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Atmospheric Chemistry and Physics Discussions

Interactive comment on "An evolution strategy to estimate emission source distributions on a regional scale from atmospheric observations" *by* P. O'Brien et al.

Anonymous Referee #1

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General

The authors present an iterative algorithm ("evolution strategy", (ES)) for solving a least-square minimisation problem and the application of this algorithm on the inverse problem of inferring source distributions from atmospheric observations.

Using three different artificial emission distributions, synthetic observations are created (by running the atmospheric model in forward mode). The algorithm is tested regarding its ability to reconstruct these emission distributions again from the synthetic observations. The results are compared with those obtained by using the singular value decomposition (SVD) method. The main conclusion of the paper is that the proposed ES algorithm is superior to the SVD method.

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The SVD method is widely used for least square minimisation of linear problems and it would be certainly an interesting finding to demonstrate that iterative algorithms like the proposed ES may yield better results. However, I am worried whether the comparison presented is really appropriate. Unfortunately the exact mathematical conditions of the inverse problem are not very well described which render a definite judgment difficult. **A central problem in the application of the SVD algorithm, however, may be the choice of W_{min}=1.0 x 10^{-4} W_{max}, as listed in Table 2.** The W_{min} parameter sets the threshold for the singular values w_i (derived from the SVD) considered in the least square minimisation, i.e. for all $w_i < W_{min}$: $1/w_i = 0$. While I cannot, of course, completely reconstruct the calculations presented in this manuscript, I run a few SVD exercises for simple matrix inversion, which directly show, that matrix inversion results dramatically deteriorate, if the ratio W_{max} / W_{min} is smaller than the condition number of the problem (which is the ratio between the largest and the smallest singular value w_i.). While limiting W_{max} / W_{min} is useful in order to minimize artefacts from e.g. limited numerical precision and measurement noise (though the latter is not considered in the paper), a too small W_{max} / W_{min} ratio will throw away significant information of the analysed system.

In order to provide a convincing proof of the main statement of the paper that the ES is superior to the SVD method it would be required to present a detailed mathematical analysis of the investigated inverse problem along with some tests of the SVD method:

1. what are the exact dimensions of the problem (number of parameters n_{para}, and number of observation n_{obs}) ?

2. discuss whether the problem is over- or underdetermined (I assume $n_{para} < n_{obs}$, however the problem may become ill-conditioned, if the data do not clearly distinguish between the base functions)

3. show the spectra of the singular values (i.e. w_i vs. i with $w_i >= w_{i+1}$)

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4. show the dependence of SVD results on choice of W_{max} / W_{min}

5. which machine precision is used (for SVD a reasonable choice of W_{max} / W_{min} may depend on the machine precision) ?

6. compare the achieved values of the cost function for SVD and ES

It would be helpful to discuss points 1-3 and 6 for all test cases presented (i.e. different model resolutions, and the three different emission maps). The paper should be considered for ACP only if the main concern about the paper (i.e. that the conclusion is mainly based on an inappropriate application of the SVD) can be invalidated.

A further general comment is that the presentation and discussion should be thoroughly revised. In its present form the manuscript contains many very vague and imprecise statements (some of which are listed in the specific comments below).

Also it is not clear from the presentation in the manuscript, to which extent the proposed ES algorithm is based on existing work and which are the novel own developments.

Further specific comments

page 1334 line 23-24: "important trace gases and other species": what is meant by "other species" ?

page 1335, line 26-27: "A popular meteorological tool to investigate emission is the transport model" should be reworded. Also, the most widely used models are probably Eulerian 3D atmospheric (chemistry) transport models, which should also be explicitly mentioned.

page 1336, line 3-4: "the model may be scaled" change to e.g. "the model parameters may be scaled".

page 1336, line 25: "a consequence of these simplifying assumptions is that the solution of real-world problems cannot be attempted " Although the authors admit that

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their model is strongly simplified a brief discussion of the general limitations of back-trajectory models should be given (such as neglecting vertical transport, the difficulties to define the baseline (see e.g. [Ryall et al., 2001]), and the assumption that the mixing ratio at the origin of the back trajectory equals the baseline)

page 1337 line 15: "independence on the timescale of the trajectory set" I assume independence of emission is meant ?

page 1337 line 17 (eq 2): what are the units of n_i and e_i ?

page 1337 line 20: "The weighting factor can be made as detailed as one feels necessary" This is probably more a question of availability of appropriate algorithms and parameterizations.

page 1338 line 6 "artificially intelligent global optimisation technique". Which characteristics of this algorithm are exactly meant by the classification of the algorithm to artificial intelligence. What is meant by "global" in this context ?

It should be mentioned that also a large number of other iterative minimisation routines exist (e.g. conjugate gradient methods).

page 1338 line 18-20: "The ES is closely related to the Genetic Algorithm ... and the distinction between these approaches is often blurred." What are the distinctions ?

page 1339 line 15ff: "In general for inverse modelling it is necessary to supply a priori information about the source activity..."

In fact it is true, that in most inverse modelling studies the original numbers of parameters (i.e. emissions from individual grid cells) to be determined is larger that the number of observations (equations) and that it is therefore necessary to include additional a priori information on the emissions (e.g. prescribing the spatio-temporal emission patterns). In the paper it is argued that the ES method allows omitting such additional a priori information. It is, however, not a question of the algorithm for solving a given least-square problem (e.g. ES vs. SVD), but a question of how the inverse problem is formulated. In the present study a central assumption is that the emissions of the individual grids cell are constant. Using then a long time series of back trajectories (with each back trajectory giving one row in eq. (2)) allows to increase the number of equations over the number of parameters.

page 1339 line 16-17 "..and perhaps more importantly the uncertainty of the emission strength..." should be further explained (or references given for this statement).

page 1342 line 1-2 "It is a matter of personal judgment what proportion of the population is discarded per generation" I would consider this proportion mainly as parameter for the ES algorithm with the optimal choice of this parameter to be derived from tests.

page 1342 line 10 "...but that solution may be of lower cost" I assume lower value of cost function ?

page 1342 line 23 ff "grid size of 200 x 200 km^2" Is the model surface a plane of a sphere ? Even for a limited domain model a plane does not seem to be appropriate given the large latitudinal coverage of the model.

page 1347 line 6 "For the operation of the ES no a priori emission data was assumed" I assume that also for the SVD no a priori data are included ?

page 1347 line 10-11 "tendency to locate false emissions at the extremes of the trajectories" This is inherently a problem of the back trajectory model and has nothing to do with the ES or SVD method.

Interactive comment on Atmos. Chem. Phys. Discuss., 3, 1333, 2003.

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