Modelling Flow-Dependent Covariances with Gaussian Integrals

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1 Introduction

Introducing flow-dependency in NWP analyses is necessary in order to better represent the actual state of the atmosphere in the initial conditions for a weather forecast. Currently, widely used methods to achieve this goal are DA by ensembles and variational algorithms like 4D-VAR. Here a new method is presented that has the appealing properties of being easy to implement and well suited for applications demanding a very high update frequency (e.g. Very Short Range NWP or NWP-NWC).

2 The Analysis Increments as a Gaussian Random Field on a Grid

The analysis increments Δ on an N-grid can be considered a Gaussian Random Field with a source term S. This statement follows immediately from a reorganization of the terms in the 3D-VAR cost function

$$2J_{3DVAR}(\Delta, y) = \Delta^T B^{-1}\Delta + (y-\Delta)^T R^{-1}(y-\Delta) = \Delta^T G^{-1}\Delta - 2\Delta^T S + y^T R^{-1} y \Rightarrow$$
$$\Rightarrow \quad 2J_S(\Delta) = \Delta^T G^{-1}\Delta - 2\Delta^T S \qquad (1)$$

with

$$G^{-1} \equiv B^{-1} + R^{-1} \quad ; \qquad S \equiv R^{-1} y = R^{-1}(ob - fg)$$

where the last term quadratic in the observation increments "(ob-fg)" in (1) has been disregarded. This amounts to consider the observation increments set as a non-random field. The source field S is just given by these increments after being duly normalized. The analysis problem becomes that of finding the Δ that maximizes the probability conditioned on a given set of observation increments :

$$P(\Delta, y) \propto \quad e^{-J_{3DVAR}} = \quad e^{-\frac{1}{2}\Delta^T G^{-1}\Delta + \Delta^T S} \; e^{-\frac{1}{2}y^T R^{-1} y} \equiv e^{-J_S(\Delta)} \; e^{-\frac{1}{2}y^T R^{-1} y} \propto P(\Delta|y)P(y)$$

and P(y) can be absorbed in the normalization, which is the so-called generating function N(S)

$$P(\Delta|y) \equiv P_S(\Delta) = \frac{e^{-J_S(\Delta)}}{N(S)} \quad ; \quad N(S) = \int d\Delta_1 \dots d\Delta_N e^{-J_S(\Delta)} = \sqrt{(2\pi)^N \|G\|} \quad e^{\frac{1}{2}S^T G S}$$

2.1 3D-VAR Results Recovered from this Formalism

The analysis is obtained by expectation of Δ as given by $P_S(\Delta)$

$$\langle \Delta_i \rangle_S = \frac{1}{N(S)} \int d\Delta_1 ... d\Delta_N \; \Delta_i \; e^{-J_S(\Delta)} = \frac{1}{N(S)} \frac{\partial}{\partial S_i} N(S) = \frac{1}{2}\left[G_{ij} S_j + S_j G_{ji} \right] = G_{ij} S_j = \langle \Delta_i \Delta_j \rangle_{S=0} S_j \quad (2)$$

where the last equality follows from the well-known property of Gaussian Integrals for G symmetric and positive definite

$$G_{ij} = \frac{1}{N(S=0)} \int d\Delta_1 \ldots d\Delta_N \; \Delta_i \Delta_j \; e^{-\frac{1}{2}\Delta^T G^{-1} \Delta} = \frac{1}{N(S=0)} \int d\Delta_1 \ldots d\Delta_N \; \Delta_i \Delta_j \; e^{-J_{S=0}(\Delta)}$$

In a similar way , one can see that the analysis error at grid point "i" is

$$\langle \Delta_i^2 \rangle_S - \langle \Delta_i \rangle_S^2 \quad = \quad \langle \Delta_i^2 \rangle_{S=0} = \quad G_{ii}$$

These results are not surprising as soon as we notice that $G^{-1} = (B^{-1} + R^{-1})$ is indeed the Hessian of the 3D-VAR problem, that is, the inverse of the 3D-VAR analysis covariance error matrix, frequently denoted by A^{-1}. The connection between the 3D-VAR algorithm and this Gaussian Integral (GI) formalism is explored further in section 4 after we next introduce a computation scheme by expansion in power series.

2.2 The Error Covariance G as Green Function. Analogy with QFT Propagators.

It is possible to make a close analogy between the calculation of the 3D-VAR solution just outline above, and common methods employed in the theory of random fields (QFT Quantum Field Theory) for the calculation of probability amplitudes for different fundamental physical processes (scattering cross sections, etc…). This analogy arises from thinking of the covariance matrix G as a kind of Green Function or, in QFT terminology, as a kind of propagator. This correspondence is just the reverse of that presented in **[1]**,**[2]**, where the similitudes between the Green Function for a variational constrained problem and covariance matrices were emphasized.

One immediate application of this idea is to consider the possibility of introducing external fields in the formalism, as is done in QFT when, for instance, one wants to take into account the effect of an ambient electromagnetic field in the correction to the energy levels of an atom. In the case of interest here, we may introduce a **V** vector field that converts the correlation function (or "2-point function" in QFT parlance) in a functional of this **V** field

$$\langle \Delta_i \Delta_j \rangle_{S=0} \left[\vec{V} \right] \quad \propto \quad \int d\Delta_1 \ldots d\Delta_N \; \Delta_i \Delta_j \; \exp\left(-\frac{1}{2} \Delta^T G^{-1} \Delta - \frac{\mu}{2} tr\left(\left[\vec{V} \cdot \vec{\nabla} \Delta \right] \left[\vec{V} \cdot \vec{\nabla} \Delta \right]^T \right) \right) \quad ; \quad \dim(\mu) = \left[\frac{error}{time} \right]^{-2} \quad (3)$$

one can say that the "free propagation" or "kinetic energy" of the error field (½ $\Delta^T G^{-1} \Delta$) is corrected by an "interaction with a background **V** field" with coupling factor μ.

3 Implementation of a Computation Algorithm and First Tests

The calculation proposed in (3) can be approximated by a power series in μ. With $\mathbf{V_p=(u_p,v_p,w_p)}$

$$\left\langle \Delta_i \Delta_j \right\rangle_{S=0}\left[\vec{V}\right] \approx \int d\Delta_1 \cdots d\Delta_N \exp\left(-\frac{1}{2}\Delta^T G^{-1}\Delta\right)\Delta_i\Delta_j\left[1-\frac{\mu}{2}\sum_{p\in(1,\dots,N)}\left(\vec{V}\cdot\vec{\nabla}\Delta\right)_p^2+O(\mu^2)\right] = \left\langle \Delta_i \Delta_j \right\rangle_{S=0} - \frac{\mu}{2}\sum_{p\in(1\dots N)} u_p^2 \left\langle \Delta_i \Delta_j \left(\partial_x \Delta\right)_p^2 \right\rangle_{S=0} + \dots$$

and the derivatives of analysis increments are approximated with finite differences on the grid. The result is that the correction to first order in μ is given by a sum over all the grid points of four-moment values, with this sum modulated by the **V** field:

$$\sum_{p\in(1\dots N)}\left(\frac{u_p}{\Delta x}\right)^2\left\langle \Delta_i\Delta_j\left(\Delta_{p(x)+1}-\Delta_{p(x)-1}\right)^2\right\rangle_{S=0} + \dots = \sum_{p\in(1\dots N)}\left(\frac{u_p}{\Delta x}\right)^2\left(\left\langle \Delta_i\Delta_j\Delta_{p(x)+1}^2\right\rangle_{S=0}+\left\langle \Delta_i\Delta_j\Delta_{p(x)-1}^2\right\rangle_{S=0}-2\left\langle \Delta_i\Delta_j\Delta_{p(x)+1}\Delta_{p(x)-1}\right\rangle_{S=0}\right) + \dots$$

These four-moment are in turn given by the matrix elements of G, because by Wick's rule

$$\left\langle \Delta_a\Delta_b\Delta_c\Delta_d \right\rangle_{S=0} = G_{ab}G_{cd} + G_{ac}G_{bd} + G_{ad}G_{bd}$$

These calculations let themselves be nicely represented by diagrams (the famous Feyman's diagrams), but the number of terms becomes quickly very high. For instance, for a 3-D **V** field, to order μ we must sum over 21 four-moments, and to order μ^2 the sum is over 126 six-moments (10 and 35 respectively if we are satisfied with a 2-D **V** field). As each four-moment gives 3 products of pairs of G matrix elements and a six-moment gives 15 products of pairs, we have 63 of such products to order μ and 1890 to order μ^2, to be sum over all grid points. This vast amount of computations can be dramatically reduced by using the fact that G is sparse (covariances of analysis errors decay with grid point separation).

A first implementation has been utilized to evaluate the potential of this technique, both in terms of its impact on the analysis and also on its feasibility given a certain amount of computation power. The algorithm scales well with the number of observations: it is not necessary to compute these "2-point functions" for all pairs of grid points, is just enough to carry it out only for each observation.

Below these lines, the deformation of an isotropic correlation (contoured on the left bottom corner) due to a vortex is shown (fig 1). On figure 2 the modulation caused by a HARMONIE-AROME wind field at level 55 on an isotropic correlation with length scale characteristic for the specific humidity variable is shown. This test with a 2-D **V** field and to order μ gave a processing time of about 1 sec/observation.

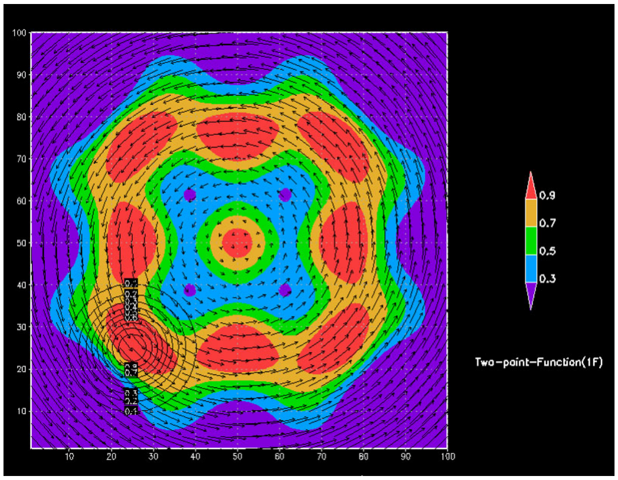

Figure 1: Correlations from 9 observations located in a vortex. Isotropic correlation for the one at the bottom-left is shown in contours, its length scale is 10 grid points.

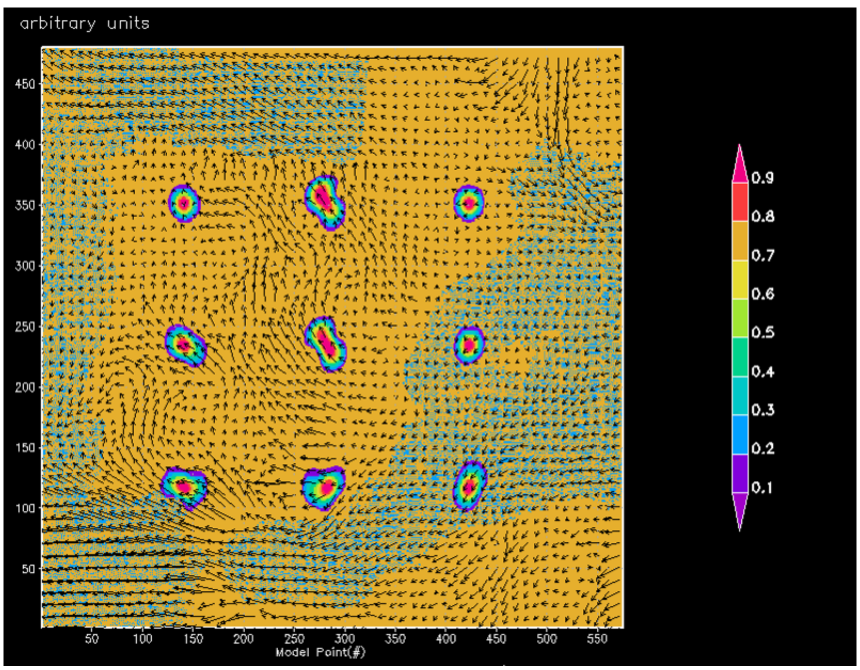

Figure 2: Horizontal correlation functions for 9 specific humidity (q) observations on an atmospheric level about 850hPa over the Iberian Peninsula, derived by coupling isotropic error correlations to the model wind field. The length scale of these isotropic correlations is determined from actual model errors.

4 Approximation to the 3D-VAR Solution with Gaussian Integrals

The 3D-VAR solution as given in (2) can be approximated by GI by decomposing the G propagator in a B propagator and a perturbation produced by the spatial distribution and correlations among the observations represented by R^{-1}. This perturbation is given in model space (R^{-1} is actually $H^T R^{-1} H$, but the simpler notation is retained for comfort). R may not exist, but this is not a problem as it is not required for the calculations that follow. Indeed, R^{-1} will have, when represented on the grid, many zeros, which actually is an advantage to reduce the number of required computations !.

The generating function

$$N_G(S) = \sqrt{(2\pi)^N \|G\|}\ e^{\frac{1}{2}S^T GS} \qquad (4)$$

can be computed for small R^{-1} by expanding in powers of it

$$N_G(S) \approx \int d\Delta^N\ e^{-\frac{1}{2}\Delta^T B^{-1}\Delta + \Delta^T S}\left(1 - \frac{1}{2}\Delta^T R^{-1}\Delta + \frac{1}{8}\left(\Delta^T R^{-1}\Delta\right)^2 + O\left(R^{-3}\right)\right) = N_B^0(S)\left(1 + N_B^1(S) + N_B^2(S) + \ldots\right)$$

where the subscripts "G" and "B" have been introduced to distinguish the "free propagator" employed in each case. Here

$$N_B^0(S) = \sqrt{(2\pi)^N \|B\|}\quad e^{\frac{1}{2}S^T BS};\quad N_B^1(S) = -\frac{1}{2}\left(Tr\left(BR^{-1}\right) + S^T\left(BR^{-1}B\right)S\right)$$
$$N_B^2(S) = \frac{1}{8}\left(Tr\left(BR^{-1}\right) + S^T\left(BR^{-1}B\right)S\right)^2 + \frac{1}{2}\left(\frac{1}{2}Tr\left(BR^{-1}BR^{-1}\right) + S^T\left(BR^{-1}BR^{-1}B\right)S\right)$$

These results can also be obtained more directly from (4) by making use of the "Neumann series" for G (see footnote), valid for linear bounded operators. This is always the case for operators on finite dimensional space, although convergence is not guaranteed.

$$G = \left(1 + BR^{-1}\right)^{-1} B = B\left(1 + R^{-1}B\right)^{-1} \approx B - BR^{-1}B + BR^{-1}BR^{-1}B + \ldots \quad (5)$$

and the following relation between determinant and trace of a matrix

$$\ln\|M\| = Tr\left(\ln M\right) \quad ; \quad M = 1 + BR^{-1} \equiv 1 + \varepsilon \quad ; \quad \ln M = \varepsilon - \frac{\varepsilon^2}{2} + O\left(\varepsilon^3\right)$$

so that

$$N_G(S=0) \approx N_B^0(S=0)\left(1 - \frac{1}{2}Tr\varepsilon + \frac{1}{8}\left(Tr\varepsilon\right)^2 + \frac{1}{4}Tr\varepsilon^2 + O(\varepsilon^3)\right)$$

or up to the ε^2 order

$$N_G(S=0) \approx N_B^0(S=0)\ e^{-\frac{1}{2}(Tr\varepsilon - \frac{Tr\varepsilon^2}{2})}$$

Now, the quantity that we need to compute is, according to (2):

(footnote) Thank you to Roel Stappers for pointing out to me this formal solution for the 3D-VAR analysis

$$\left\langle \Delta_i \Delta_j \right\rangle_{G,S=0} \approx \frac{1}{N_G(S=0)} \int d\Delta^N \; \Delta_i \Delta_j \; e^{-\frac{1}{2}\Delta^T B^{-1}\Delta} \left(1 - \frac{\Delta^T R^{-1}\Delta}{2} + \frac{(\Delta^T R^{-1}\Delta)^2}{8} + \ldots \right) =$$

$$\frac{e^{\frac{1}{2}\left(Tr\varepsilon - \frac{tr\varepsilon^2}{2}\right)}}{N_B(S=0)} \int d\Delta^N \; \Delta_i \Delta_j \; e^{-\frac{1}{2}\Delta^T B^{-1}\Delta} \left(1 - \frac{\Delta^T R^{-1}\Delta}{2} + \frac{(\Delta^T R^{-1}\Delta)^2}{8} + \ldots \right) =$$

$$e^{\frac{1}{2}\left(Tr\varepsilon - \frac{tr\varepsilon^2}{2}\right)} \left(\left\langle \Delta_i \Delta_j \right\rangle_{B,S=0} - \frac{1}{2} \left\langle \Delta_i \Delta_j \Delta^T R^{-1}\Delta \right\rangle_{B,S=0} + \frac{1}{8} \left\langle \Delta_i \Delta_j (\Delta^T R^{-1}\Delta)^2 \right\rangle_{B,S=0} + \ldots \right) =$$

$$e^{\frac{1}{2}\left(Tr\varepsilon - \frac{tr\varepsilon^2}{2}\right)} \left(\begin{array}{l} B_{ij} \left(1 - \frac{1}{2} Tr\varepsilon + \frac{1}{8} \left(Tr\varepsilon\right)^2 + \frac{1}{4} Tr\varepsilon^2 + O(\varepsilon^3) \right) - (BR^{-1}B)_{ij} (1 - \frac{1}{2} Tr\varepsilon + O(\varepsilon^2)) + \\ (BR^{-1}BR^{-1}B)_{ij} (1 + O(\varepsilon)) + \ldots \end{array} \right) =$$

$$\left(B_{ij} \left(1 + O(\varepsilon^3) \right) - (BR^{-1}B)_{ij} (1 + O(\varepsilon^2)) + (BR^{-1}BR^{-1}B)_{ij} (1 + O(\varepsilon)) + \ldots \right)$$

which is the 3D-VAR solution as given by (5) to second order in R^{-1}

5 References

[1] C. Geijo and B. Escribá: "Variational Constraints for Data Assimilation in ALADIN-NH Dynamics". 11th ALADIN-HIRLAM Newsletter, Aug. 2018 . http://www.umr-cnrm.fr/aladin/IMG/pdf/nl11.pdf also available in: https://www.researchgate.net/publication/326479446_Variational_Constraints_for_Data_Assimilation_in_ALADIN-NH_Dynamics

[2] C. Geijo: "ANNEX to Variational Constraints for DA in ALADIN-NH dynamics", Aug 2018 https://www.researchgate.net/publication/327117950_ANNEX_to_Variational_Constraints_for_DA_in_ALADIN-NH_Dynamics