is (i) a raw inversion (ii) how well the inversion is capable to reproduce the data. We never see any simulated of measured time-series in the paper.

Page 4803: top. Here biases are discussed. However, hardly any conclusions are drawn concerning biases. This makes the paper lengthy and messy.

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Page 4805: r_max could be determined by one region, e.g. a large correlation between emissions in one region and a neighboring region. Should r_max not reflect an average correlation between state vector elements?

Page 4806: discussion is very detailed (e.g. bias vs. filtering). I loose the view on the most important aspects of the paper.

Page 4807, line 4: dominates → dominate

Page 4808, line 19: the closest to the observation network: unclear sentence.

Page 4809: I like the comparison with the "frozen" error matrices. I miss however the connection with the earlier statement that this leads to an "underestimation of errors" when diagonal matrices are used. Anyhow, you should specify here whether the matrices are diagonal and the grid is reduced. A comparison with the classical inversions should employ the classical correlations I guess, and also present the ML solution.

Page 4825: component → components

Page 4826: plain→ solid

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Interactive comment on Geosci. Model Dev. Discuss., 7, 4777, 2014.