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Atmospheric Measurement Techniques Discussions

Interactive comment on "A novel gridding algorithm to create regional trace gas maps from satellite observations" *by* G. Kuhlmann et al.

G. Kuhlmann et al.

yunflam@cityu.edu.hk

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We thank the reviewer for the careful review of our manuscript and the valuable comments, suggestions and commentary. We replied to the comments below. The updated manuscript has been attached as supplement. The changes are highlighted in red for changes based on reviewer #1, in green for changes based on reviewer #2 and blue for changes based on comments from both reviewers.

Main comments

1. Section 2.4.1 is a little bit confusing. I would suggest to clarify the following aspect:

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"The undetermined equation Cx=0 reflects the continuity condition for the first derivative. This equation can be used as a constraint (see Section 2.4.2), or, if the mean values d(i) are known, it can be used to compute the n+1 coefficients p(i)"

Reply: The sentence has been included into Sec. 2.4.1:

> ... with $\alpha_i = 1/h_i$. Equation (16) can be used as a constraint (see Section 2.4.2), or, if the mean values d_i are known, it can be used to compute the $n + 1$ coefficients p_i.In the latter case, matrix $\mathbf{C}$ can be simplified to a tridiagonal matrix.

2. In Section 2.4.3, the method for solving the quadratic programming problem (30) is not the best choice if the problem is severely ill-posed. The discrete ill-posedness come from the large condition number of the matrix M, and so, when computing H, we have cond(MˆT*M) = cond(M)**2. In general, it is recommended to avoid the computation of MˆT*M. This can be done by using the null-space approach: a. Let Z be a matrix whose column vectors form a basis for the null space of C. Then, the solution x is a linear combination of the column vectors of Z, that is, x = Zy. The constrained minimization problem reduces to an unconstrained minimization problem of lower dimension, with the solution ZˆT*H*Z*y = -ZˆT*g Since, ZˆT*H*Z = 2*ZˆT * [MˆT * Sˆ(-1) * M + gamma * LˆT * Bˆ(-1) * L] * Z, the generalized singular value of the matrix pair (Sˆ(-1/2) * M * Z, Bˆ(-1/2) * L * Z) can be used to compute a stable solution of the above equation. b. The matrix Z can be computed by a QR factorization of CˆT, or by using the variable reduction technique. My feeling is that the problem is not too ill-posed, and so, the brute force method (similar to the range-space method) do a a good job.

Reply: We agree that more sophisticated techniques are available to solve the quadratic programming problem. However, our study of the problem shows that the

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ill-posedness is not the result of a large condition number, but caused by measurement noise. The computed splines still fulfil Eq. (22), but due to the strong oscillation of the coefficients, the solutions are not useful. The first paragraph of Sec. 2.4.3 has been modified to clarify this:

> The inverse problem is ill-posed, i.e. very sensitive to measurement noise, if the FWHM of the instrument function is about twice the length of the pixel size.

Therefore, the use of e.g. the null-space approach is not necessary in current algorithm. The detailed cause of the ill-posedness has not been analysed yet. We add the following paragraph to the conclusion (Sect. 5):

> The reason for the sensitivity of the inverse problem to measurement noise has not been analysed in detail in this paper. Our analysis suggests that the inverse problem becomes undetermined, because the measurement noise and the wide instrument function reduce the "effective" rank of the problem. In addition, the parametrisation of the distribution by parabolic splines may favour the oscillation of the mean values, because the spline is created by combining parabolas with continuous first derivatives. In this study, we used parabolic splines, because they are the simplest parametrisation. A different parametrisation, for example higher-order polynomials, could make the inversion more stable.

3. In Section 2.4.4, I would suggest to summarize the method using a mathematical language. For example: - Step 1: For each i=0,..., n-1, solve Eq.(32), for x=[...], y=[...], and S(k,k) = ... - Step 2: For each j=0,...,m-1, solve Eq.(16), for x=[...], where the entries ... of x are known. - Step 3: Solve Eq.(16), for x=[...], where the entries ... of x are known.

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Reply: Section 2.4.4 has been rewritten to include this suggestion (see supplement to this comment).

4. The regularization parameter gamma is chosen by using an a priori parameter choice method. The method is based on synthetic data, and in contrast to a posteriori parameter choice methods or to error-free parameter choice methods, the method may fail for real data. As I know, this selection criterion should be organized as follows:
- for each realization of the data vector, compute the regularization parameter as the minimizer of solution error, and then
- average the regularization parameter over configurations.
It is not clear for me if the authors used this technique. However, it seems that the method works very good in practice.

Reply: Different methods to determine the regularisation parameter are possible. In this study, the parameter is chosen empirically using synthetic data from, for instance, a chemistry transport model. We think our approach is justified, because the model creates very realistic synthetic data.

Minor comments

1. From Eq.(18), I cannot understand the structure of the matrix C.
Reply: The structure of matrix $\mathbf{C}$ can be seen in Fig. 1 of this comment.

2. In Eq. (19), replace the index n by the index m.
Reply: Done

Please also note the supplement to this comment:

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http://www.atmos-meas-tech-discuss.net/6/C3396/2013/amtd-6-C3396-2013-supplement.pdf

Interactive comment on Atmos. Meas. Tech. Discuss., 6, 7867, 2013.

$$\mathbf{C} = \begin{bmatrix} 2\alpha_0 & -3\alpha_0 & \alpha_0 & & & & & & \\ \alpha_0 & -3\alpha_0 & 2(\alpha_0+\alpha_1) & -3\alpha_1 & \alpha_1 & & & & \\ & & \alpha_1 & -3\alpha_1 & 2(\alpha_1+\alpha_2) & -3\alpha_2 & \alpha_2 & & \\ & & & & & \cdots & & & \\ & & & & \alpha_{n-2} & -3\alpha_{n-2} & 2(\alpha_{n-2}+\alpha_{n-1}) & -3\alpha_{n-1} & \alpha_{n-1} \\ & & & & & & \alpha_{n-1} & -3\alpha_{n-1} & 2\alpha_{n-1} \end{bmatrix}$$

Fig. 1.

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