An Approach to Assess Observation Impact Based on Observation-minus-Forecast Residuals

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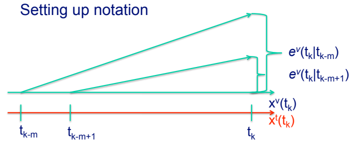
Abstract

Langland and Baker (2004) introduced an approach to assess the impact of observations on the forecasts. In that, a *state-space* aspect of the forecast is defined and a procedure is derived that relates changes in the aspect with changes in the forecast initial conditions due to the assimilation of observations, ultimately providing information of the impact of individual observations on the forecast. Though very instructive, this approach has its limitations. Typical choices of forecast aspect are rather arbitrary and generally lead to an incomplete assessment of the observing system. Furthermore, the state-space forecast aspect requires availability of a verification state that should ideally be uncorrelated with the forecast but in practice is not. And lastly, the approach involves the adjoint operator of the entire data assimilation system and as such it is constrained by the validity of this operator. The present work examines an *observation-space* metric that, for a relatively time-homogeneous observing system, allows for observation impacts to be derived without these limitations. Specifically, using observation-minus-forecast residuals leads to an approach with the following advantages: (i) it suggests a rather natural choice of forecast aspect directly related to the analysis system and that provides full assessment of the observing system; (ii) it naturally avoids introducing undesirable correlations in the forecast aspect by verifying against the observations; and (iii) it does not involve linearization and use of adjoints, therefore being applicable to any length of forecast. The observation-space approach has the additional advantage of being nearly cost-free and very simple to implement. The state- and observation-space approaches might be complementary to some degree, but their limitations and complexities are substantially different. Illustrations comparing these two approaches are given here using the NASA GEOS-5 data assimilation system.

Setting up notation



Three error measures considered here:

True state-space error: $e_{k|\ell} \equiv (\mathbf{x}^f_{k|\ell} - \mathbf{x}^t_k)^T \mathbf{T}_k (\mathbf{x}^f_{k|\ell} - \mathbf{x}^t_k)$

Perceived state-space: $e^v_{k|\ell} \equiv (\mathbf{x}^f_{k|\ell} - \mathbf{x}^v_k)^T \mathbf{T}_k (\mathbf{x}^f_{k|\ell} - \mathbf{x}^v_k)$

Observation-space residual: $e^y_{k|\ell} \equiv \left[\mathbf{h}_k(\mathbf{x}^f_{k|\ell}) - \mathbf{y}^o_k\right]^T \mathbf{C}_k \left[\mathbf{h}_k(\mathbf{x}^f_{k|\ell}) - \mathbf{y}^o_k\right]$

Forecast model: $\mathbf{x}^f_{k|k-m+1} = \mathbf{m}_{k,k-m+1}(\mathbf{x}^a_{k-m+1|k-m+1})$

Suboptimal analysis update:

$$\mathbf{x}^a_{k-m+1|k-m+1} = \mathbf{x}^b_{k-m+1|k-m} + \tilde{\mathbf{K}}_{k-m+1|k-m}[\mathbf{y}^o_{k-m+1} - \mathbf{h}_{k-m+1}(\mathbf{x}^b_{k-m+1|k-m})]$$

Observation-minus-background residual: $\mathbf{d}_{k-m+1|k-m} \equiv \mathbf{y}^o_{k-m+1} - \mathbf{h}_{k-m+1}(\mathbf{x}^b_{k-m+1|k-m})$

State-space forecast error reduction: $\delta e^v_k \equiv e^v_{k|k-m+1} - e^v_{k|k-m}$

Observation-space forecast error reduction: $\delta e^y_k \equiv e^y_{k|k-m+1} - e^y_{k|k-m}$

Remarks:

- The sub-optimality of the analysis update accommodates the weakly non-linear case
- Here, we'll be talking about the 1-day forecast error and corresponding error reduction

State-space (Adjoint) Approach

Question 1: How does the forecast error change with a change of initial condition?

Answer to Q1: Treat change of initial condition as infinitesimal and derive approximate formulae expressing the change in forecast error to various orders of accuracy. For example, a first-order expression involves:

$$\nabla_{\mathbf{x}^a} e^v_{k|\ell} = 2\mathbf{M}^T_{g;k,k-m+1}\mathbf{T}_k[\mathbf{x}^f_{k|\ell} - \mathbf{x}^v_k]$$

$$\mathbf{M}_{g;k,k-m+1} = \left.\frac{\partial \mathbf{m}_{k,k-m+1}(\mathbf{x})}{\partial \mathbf{x}}\right|_{\mathbf{x}=\mathbf{x}^g}$$

Question 2: How does the forecast error change when the initial condition changes as a consequence of assimilating observations?

Answer to Q2: Similarly to addressing Q1, treat change of initial condition as infinitesimal and derive approximate formulae expressing the change in forecast error to various orders of accuracy. For example, first and second order approximations give:

$$\delta e^{v,1}_k = \mathbf{d}^T_{k-m+1|k-m}\tilde{\mathbf{K}}^T_{k-m+1|k-m}\nabla_{\mathbf{x}^a} e^v_{k|k-m},$$

$$\delta e^{v,2}_k = \frac{1}{2}\mathbf{d}^T_{k-m+1|k-m}\tilde{\mathbf{K}}^T_{k-m+1|k-m}\left[\nabla_{\mathbf{x}^a} e^v_{k|k-m} + \nabla_{\mathbf{x}^a} e^v_{k|k-m+1}\right]$$

Observation-space Approach

Calculating the error reduction requires no approximation: $\delta e^y_k \equiv e^y_{k|k-m+1} - e^y_{k|k-m}$

Following Errico (2007) or Daescu and Todling (2009) one could write down approximations to this error reduction to various orders, but they are unnecessary.

Insights on State- vs Observation-space Approaches

For the sake of argument, consider the linear *suboptimal* case.

Define the forecast error covariance difference: $\Delta\mathbf{P}^f_k \equiv \mathbf{P}^f_{k|k-m+1} - \mathbf{P}^f_{k|k-m}$

Then:

$$< \delta e_k > = \mathrm{Tr}\left\{\mathbf{T}_k \Delta\mathbf{P}^f_k\right\}$$

$$< \delta e^y_k > = \mathrm{Tr}\left\{\mathbf{H}^T_k \mathbf{C}_k \mathbf{H}_k \Delta\mathbf{P}^f_k\right\}$$

Remark: Probabilistic approach has very clear notion of improvement: $\Delta\mathbf{P}^f_k < 0$.

Useful definitions for what follows:

Observation-minus-forecast residual covariance matrix:

$$\mathbf{\Gamma}_{k|k-m} = \mathbf{H}_k \mathbf{P}^f_{k|k-m}\mathbf{H}^T_k + \mathbf{R}_k$$

Difference between a general, *suboptimal* gain, and the Kalman gain:

$$\Delta\mathbf{K}_k \equiv \tilde{\mathbf{K}}_k - \mathbf{K}_k$$

One can derive the following basic results:

1. For optimal systems, the *expected* forecast error reduction always corresponds to positive impact – assimilation of data always leads to improvement in the expected mean sense.

$$< \delta e_k > \overset{opt}{\leq} 0$$

$$< \delta e^y_k > \overset{opt}{\leq} 0.$$

2. For optimal systems, and a suitable choice of weighting matrix $\mathbf{T}_k$, the state-space *expected* forecast error reduction produces the same estimate as that obtained in observation-space.

$$< \delta e_k(\mathbf{T}_k = \mathbf{H}^T_k\mathbf{C}_k\mathbf{H}_k) > \overset{opt}{=} < \delta e^y_k >$$

Since $rank(\mathbf{T}_k) \geq rank(\mathbf{C}_k)$ there is only so much the measure in observation-space can capture when compared with that in state-space, however, the remaining part is not accessible to us.

3. In general, for suboptimal systems, verifying against a state other than the truth introduces a correlation (covariance) between the observation-minus-background residual and the error in the verification, $\boldsymbol{\epsilon}^v_k \equiv \mathbf{x}^v_k - \mathbf{x}^t_k$

$$< \delta e^v_k > = < \delta e_k > -2\mathrm{Tr}\left[\tilde{\mathbf{K}}^T_{k-m+1}\mathbf{M}^T_{k,k-m+1}\mathbf{T}_k < \boldsymbol{\epsilon}^v_k \mathbf{d}^T_{k-m+1|k-m} >\right]$$

4. In general, for suboptimal systems, if the verification is chosen to be the underlying analysis all intermediate residual correlations (covariances) participate

$$< \delta e^{v=a}_k > = < \delta e_k >$$

$$-2\mathrm{Tr}\left[\tilde{\mathbf{K}}^T_{k-m+1}\mathbf{M}^T_{k,k-m+1}\mathbf{T}_k\left(\mathbf{M}_{k,k-m+1}\Delta\mathbf{K}_{k-m+1}\mathbf{\Gamma}_{k-m+1} + \sum_{j=0}^{m-2}\mathbf{M}_{k,k-j}\tilde{\mathbf{K}}_{k-j} < \mathbf{d}_{k-j|k-j-1}\mathbf{d}^T_{k-m+1|k-m} >\right)\right]$$

5. Therefore, only in the optimal case, use of the verification is equivalent to use of the unknown true state to obtain the expected error change of interest.

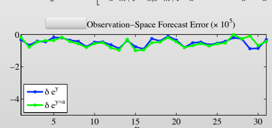
Experimental Setup with GEOS-5 DAS

- 2x2.5x72 resolutio
- IAU-based 3DVAR
- Statistics collected over 31 00Z 24-hr forecasts for August 2007
- Broad LPO excluding only top layers of model

The Role of the Verification

The role of the verification can be precisely tested in observation-space. Similarly, to the result obtained in state-space, when the verification is chosen to be the analysis, now projected onto observation space, the following holds:

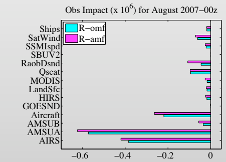
$$< \delta e^{y=a}_k > = < \delta e^y_k > -2\mathrm{Tr}\left[\tilde{\mathbf{K}}^T_{k-m+1}\mathbf{M}^T_{k,k-m+1}\mathbf{H}^T_k\mathbf{C}_k\mathbf{H}_k < \boldsymbol{\epsilon}^{v=a}_k\mathbf{d}^T_{k-m+1|k-m} >\right]$$



The result with GEOS-5 DAS indicates that in the light of this global measure, the system is nearly optimal, and using the analysis as a proxy for the observations is reasonable most of the time. Indeed, this provides a test of optimality.

The Role of the Verification

Although from an global measure perspective the system behaves as if it were optimal so that verification can be accomplished by comparing against either the observations or the analysis, a closer look indicates this cannot be pushed too far.

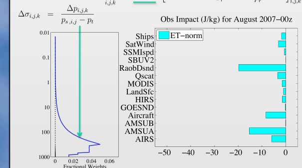


Examination of the observation-space impacts when either the observations or the analyses are used for verification reveals that use of the analysis has the tendency to overestimate the impact of observations on the forecast.

Observation Impacts and Choice of Norm

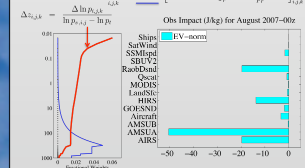
$$e_t \equiv \mathbf{x}^T_1\mathbf{T}_t\mathbf{x}_2 = \frac{1}{2}\sum_{i,j,k}\Delta H_{i,j}\Delta\sigma_{i,j,k}\left[u'_1u'_2 + v'_1v'_2 + \frac{c_p}{T_r}T'_1T'_2 + \frac{RT_r}{p^2_r}p'_{s1}p'_{s2}\right]_{i,j,k}$$

$$\Delta\sigma_{i,j,k} = \frac{\Delta p_{i,j,k}}{p_{s,i,j} - p_t}$$



$$e_t \equiv \mathbf{x}^T_1\mathbf{T}_t\mathbf{x}_2 = \frac{1}{2}\sum_{i,j,k}\Delta H_{i,j}\Delta z_{i,j,k}\left[u'_1u'_2 + v'_1v'_2 + \frac{c_p}{T_r}T'_1T'_2 + \frac{RT_r}{p^2_r}p'_{s1}p'_{s2}\right]_{i,j,k}$$

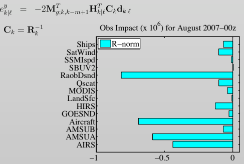
$$\Delta z_{i,j,k} = \frac{\Delta \ln p_{i,j,k}}{\ln p_{s,i,j} - \ln p_t}$$



$$\delta e^y_k \approx \delta e^{y,2}_k = -\frac{1}{2}\mathbf{d}^T_{k-m+1|k-m}\tilde{\mathbf{K}}^T_{k-m+1|k-m}\left[\nabla_{\mathbf{x}^a}e^y_{k|k-m} + \nabla_{\mathbf{x}^a}e^y_{k|k-m+1}\right]$$

$$\nabla_{\mathbf{x}^a}e^y_{k|\ell} = -2\mathbf{M}^T_{g;k,k-m+1}\mathbf{H}^T_k\mathbf{C}_k\mathbf{d}_{k|\ell}$$

$$\mathbf{C}_k = \mathbf{R}^{-1}_k$$

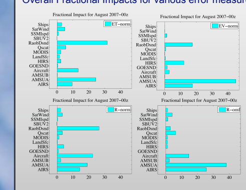


Applying the state-space (adjoint-based) approach, these three panels illustrate the consequences of using different norms to derive observation impacts. The typical norm employed thus far in related works is based on a linearized total (dry) energy expression whose weights largely emphasize the troposphere (top) and neglect the stratosphere. Possible alternatives are to use the linearized total (dry) energy norm written in such a way that it more evenly weighs the vertical grid (middle), or yet to use a norm that weights the forecast aspect according to how the analysis system weights the observations (bottom). These three norms amount to distinct assessments of the impact of observations on the 24-hr forecast. For example, when the troposphere is emphasized the radiosonsode network shows as the primary observing system followed closely by AMSU-A; not surprisingly, when the norm evenly weighs the vertical AMSU-A becomes the primary contributor to the 24-hr forecast error reduction and the radiosonde network plays a secondary role together with AIRS; when the weights are made consistent with the analysis weighting of observations the radiosonde network becomes again the primary player followed now by Aircraft observations which seem to contribute more to error reduction than AMSU-A. The conclusion being that observation impacts are largely a function of the definition of forecast aspect.

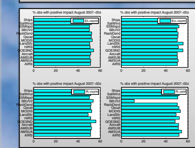
References:

Daescu, D. N., and R. Todling, 2009: Adjoint estimation of the variation in a model functional output due to assimilation of data. Mon. Wea. Rev., 1705-1716.
Errico, R. M., 2007: Interpretation of an adjoint-derived observational impact measure. Tellus, 59A, 273-276.
Langland, R., and N. L. Baker, 2004: Estimation of observation impact using the NRL atmospheric variational data assimilation adjoint system. Tellus, 56A, 189-201.

Overall Fractional Impacts for various error measures

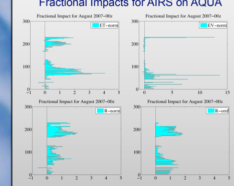


The figure on the left gives a summary of the observation impacts on the 24-hr forecast for the individual main observing systems used in GEOS-5 DAS. The panels show the fractional impacts when the state-space (adjoint-based) approach is used with three different norms: tropospheric-centric total (dry) energy norm (top-left), evenly-weighted total (dry) energy norm (top-right); and inverse observation error covariance norm (bottom-left). Also, the impacts as derived from the adjoint-free, observation-space approach are shown in the bottom-right panel, where the norm is based on the inverse observation error covariance matrix. At first glance, results from the two approaches look quite similar, especially when it comes to the relative impact among different observing systems. Looking more closely, there differences. The most dramatic difference being the less significant impact of the radiosonde network suggested by the observation-space approach versus what is indicated by the state-space approach.



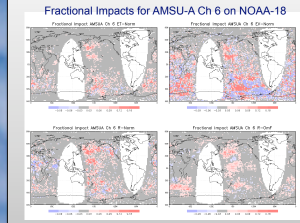
The figure on the left shows that, independently of the norm, about 50% of the data contribute positively to the 24-hr forecast error reduction. The only exception is indicated by the observation-space measure (bottom-right panel) when it comes to use of SBUV ozone observations, when only 10% of the observations seem to help reduce forecast error. Indeed, it is surprising that the state-space measures based on total energy claim 50% of ozone observations to contribute to forecast error: the energy expression does not even account for errors in ozone. When the state-space approach uses the inverse of R to define the error norm, the results still seem to say that 50% of the ozone observation contribution to forecast error reduction. The conclusion is that this is a spurious result coming from high sensitivity of the (adjoint) analysis to ozone observations.

Fractional Impacts for AIRS on AQUA



An even closer look at the results reveals more differences among the various forecast error measures and the two approaches. The figure on the left looks at the impacts of the individual channels of AIRS. When using the state-space (adjoint-based) approach with a measure that emphasizes the troposphere, the troposphere-peaking channels of AIRS are the ones that show the largest impacts; when the stratosphere is emphasized, most of the AIRS impacts come from the channels peaking there. When the forecast error measure is based on a norm that uses weights compatible with the weights given to the observations by the analysis (for either approach) the impacts are more evenly spread among the various channels of AIRS.

Fractional Impacts for AMSU-A Ch 6 on NOAA-18



Lastly, the figure above shows maps of the fractional impacts of channel 6 for the AMSU-A instrument on NOAA-18 as calculated by the various norms and the two approaches. For this particular channel, the fractional impacts are not dramatically distinct, even though sometimes their amplitudes are. Only when the stratosphere is emphasized in the measure and the adjoint-based approach is used one sees large mixed, positive and negative, impacts in the Southern Pacific Ocean; elsewhere the fractional impacts are positive or relatively small.

Limitations of the observation-space approach

- Observation-space measures capture only a part of the forecast error – that part projecting onto the space of observations – unfortunately, this is *only* part accessible to us.
- In practice, since observations are bias-corrected, there is still a correlation in the observation-space forecast aspect between the forecast and the verification (i.e., bias-corrected observations in this case).
- The observing system must be relatively homogenous at the initial and final (verification) times (which is the case in most applications).

Conclusions

- A fair assessment of the observing system impact on the forecast requires careful choice of a forecast error measure. Statements about specific observing systems are largely subject to the choice of norm.
- Observation impacts derived from the sequence of observation-minus-forecast residuals provide reliably similar information to that obtained with adjoint-based techniques with considerably less restrictions and complexities.

Background photo from Cloud Appreciation Society by: Katrin Pfeifer, Afternoon sky with the moon, taken in Castagneto Carducci, Tuskany, Italy.