Interactive comment on “Technical Note: Spectral representation of spatial correlations in variational assimilation with grid point models and application to the Belgian assimilation system for chemical observations (BASCOE)” by Q. Errera and R. Ménard

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Review of Technical Note: Spectral Representation of spatial Correlations in Variational Assimilation with Grid Point Models and Application to the Belgian Assimilation System for Chemical ObsErvations (BASOE)

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General comments

This paper is essentially a review of the spectral method as used to model efficiently horizontal correlations of background errors data assimilation. It applies the method to a tracer problem (with real data) of stratospheric ozone data assimilation. The spectral method to model homogeneous and isotropic background error correlations is well established in data assimilation, but this paper is a reasonably comprehensive collection of useful references for the practitioner of data assimilation. It is accessible to mathematicians and non-mathematicians alike. While most of the contents of this paper are not new, I think that it will be a very useful and well-cited source.
Specific comments

This is a list of issues that the authors might like to think about or do. I do not suggest that all need to be done to make the paper publishable.

In the assimilation experiments with the single observation, is the observation always exactly on a grid point in both the LL and GG cases? It would also be interesting to see how the results change as the observation location is increased in latitude to see how the interpolation errors introduced by the G-operator change.

The paper states (P. 16782, line 372) that the reason for the difference in the fitted correlation lengthscales to the true lengthscale is not known. Would any light be shed on this problem by repeating the experiment with different grid resolutions? If the resolution is difficult to control in this system, then a similar experiment could be performed by changing the correlation lengthscale instead, where the \( L_n \) (grid length) would be the important quantity.

The discussion of fig 2 (P. 16782, line 26 - P. 16783, line 8), there appears to be an underlying assumption that the higher the value of the power, the better, as more information is being provided by the observations. I would say that there is an optimal size of the power spectrum - over and under this value would represent a suboptimal-ity of the assimilation. I would suggest (either for this paper or for future work) that the authors attempt some analytic work (or at least some numerical work on a very high resolution grid which introduces negligible finite-size errors) to derive an optimal spectrum.

The authors may wish to interpret the improved impact of the CORREL results over the DIAG results in figs 3-6 in the following way. The structure functions in CORREL are broader than in DIAG, but (presumably) have the same amplitude as the delta-function-shaped structure functions in DIAG. (What I mean by structure functions is the following: structure functions are like correlation functions, but relate to covariance instead or correlation.) This means that each observation in CORREL is responsible for giving rise to larger total analysis increments when integrated over a region. When observations are biased with respect to the background (as is hinted to here for MIPAS, P. 16785, line 14), this means that the effect of neighbouring observations don’t act to ‘cancel each other out’ over a region, and so the effect is enhanced. It would be interesting to see how the results compare when the MIPAS observations are bias corrected. Also would an increased \( \Sigma \) in Eq. (36) have the same effect? An experiment comparing DIAG (with an increased \( \Sigma \)) with CALLIB (with the normal \( \Sigma \)) would be interesting to see. The increased \( \Sigma \) value would be chosen such that the area under each structure function is the same for CALLIB and DIAG.

The first part of appendix A4 is very useful, but I think that it could be improved. It attempts to show that if error covariances on the sphere are homogeneous and isotropic then the error covariance between the spectral modes is diagonal. In going from (A18) to (A19) a result is used from an earlier part of the paper Eq. (21) which is valid when one of the points (to compute covariance with) is at the pole. As it stands this is therefore not a proof of homogeneity; unless it can be shown that (21) is valid for any two points. An easier way may be to show that homogeneity and isotropy follow from the imposition of a diagonal covariance matrix in spectral space. This may be done as follows. Equation (A.17) is the structure function between points \( \Omega \) and \( \Omega' \) (thinking of \( \Omega' \) as fixed and the structure function being a function of \( \Omega \)):

\[
\langle \epsilon(\Omega) | \epsilon(\Omega') \rangle^* = \sum_{n=0}^{N} \sum_{m=-n}^{n} \sum_{n'=0}^{N} \sum_{m'=-n'}^{n'} \langle \delta_n \delta_{n'} m m' \rangle Y_{n}^{m}(\Omega) [ Y_{n'}^{m'}(\Omega') ]^*.
\]

When the covariance matrix in spectral space is diagonal, then (A.21) holds giving:

\[
\langle \epsilon(\Omega) | \epsilon(\Omega') \rangle^* = \sum_{n=0}^{N} \sum_{m=-n}^{n} \sum_{n'=0}^{N} \sum_{m'=-n'}^{n'} h_{nm} \delta_{n} \delta_{n'} m m' Y_{n}^{m}(\Omega) [ Y_{n'}^{m'}(\Omega') ]^*.
\]
= \sum_{n=0}^{N} \sum_{m=-n}^{n} b_n Y_n^m(\Omega)\overline{Y_n^m(\Omega')}^*.

The addition theorem (A.15) then results in:

\langle \epsilon(\Omega)\epsilon(\Omega')^* \rangle = \sum_{n=0}^{N} b_n (N_n^d)^2 P_n(\cos \theta),

where $\theta$ is the angular separation between $\Omega$ and $\Omega$. This is a general result and does not rely on (21).

In table 1, the expected value of $J$ is quoted as 1. I think that the value should be 1/2 for a single observation (half of the number of observations). This is a statistical expectation and not a precise result expected every time. This is a chi-squared statistic and so a little needs to be done to assess which of the results (i.e. LL or GG) is best (or if they are distinguishable). The reason for the empirical values close to 1, rather than 1/2, may be an omission of the 1/2 in the definition of the cost function that has been coded-up.

Technical corrections

I have found a number of minor points with the paper, but each is very easy to correct.

1. P. 16764, line 9: "interpolating on" change to "interpolating to".

2. P. 16764, line 22: The paper says that two approaches have been developed to represent spatial correlations in variational data assimilation (spectral and diffusion operators). A third approach is also known, namely recursive filters (see e.g. Purser et al., 2003, MWR 131, 1524-1535).

3. P. 16765, line 9: "done" change to "made".

4. P. 16766, line 9: The paper states that the inverse transform is not needed in variational data assimilation. This is true if a calibration step is not completed (see point x below) and if the ‘guess’ (or reference) state is the same as the background state. The calibration step requires a population of forecast errors to be known in spectral space (from model space) so the vertical covariance matrices and spectral coefficients of the horizontal spectra can be determined. If the ‘guess’ state, $x_g$ is not the same as the background then the difference between $x_b$ and $x_g$ needs to be put in control variable space (call this $\chi_b$), where the right hand side of (31) becomes $(\chi - \chi_b)^T(\chi - \chi_b)$. The inverse transform is need to do this.

5. After Eq. (1): Please define how $\mu$ is related to latitude.

6. In connection with Eqs. (8) and (10): In practice, a fast Fourier transform will be done instead of literal evaluations of the summations shown. This warrants a mention in the paper.

7. P. 16769, line 8: Here and at many other points in the paper the "spectral grid" referred to seems to be a lat/long space that is used immediately before/after performing the spectral transform. This is not in spectral space and so I am puzzled why it is called a spectral grid. In my mind the spectral grid is the set of $n$ and $m$ values, but then I might not know what the convention is for this.

8. Before Eq. (11): I think that it would aid some readers if the Gaussian quadrature formula is given in general form (ie for an arbitrary integrand), which will lead to the derivation of (11).

9. P. 16770, line 19: Replace "allows" with "allows one" or "allows us".
10. P. 16771, line 6: Here it states that "Since $\psi(\lambda, \mu)$ is real we have $S^* = S^T$. Although $\psi(\lambda, \mu)$ is real, this does not mean that $S$ is a real-valued operator. Indeed (8) shows that this operator is complex.

11. Eqs. (16) and (17): These are adjoint equations and so they no longer relate to $\psi$ fields. The notation that I am familiar with is to add hats, ie $\hat{\psi}$, to show that they are 'adjoint variables' (i.e. derivatives with respect to $\psi$, i.e. $\hat{\psi} = \partial J/\partial \psi$).

12. P. 16772, line 22: Replace "allows" with "allows one" or "allows us".

13. Eq. (19), and all equations that use expectation. The second item should be subject to a * operator to indicate transpose and complex conjugate. This is not necessary when the second element is real (as in (19)), but is a good habit to get into. It is necessary in, eq. (22) and many of the equations in appendix A.

14. Eq. (30): This should read $B = LL^T$ (or more strictly $B = LL^*$).

15. Eq. (35): The derivative of $H$ should be with respect to $x$ and not to $\chi$.

16. P. 16777, line 10: If not converged, the algorithm should go back to step 2, not step 3.

17. P. 16778, line 13: Replace "allows" with "allows one" or "allows us".

18. Eq. (39) and comment that follows it: $\Lambda$ is a symmetric matrix, but $\Lambda^{1/2}$ need not be. Such matrices have an infinite number of valid square-roots. Some of them are symmetric, in which case $\Lambda^{1/2} = \Lambda^{1/2*}$. Unless the authors are restricting the square-root to a symmetric case then (39) holds, otherwise a * should be added to $\Lambda^{1/2}$.

19. P. 16779, line 11: Replace "allow" with "allow one" or "allow us".

20. P. 16779, line 16: Replace "never" with "not yet".

21. P. 16779, line 25: Replace "matrix" with "matrices".

22. P. 16782, lines 10-11: Since the lines on fig 1 are so close to each other, why not plot differences?

23. P. 16786, line 7: Replace "in" with "of".

24. P. 16787, lines 2-3 (two occurrences): Replace "allow" with "allow one" or "allow us".

25. P. 16787, line 8: Replace "in" with "of".

26. P. 16787, line 9: Replace "method" with "methods".

27. P. 16788, line 8: Replace "value" with "values".

28. P. 16789, line 11: Replace "introduced" with "introduce".

29. Eq. (A14): I think that the $\mu$ and $\mu'$ in this equation should be $\phi$ and $\phi'$ respectively.

30. Eq. (A20): The $m$ summation index should be $m$.

I hope that these comments are useful to the authors. R.N.Bannister.