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

Anonymous Referee #2

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The paper presents a new gridding algorithm to improve the accuracy and spatial resolution of trace gas maps obtained from satellite measurements. The algorithm is based on the parabolic spline method. The proposed method is very interesting and it seems to work very efficiently. Some minor comments are listed below.

1. Section 2.4.1 is a little bit confusing. I would suggest to clarify the following aspect: "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 $p(i)$"

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.

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.

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.

And now, some very minor observations: 1. From Eq.(18), I cannot understand the structure of the matrix C.

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

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