ERROR COVARIANCE PROPAGATION AND 4D-VAR

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1. INTRODUCTION

One of the challenges of data assimilation is to construct a realistic representation of the background error covariance matrix. This matrix is important to represent accurately as it characterizes the uncertainties of the background state, and the correlations within it. This has an impact on the weights assigned to the normal modes in the atmosphere, and to the way that information from the observations is spread-out in space in the resulting analysis.

In many forms of data assimilation such as 3d-Var., the background error covariance matrix is independent of time*. In 4d-Var., the background model state is propagated explicitly to the time of each observation so that the model's version of the observation can be computed. It is widely believed that the method similarly propagates the background error covariance matrix. Unlike the background state vector, the background error covariance matrix is though to evolve implicitly, so that we have to do some simple analysis to reveal this.

This propagation is done in a way that is consistent with the (linearized) dynamics of the model (as in the Kalman filter). If $\mathbf{B}$ is the background error covariance matrix, and the time integration model takes the background state from time $t = 0$ ($\boldsymbol{x}_B$) to a later time t ($\boldsymbol{x}_B(t)$),

$$\boldsymbol{x}_B(t) = \boldsymbol{M}_t \boldsymbol{M}_{t-\delta t} \ldots \boldsymbol{M}_{\delta t} \boldsymbol{x}_B, \tag{1.1}$$

(where δt is the timestep as in [1]), then the propagated background error covariance matrix is,

$$\mathbf{B}(t) = \mathbf{M}_t \mathbf{M}_{t-\delta t} \ldots \mathbf{M}_{\delta t} \, \mathbf{B} \, \mathbf{M}_{\delta t}^T \ldots \mathbf{M}_{t-\delta t}^T \mathbf{M}_t^T, \tag{1.2}$$

(see [2] for the justification of why covariance matrices are propagated like this). In Eq. (1.2), $\mathbf{M}_t$ is the linearization of $\boldsymbol{M}_t$ (as in Eq. (1.1)), and can, in principle, be written as a matrix.

It is easy to prove that this transformation on $\mathbf{B}$ is in an implicit part of 4d-Var. in the special case that all observations are made at a common time [3]. In the more general case of observations spread over many times, the relevance of this proof is uncertain, as outlined in these notes.

* In some implementations of 3d-Var., seasonal dependence of the background error covariance matrix has been imposed in a somewhat artificial manner.

2. RECAP OF THE COST FUNCTION AND ITS GRADIENT

The standard cost function for 4d-Var. can be written [1],

$$J[\boldsymbol{x}] = \frac{1}{2}(\boldsymbol{x}_B - \boldsymbol{x}(0))^T \mathbf{B}^{-1}(\boldsymbol{x}_B - \boldsymbol{x}(0)) + \frac{1}{2}\sum_{t=0}^{\Delta t}(\boldsymbol{y}(t) - \boldsymbol{H}_t^o[\boldsymbol{x}(t)])^T \mathbf{E}^{-1}(\boldsymbol{y}(t) - \boldsymbol{H}_t^o[\boldsymbol{x}(t)]), \quad (2.1)$$

where $\boldsymbol{x}$ is the state for which the cost function is evaluated (the particular $\boldsymbol{x}$ that gives the smallest J is referred to as the analysis), $\boldsymbol{y}(t)$ are the vectors of the observations made at time t, for which $\boldsymbol{H}_t^o[\boldsymbol{x}(t)]$ are the model equivalents, $\mathbf{E}$ is the observation error covariance matrix, and Δt is the duration of the 4d-Var. time window. Differentiating Eq. (2.1) with respect to the vector $\boldsymbol{x}$ gives [1],

$$\nabla_x J \approx -\mathbf{B}^{-1}(\boldsymbol{x}_B - \boldsymbol{x}(0)) - \sum_t (\mathbf{M}_t \mathbf{M}_{t-\delta t} \dots \mathbf{M}_{\delta t})^T \mathbf{H}_t^{oT} \mathbf{E}^{-1}(\boldsymbol{y}(t) - \boldsymbol{H}_t^o[\boldsymbol{x}(t)]), \quad (2.2)$$

where the observation Jacobian matrices $\mathbf{H}_t^o$, relevant to time t, are defined as,

$$\mathbf{H}_t^o = \frac{\mathrm{d}\boldsymbol{H}_t^o[\boldsymbol{x}(t)]}{\mathrm{d}\boldsymbol{x}(t)}. \quad (2.3)$$

3. THE ANALYSIS

The background error covariance matrix, and the observation and time evolution operators are too large to represent explicitly, or to invert. In variational analysis, the solution that minimizes the cost function, Eq. (2.1), is found by iteration so that small increments in $\boldsymbol{x}$ progressively move 'down hill' towards the analysis state. The procedure needed to achieve this requires only the ability to act with the operators (and their adjoints) with no need to invert any operators. This procedure is complicated and requires an extra preconditioning step. Often however when one wishes to assess the behaviour of the assimilation scheme's formulation, we can skip the variational part of the problem and write matrix inverses symbolically. This method jumps straight to the analysis, and will give the same solution as 4d-Var. in the case of all operators being linear.

Setting the gradient of the cost function, Eq. (2.2), to zero (for the minimum) yields,

$$\mathbf{B}^{-1}(\boldsymbol{x}(0) - \boldsymbol{x}_B) = \sum_t (\mathbf{M}_t \mathbf{M}_{t-\delta t} \dots \mathbf{M}_{\delta t})^T \mathbf{H}_t^{oT} \mathbf{E}^{-1}(\boldsymbol{y}(t) - \boldsymbol{H}_t^o[\boldsymbol{x}(t)]), \quad (3.1)$$

$$= \sum_t (\mathbf{M}_t \mathbf{M}_{t-\delta t} \dots \mathbf{M}_{\delta t})^T \mathbf{H}_t^{oT} \mathbf{E}^{-1}(\boldsymbol{y}(t) - \boldsymbol{H}_t^o[\boldsymbol{M}_t \boldsymbol{M}_{t-\delta t} \dots \boldsymbol{M}_{\delta t}\boldsymbol{x}(0)]). \quad (3.2)$$

We proceed by setting $\boldsymbol{x}(0) = \boldsymbol{x}_B + (\boldsymbol{x}(0) - \boldsymbol{x}_B)$ in Eq. (3.2), and assume that the time evolution and observation operators are linear (ie $\boldsymbol{M}_t \approx \mathbf{M}_t$ and $\boldsymbol{H}_t^o \approx \mathbf{H}_t^o$). The resulting equation, trivially rearranged is,

$$\left\{\mathbf{B}^{-1} + \sum_t (\mathbf{M}_t\mathbf{M}_{t-\delta t}\ldots\ \mathbf{M}_{\delta t})^T \mathbf{H}_t^{o^T}\mathbf{E}^{-1}\mathbf{H}_t^o\mathbf{M}_t\mathbf{M}_{t-\delta t}\ldots\ \mathbf{M}_{\delta t}\right\}(\boldsymbol{x}(0) - \boldsymbol{x}_B)$$

$$= \sum_t (\mathbf{M}_t\mathbf{M}_{t-\delta t}\ldots\ \mathbf{M}_{\delta t})^T \mathbf{H}_t^{o^T}\mathbf{E}^{-1}(\boldsymbol{y}(t) - \mathbf{H}_t^o\mathbf{M}_t\mathbf{M}_{t-\delta t}\ldots\ \mathbf{M}_{\delta t}\boldsymbol{x}_B) \qquad (3.3)$$

Acting on each side with **B**,

$$\left\{\mathbf{I} + \sum_t \mathbf{B}(\mathbf{M}_t\mathbf{M}_{t-\delta t}\ldots\ \mathbf{M}_{\delta t})^T \mathbf{H}_t^{o^T}\mathbf{E}^{-1}\mathbf{H}_t^o\mathbf{M}_t\mathbf{M}_{t-\delta t}\ldots\ \mathbf{M}_{\delta t}\right\}(\boldsymbol{x}(0) - \boldsymbol{x}_B)$$

$$= \sum_t \mathbf{B}(\mathbf{M}_t\mathbf{M}_{t-\delta t}\ldots\ \mathbf{M}_{\delta t})^T \mathbf{H}_t^{o^T}\mathbf{E}^{-1}(\boldsymbol{y}(t) - \mathbf{H}_t^o\mathbf{M}_t\mathbf{M}_{t-\delta t}\ldots\ \mathbf{M}_{\delta t}\boldsymbol{x}_B), \qquad (3.4)$$

and the analysis increment, $(\boldsymbol{x}(0) - \boldsymbol{x}_B)$, is found by acting on each side with the inverse operator, $\{\mathbf{I} + \Sigma_t\mathbf{B}(\mathbf{M}_t\mathbf{M}_{t-\delta t}\ldots\mathbf{M}_{\delta t})^T\mathbf{H}_t^{o^T}\mathbf{E}^{-1}\mathbf{H}_t^o\mathbf{M}_t\mathbf{M}_{t-\delta t}\ldots\mathbf{M}_{\delta t}\}^{-1}$. Equation (3.4) takes us only half way to proving that 4d-Var. implicitly propagates in time the error covariance matrix **B**.

Following [3], it is straightforward to show that this property of 4d-Var. is carried through in the case of observations present at only one time. Let the time that all observations made be t. Equation (3.4) then simplifies to,

$$\left\{\mathbf{I} + \mathbf{B}(\mathbf{M}_t\mathbf{M}_{t-\delta t}\ldots\ \mathbf{M}_{\delta t})^T \mathbf{H}_t^{o^T}\mathbf{E}^{-1}\mathbf{H}_t^o\mathbf{M}_t\mathbf{M}_{t-\delta t}\ldots\ \mathbf{M}_{\delta t}\right\}(\boldsymbol{x}(0) - \boldsymbol{x}_B)$$

$$= \mathbf{B}(\mathbf{M}_t\mathbf{M}_{t-\delta t}\ldots\ \mathbf{M}_{\delta t})^T \mathbf{H}_t^{o^T}\mathbf{E}^{-1}(\boldsymbol{y}(t) - \mathbf{H}_t^o\mathbf{M}_t\mathbf{M}_{t-\delta t}\ldots\ \mathbf{M}_{\delta t}\boldsymbol{x}_B). \qquad (3.5)$$

Operating now on each side with the operator $\mathbf{M}_t\mathbf{M}_{t-\delta t}\ldots\mathbf{M}_{\delta t}$, and compacting using Eq. (1.2) gives,

$$\left\{\mathbf{M}_t\mathbf{M}_{t-\delta t}\ldots\ \mathbf{M}_{\delta t} + \mathbf{B}(t)\mathbf{H}_t^{o^T}\mathbf{E}^{-1}\mathbf{H}_t^o\mathbf{M}_t\mathbf{M}_{t-\delta t}\ldots\ \mathbf{M}_{\delta t}\right\}(\boldsymbol{x}(0) - \boldsymbol{x}_B)$$

$$= \mathbf{B}(t)\mathbf{H}_t^{o^T}\mathbf{E}^{-1}(\boldsymbol{y}(t) - \mathbf{H}_t^o\mathbf{M}_t\mathbf{M}_{t-\delta t}\ldots\ \mathbf{M}_{\delta t}\boldsymbol{x}_B), \qquad (3.6)$$

which shows that all occurrences of **B** are replaced naturally with $\mathbf{B}(t)$, thus proving the point in this case. The difficulty for the case of observations present at more than one time is the summation over time, blocking the use of the step leading to Eq. (3.6). It is thus unproven here that the general 4d-Var. process propagates **B** in a manner consistent with the linearized dynamics.

REFERENCES

[1] Bannister R.N., Elementary 4d-Var. (DARC technical report No. 2), http://www.met.rdg.ac.uk/~ross/Documents/Var4d.html (2001).

[2] Bannister R.N., Linear algebra notes, http://www.met.rdg.ac.uk/~ross/Documents/

Basis.html (2000).

[3] Fisher M., Assimilation techniques: 4d-Var., *http://wms.ecmwf.int/newsevents/training/rcourse_notes/DATA_ASSIMILATION/ASSIM_TECHNIQUES_4dVAR/Assimilation_techniques_4dVar.html*