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Atmospheric Chemistry and Physics Discussions

Interactive comment on "Towards better error statistics for atmospheric inversions of methane surface fluxes" *by* A. Berchet et al.

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General comments

This is paper represents an important advance if the technical issues noted below can be addressed. In the 20 years since Bayesian inversions were described, the refinement of the statistical basis has been quite slow. My own view is that for regional inversions, it will probably be appropriate to go beyond the assumption of normally distributed errors, (see for example the Cape Grim CO_2 data set plotted in Enting (2002)).

Context

A point that is emphasised by Enting (2002) and more recently by Enting et al. (2012) is that in terms of statistical analysis, the inverse problem should be seen as one of

statistical estimation. In order to better integrate with the statistics community, and draw from the wider literature, the use of standard statistical notation and terminology is highly desirable. A particularly important aspect is the use of the 'hat' notation, to denote estimates as, for example, $\hat{\mathbf{x}}$. (As an example of the importance of the distinction, things such as expressing the mean square error of an *estimate* as $\mathrm{E}[(\hat{x}-x)^2]$ become much more complicated and/or obscure without such a distinction.) Similarly E[.] is termed the 'expectation' not (as is done in the paper) the 'expectancy'. As a minor point, since E is not a mathematical variable (unlike in $E = mc^2$) an upright font should be used.

Review

Comments on presentation

- The paper seems not to come to grips with an essential question: how much information about $(\mathbf{R}, \mathbf{B})$ can be obtained from the observations. The cases seem to be:
  - Desroziers: $(\mathbf{R}, \mathbf{B})$ are taken as diagonal and then the data/state vectors are stratified so that 41 (26+15) variances are to be estimated. Conceptually, this seems similar to the approach of Michalak et al. (2005): characterise $(\mathbf{R}, \mathbf{B})$ using a physically-based stratification using a small number of parameters (except that Michalak et al. (2005) do a joint estimation of state and error parameters).
  - Maximum likelihood: This case raises a range of questions. The implication is that although $(\mathbf{R}, \mathbf{B})$ are still taken as diagonal, *all* diagonal elements are being estimated independently, estimating more quantities than the number of data — this would seem to be insufficiently robust to be useful.
  - Observation space diagnostics: In this case, many more quantities are being estimated than the available date and again would seem to be insufficiently

robust to be useful. This would imply a χ^2 test with a negative number of degrees of freedom. There is a need to explain more clearly what is being done. Other technical issues with the description are noted below.

Issues

- While I think this work is an important advance, I am unhappy to see it described as *optimal*. Indeed I think that such a description is meaningless in the absence of any specification of the criteria (e.g. minimising a specified objective function) against which is being optimised. (The title of the paper merely says 'better'.)
- What is going on here, in at least some of the cases, is the use of the observations to estimate the tuple $(\mathbf{R}, \mathbf{B})$ and then to use the **same** data to estimate the state as if $(\mathbf{R}, \mathbf{B})$ is known exactly. I think that this is technically unsound, although numerically it might not be important. The issue should at least be noted, even if actual tests (e.g. by Monte Carlo) are left to a later study.
- I am having great difficulty analysing the procedure associated with relations (8)
  - a specific reference to equations in (Desroziers et al., 2005) would be helpful;
  - as an iterative procedure, this only seems to make sense if the subscripts on the left hand sides of lines 2 and 3 of relation (8) are $k+1$ rather than k.
  - Desroziers et al. (2005) state that they are solving a non-linear fixed point relation. It would be helpful of the authors could say what they are solving. My guess is
  $$\mathsf{E}[\left(\mathbf{y}^{\mathsf{o}} - \mathbf{H}\hat{\mathbf{x}}(\mathbf{y}^{\mathsf{o}}, \mathbf{R}, \mathbf{B})\right)\left(\mathbf{y}^{\mathsf{o}} - \mathbf{H}\mathbf{x}^{\mathsf{b}}\right)] = \mathbf{R}$$
  where $\hat{\mathbf{x}}(\mathbf{y}^{\mathsf{o}}, \mathbf{R}, \mathbf{B})$ indicates that $\hat{\mathbf{x}}$ (i.e. $\mathbf{x}^{\mathsf{a}}$) depends on $(\mathbf{y}^{\mathsf{o}}, \mathbf{R}, \mathbf{B})$ because of eqn (2).

  - Desroziers et al. (2005) appear to be estimating the expectation from a sum over the observational data set. It is not clear to me that the Monte Carlo technique used here is a valid way of evaluating the expectation for the purposes of solving the non-linear fixed point relation. It seems that the expectations are being calculated over random variables from two different realisations from (approximately) the same distribution: firstly a fixed sample of observations and secondly samples from a Monte Carlo simulation. Any terms in (7) that represent products of such random variables should have zero expectation if the variables come from different realisations, but will in general have non-zero expectation if the random variables come from the same realisation. The analysis given here needs to be justified by a term by term expansion that captures these distinctions. (I may be able to comment more later in the discussion period if the authors are able to confirm that they are trying to solve a fixed point relation (and clarify relation (8)).

Queries

- **P 3745, L 1** Should 'maximizing' really be 'minimizing'?
- **P 3745, L 2** Should $J^{\mathsf{a}}(\mathbf{x}^{\mathsf{a}})$ really be $J^{\mathsf{b}}(\mathbf{x}^{\mathsf{a}})$?
- **P 3749, eqn 4**, The subscript n on the identity matrix should not be bold font.

Wording

- **P 3739 L 28**, to inverse → to invert
- **P 3741, L 2**, life time → lifetime
- **P 3746, L 13**, converges to Eq (4) → converges to a tuple that satisfies Eq (4)

- **P 3748, L 16**, hence the ML algorithm → hence the constrained ML algorithm
- **P 3749, L 5**, $\mathbf{d}_\mathrm{b}^\mathrm{o}$ is an innovation vector, but in this context, $\mathbf{d}_\mathrm{a}^\mathrm{o}$
- **P 3749, L 12, 20**, criterium → criterion
  (criterium refers to bicycle races). Also p3750, L14.
- **P 3750, L 10**, constraints → constrains

Other

Finally there are a small number of places where minor changes might better reflect English idiom. Some *suggestions* are:

- **P 3737, L 18**, to close → for closing
- **P 3739, L 7**, takes benefit of → exploits
- **P 3739, L 15-16**, punctual → point
- **P 3741, L 6**, In all the study → Throughout the study
- **P 3745, L 14**, follows → satisfies
- **P 3750, L 1**, with → based on
- **P 3763, L 14**, influent → influentual
- **P 3764, L 22**, implementation → inclusion
- **P 3755, L 4**, should be subdued → is unlikely to apply
- **P 3762, L 17**, Totalizing → Summing

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File berchet4acp.tex, tested by inclusion in file shell.tex.

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