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Improved assimilation of trace gas retrievals from satellite

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Abstract : An interface between satellite retrievals and the incremental 4D Variational assimilation is developed, making full use of the information content of satellite measurements. We derive the expressions of the observation operator, together with its tangent linear version and its adjoint, for application in Numerical Weather Prediction models.

1. Introduction:

When satellite data are assimilated in the form of retrieved quantities (e.g., trace gas concentrations, for example ozone), the current assimilation methods do not give optimal results. The main difficulty related to the use of satellite retrievals is that an estimate of the profile of a given atmospheric constituent will necessarily result from the combination of observational and prior information. This means that when retrievals are assimilated, there is a risk of assimilating prior information rather than information from the measurements. Eq. (1) describes the dependency of a satellite retrieval $\mathbf{y}_{\mathbf{retrieved}}$ on the true state of the atmosphere $\mathbf{y}_{\mathbf{true}}$ and the a priori state $\mathbf{y}_{\mathbf{apriori}}$, with **A** being the averaging kernels and ε the error.

2. Quasi-optimal Assimilation:

To improve the variational assimilation of trace gas retrievals (e.g., ozone profiles) we propose to assimilate them by using the Quasi-Optimal Assimilation (QOA) approach [1]. Here satellite retrievals are transformed according to eq. (2) resulting in vertically independent observation errors which are uncorrelated with the errors in the forecast. The prior information is subtracted from the retrievals, and the resulting observation vector is then multiplied by the inverse of the square root of the observation error covariance **E** (assumed to be non-singular). We assimilate $\hat{\mathbf{y}}$, the estimates of measurements for ($\mathbf{A}\,\mathbf{y}_{\mathbf{true}}$) with error covariance equal to a unit matrix (i.e., errors on $\hat{\mathbf{y}}$ are uncorrelated). In this way, $\hat{\mathbf{y}}$ can be efficiently assimilated in ordinary data assimilation systems. A further improvement with the QOA approach is that the interpolation between the model and observation grids is optimized to minimize information loss [1] as the vertical interpolation $\mathbf{W}^*$ is defined from the model to the observation grid whereas **W** is the vertical interpolation from the observation grid to model grid. Note that for eq. (3) to be meaningful, **W** needs to be full rank. This is the case if the model grid is finer than the observation grid.

3. Incremental 4D-Var:

In incremental 4D-Var [2], the best model trajectory **x** for describing the atmosphere is found using the model background $\mathbf{x}_\mathbf{b}$ and the observations **y** by minimizing a cost function $J(x)$ expressed in terms of increments $\boldsymbol{\delta}\mathbf{x} = \mathbf{x} - \mathbf{x}_\mathbf{b}$, see eq (4). The cost function in discrete form sums over all time steps i where the innovation d_i= $\mathbf{y}_i - \mathcal{H}_i(\mathbf{x}_\mathbf{b})$ measures the difference between the observation and the model background value. For this, the model values are transformed into observation space by the observation operator $\mathcal{H}_i$. $\mathbf{R}_i$ is the associated error covariance matrix (in our case equal to the unit matrix) and $\mathbf{B}_i$ is the initial forecast error covariance matrix. The full (non-linear) operators are usually expensive to calculate. In incremental 4D-Var, computing is facilitated by applying the linearized observation operator **H** (see eq. (5)) to the model increment $\boldsymbol{\delta}\mathbf{x}$ which has been propagated by the linearized (and lower resolution) model **M** from the initial conditions to obtain the increment in observation space.

4. Quasi-optimal incremental 4D-Var:

For QOA compliant incremental 4D-Var, we have to develop the full observation operator $\mathcal{H}$ (given in eq. (6)) for the trace gas of interest, e.g., ozone $\mathbf{x}_\mathbf{oz}$. The tangent linear observation operator is the derivative of the full observation operator with respect to the model state vector (see eq. (8)). In our application we only need to consider derivatives with respect to ozone as well as pressure (because of the interpolation). The term dependent on pressure and its derivative are given in eqs. (3) and (7), respectively. Examples of the tangent linear operator, together with the full (non-linear) operator is shown in Fig. 1 and 2. The observation grids can be reduced to make **W** having full rank so that **H** exists [3]. The adjoint operator can be obtained simply by transposing the matrix constituting the tangent linear operator. We plan to implement the solution in the ECMWF's IFS for testing with real data.

References

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$$\mathbf{y}_{\mathbf{retrieved}} - \mathbf{y}_{\mathbf{apriori}} = \mathbf{A}(\mathbf{y}_{\mathbf{true}} - \mathbf{y}_{\mathbf{apriori}}) + \epsilon \quad (1)$$

$$\hat{\mathbf{y}} = \mathbf{E}^{-1/2}\left[\mathbf{y}_{\mathbf{retrieved}} - (\mathbf{I} - \mathbf{A})\mathbf{y}_{\mathbf{apriori}}\right] \quad (2)$$

$$\mathbf{W}^* = (\mathbf{W}^T\mathbf{W})^{-1}\mathbf{W}^T \quad (3)$$

$$J(x) = \frac{1}{2}\delta\mathbf{x}^T\mathbf{B}^{-1}\delta\mathbf{x} + \frac{1}{2}\sum_i(\mathbf{H}_i\mathbf{M}_i\delta\mathbf{x} - \mathbf{d}_i)^T\mathbf{R}_i^{-1}(\mathbf{H}_i\mathbf{M}_i\delta\mathbf{x} - \mathbf{d}_i) \quad (4)$$

$$\delta\mathbf{y}_{\mathbf{modelobs}} = \mathbf{H}\delta\mathbf{x}. \quad (5)$$

$$\mathbf{y}_{\mathbf{modelobs}} = \mathcal{H}\mathbf{x} = \mathbf{A}\mathbf{W}^*\mathbf{x}_{\mathbf{oz}} \quad (6)$$

$$\partial\mathbf{W}^* = \partial[(\mathbf{W}^T\mathbf{W})^{-1}\mathbf{W}^T]$$

$$\partial\mathbf{W}^* = (\mathbf{W}^T\mathbf{W})^{-1}(\partial\mathbf{W})^T[\mathbf{I} - \mathbf{W}\mathbf{W}^*] - \mathbf{W}^*(\partial\mathbf{W})\mathbf{W}^* \quad (7)$$

$$\mathbf{H} = \frac{\partial\mathcal{H}}{\partial\mathbf{x}} = \mathbf{A}\left[\mathbf{W}^*, \frac{\partial(\mathbf{W}^*)}{\partial p_1}\mathbf{x}_{\mathbf{oz}}, \frac{\partial(\mathbf{W}^*)}{\partial p_2}\mathbf{x}_{\mathbf{oz}}, \cdots, \frac{\partial(\mathbf{W}^*)}{\partial p_m}\mathbf{x}_{\mathbf{oz}}\right] \quad (8)$$

Full $\mathcal{H}(\mathbf{x})$ and tangent linear TL= $\mathcal{H}(\mathbf{x}_\mathbf{b}) + \mathbf{H}\,\boldsymbol{\delta}\mathbf{x}$ observation operators calculated for an example test case. Note that the model pressure grid x_p needs to be finer than the observation grid p_r , the violation of which produces pathological cases (Fig. 1) which can be avoided by dropping observation levels (Fig. 2), an approach especially suitable for retrievals which are often recorded on too many levels compared to their information content [3].

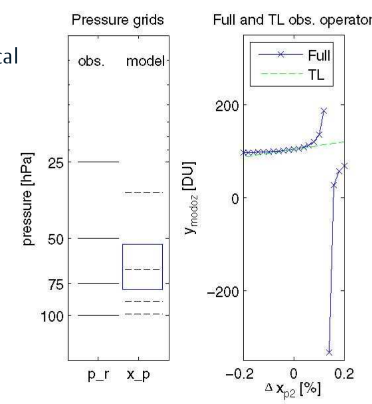

Fig. 1: Pathological case. Incremental varying of the second model pressure level x_{p2} results in a non-differentiable observation operator $\mathcal{H}(\mathbf{x})$.

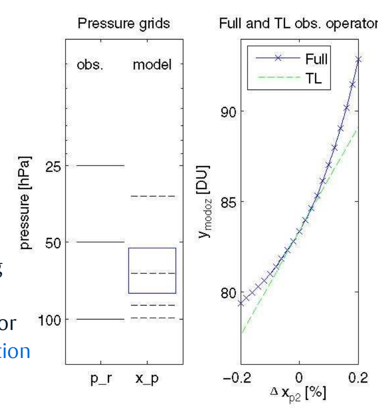

Fig. 2: Reducing the grid (i.e., dropping the appropriate observation pressure level) overcomes the problem, with the TL providing a useful approximation for the Full observation operator.