Interpreting Adjoint and Ensemble Sensitivity toward the Development of Optimal Observation Targeting Strategies

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Abstract

Two general methods, adjoint or singular vector methods, and ensemble-based methods, have been previously investigated to identify locations where observations would have a significant positive impact on a numerical weather model forecast. In this paper, we perform a basic comparison of targeting regions chosen to reduce the expected variance of a chosen forecast response function within an ensemble Kalman filter (EnKF) based on both an adjoint and an ensemble method. Ensemble sensitivity is defined by linear regressions of a chosen forecast response function onto the model initial-time state variables, and is used to calculate variance reduction fields to provide targeting guidance for the ensemble-based method. Adjoint sensitivity is used to provide targeting guidance for the adjoint-based method. 90 ensemble forecasts are considered over a 24-hour forecast period, and the response function is chosen to represent the sea-level pressure at a single point in the Pacific Northwest United States.

Targeting by ensemble guidance is shown to be a function of ensemble sensitivity and both the initial-time model state and observation variance. We find that large areas of variance reduction exist away from regions of large ensemble sensitivity, adjoint sensitivity, and the initial-time variance of the model state. Both ensemble-guided and adjoint-guided targeting regions are investigated here to gain insight into which is potentially better for observation targeting.

Considering hypothetical aircraft which could be used to gather observations, it is shown that ensemble guidance is superior to adjoint guidance for 850-hPa temperature observations. This advantage increases as the number of flight tracks increases. In all
cases, as more flight tracks are considered, diminishing returns on response function variance reduction are realized. The implications of these results for the development of targeting strategies are discussed.
I. Introduction

Adaptive atmospheric data assimilation involves gathering observations above and beyond the routine observational network that may significantly improve the prediction of a specific forecast aspect. The adaptive nature of this type of data assimilation is due to the fact that target regions will likely vary with both flow situation and the chosen specific forecast aspect that the targeted observations are meant to improve. With the recent development of adaptive observing platforms, such as dropsondes, rocketsondes, and unmanned aircraft, adaptive data assimilation has the potential to improve the prediction of significant weather events that pose a significant risk to people and property.

Targeting regions should ideally incorporate error growth dynamics, analysis and observational error, and the data assimilation system used to assimilate the targeted observations (Berliner et al. 1999). One type of targeting method that has been proposed, the singular vector, or adjoint sensitivity method (Buizza and Montani 1999, Gelaro et al. 1999, Langland et al. 1999), operates under the assumption that although only a fraction of initial analysis error may project onto the fastest growing regions, it is this fraction that will dominate the forecast error. Targeting regions based on this approach are identified by leading singular vectors or regions of significant adjoint sensitivity. Further development of this method accounted for initial-condition uncertainty, and it was shown that leading total energy singular vectors shifted when analysis uncertainty was considered (Gelaro et al. 2002). A second type of targeting method is an ensemble-based approach called the ensemble transform Kalman filter (ETKF) method (Bishop et al. 2002).
Targeting regions based on the ETKF method are formulated from the ensemble forecasts in order to reduce forecast error variance. Ancell and Hakim 2007 (hereafter AH2007) developed a methodology that is able to compare targeting regions based on both the adjoint sensitivity and ensemble approach. This comparison is possible due to a quantity called ensemble sensitivity, which is defined by the linear regression of a forecast aspect onto the model initial condition variables. This formulation of ensemble sensitivity in AH2007 is developed from a similar quantity introduced in Hakim and Torn 2005. AH2007 show that ensemble sensitivity is related to adjoint sensitivity through the statistics of the initial state, and reveal how ensemble sensitivities can be manipulated to produce response function variance reduction fields due to hypothetical observations within an ensemble Kalman filter (EnKF). This paper goes beyond AH2007 in further interpreting the variance reduction fields guided by the ensemble sensitivity method. AH2007 also show that maxima in the ensemble-guided variance reduction fields exist away from regions of significant adjoint sensitivity, indicating that targeting regions guided by adjoint and ensemble methods are different within an EnKF data assimilation system. A more thorough examination of the targeting regions associated with both ensemble and adjoint methods is performed here to assess the potential of each method in reducing forecast error variance in a practical, real-time environment.
II. Background

A. Relationship of Adjoint and Ensemble Sensitivities

Following the methodology in LeDimet and Talagrand 1986, AH2007 review the formulation for the adjoint sensitivity of a chosen forecast response function $J$ with respect to the initial conditions of an atmospheric numerical weather prediction model. It is shown that the adjoint sensitivity $\partial J / \partial Y_o$ can be formulated as:

$$\partial J / \partial Y_o = R^T \cdot \partial J / \partial Y_T$$ (1)

where $\partial J / \partial Y_T$ is the gradient of the response function with respect to the model forecast state variables, $Y_T$, and $R$ is the resolvent matrix, derived from the nonlinear model, which maps initial-time perturbations to forecast time. Such perturbation evolution is a tangent linear approximation about a previously-run forecast, and the accuracy of adjoint sensitivity depends on the accuracy of this linear approximation.

Following the derivation in AH2007, the ensemble sensitivity of the response function with respect to the initial conditions, $\partial J_e / \partial Y_o$, can be formulated as:

$$\partial J_e / \partial Y_o = D^{-1} \cdot \text{Covariance}(J,Y_o)$$ (2)

where $D$ is a diagonal matrix containing the variance of each initial-time model state variable, which is an estimate of the error variance, and the covariance of the indicated
arguments is a column vector of covariances between the response function and each initial-time model state variable. In practice, ensemble sensitivity is calculated from an ensemble of size much smaller than the number of model state variables. Such a small sample size implies sampling error may exist in the ensemble sensitivity values. Statistical confidence measures may be used to address such sampling error, and these methods are discussed in AH2007.

AH2007 show that under the assumption of linear perturbation evolution, the covariance term in equation (2) can be written in terms of the initial-time analysis error covariance matrix (A) and the adjoint sensitivity of the response function calculated about a forecast trajectory begun from the mean initial condition. Thus, the relationship between ensemble and adjoint sensitivity can be written as:

\[ \frac{\partial J_e}{\partial Y_o} = D^{-1} \ast A \ast \frac{\partial J_a}{\partial Y_o} \]

Equation (3) shows that the ensemble sensitivity is a product of an initial-time statistical term (\(D^{-1} \ast A\)) and the adjoint sensitivity. This results in each ensemble sensitivity value predicting the change in response function through a product of an initial-time perturbation to a single model state variable, spread throughout the domain by the statistics of the initial state, and projected onto the entire adjoint sensitivity field. On the contrary, each adjoint sensitivity value predicts the change in response function due to the perturbation with respect to only that single model state variable.
B. Targeting Observations within an EnKF Using Ensemble Sensitivity

The EnKF utilizes the Kalman filter update equations for how a set of ensemble members are updated with observations. One equation provides an ensemble-mean analysis based on observation values, and the second equation provides an ensemble of perturbations about the mean based on the observation statistics, but not the observation values. Since the values of observations are not known when selecting targeting locations, only the equation that updates the statistics of the ensemble set will be considered here for the development of observation targeting strategies. This equation shows how the background error covariance matrix (B, typically supplied by a previous forecast) is updated to the analysis error covariance matrix (A) through the assimilation of observations:

\[
A = (I - KH) \ast B \quad (4)
\]

\[
K = B \ast H^T \ast (H \ast B \ast H^T + O)^{-1} \quad (5)
\]

In the above equations, H is a linearized observation operator that maps the background to the observations, I is the identity matrix, and O is the observation error covariance matrix, assumed to be diagonal under the assumption that the observations are uncorrelated.

Assuming that routine observations have been assimilated at the initial time, AH2007 formulate an expression for the reduction in forecast response function variance due to hypothetical targeted observations:
\[ \Delta \text{Variance}(J) = (H \ast D \ast \frac{\partial J_e}{\partial Y_o})^T \ast E^{-1} \ast (H \ast D \ast \frac{\partial J_e}{\partial Y_o}) \] (6)

where E represents the innovation error covariance matrix \((H^A \ast H^T + O)\). By allowing \(H=I\), and assuming typical observation error variances, equation (6) provides a computationally cheap way to estimate the response function variance reduction from a single hypothetical observation at every model grid point. In this case, equation (6) reduces to \((d_i \ast \frac{\partial J_e}{\partial Y_{oi}})^2 / (d_i + o_i)\) where \(d_i\), \(\frac{\partial J_e}{\partial Y_{oi}}\), and \(o_i\) are values of the initial condition variance, ensemble sensitivity, and observation variance at a single grid point with respect to a single model state variable. Furthermore, equation (6) makes it easy to estimate the response function variance reduction due to various sets of observations, such as observations along different flight tracks. AH2007 show how it is also possible to easily determine the next largest response function variance reduction of a hypothetical observation conditioned on the simultaneous assimilation of other observations already chosen.

III. Methodology

Ensemble sensitivity is calculated here using the same ensemble members in AH2007, which come from a 90-member limited area, operational EnKF system run at the University of Washington. This EnKF uses the Weather Research and Forecasting (WRF) model on a 6-hour update cycle assimilating observations from satellite-derived winds, aircraft, radiosondes, buoys, ships, and land-based stations. This WRF model
ensemble is interpolated to the PSU/NCAR MM5 Version 3 model. The ensemble sensitivities are calculated using these MM5 initial conditions and forecasts. Lateral boundary conditions for the ensemble mean are provided by the Global Forecast System (GFS) for all 90 forecasts; ensemble perturbation boundary conditions are set to zero, which has little effect on the results over the short forecast lead time. Adjoint sensitivity is also calculated as in AH2007 with the adjoint of the MM5 Version 3 model (Ruggiero et al. 2002), using the basic-state begun from the mean initial condition of the MM5 forecasts. The model physics used for the forward ensemble forecasts, the basic-state for the adjoint integration, and the adjoint model are identical. These physics are the Anthes-Kuo cumulus parameterization, the Burk-Thompson planetary boundary layer scheme, the stable precipitation explicit moisture scheme, and the simple cooling radiation scheme. The experiments are performed at 45-km horizontal resolution with 33 vertical sigma levels. The forecast period is 24 hours, and the response function is defined to be the lowest sigma level perturbation pressure at a single point over the Puget Sound in western Washington State.

The synoptic situation described by the ensemble-mean forecast for the 24-hr period under investigation from 1200 UTC 3 February to 1200 UTC 4 February 2005 is shown in Figure 1. At 1200 UTC 3 February, the flow was dominated by a large trough along 150°W in the 500-hPa field. At the surface, an occluded system was positioned over the Gulf of Alaska, and high pressure dominated the surface pressure pattern to the south. As the 500-hPa trough moved east over the next 24 hours, it appears the surface cyclone developed down the Canadian coastline in association with the northern portion of the trough aloft. At 24-hr forecast time, the 500-hPa trough sits just offshore and the
only discernable weather feature in the vicinity of the response function is a weak trough extending southwest from Washington State. The location of the response function is shown by the black dot in Figure 1f.

IV. Results and Discussion

A. Comparison of Adjoint and Ensemble Sensitivity

Adjoint and ensemble sensitivities are related by the statistics of the initial state, and it may be expected that these two types of sensitivities could be significantly different. AH2007 provide a thorough discussion of the differences in structure, magnitude, and location among adjoint and ensemble sensitivities for this case. Adjoint sensitivities were shown to be wave-like, subsynoptic-scale structures that tilt upshear and maximize in the lower troposphere, similar to what has been found in previous studies of leading singular vectors or adjoint sensitivities (Errico and Vukicevic 1992, Langland et al. 1995, Rabier et al. 1996, Zou et al. 1998, Hoskins et al. 2000). Ensemble sensitivity, however, exhibited a synoptic-scale structure throughout the depth of the troposphere, tilting slightly upshear with height. The magnitudes of the ensemble sensitivity values are roughly three orders of magnitude larger than those of the adjoint sensitivities.

AH2007 interpret the difference between ensemble and adjoint sensitivity by graphically comparing the terms in equation (3). For a selected value of ensemble
sensitivity with respect to 850-hPa temperature, AH2007 show the statistically-spread perturbation from that point (a single row of $D^{-1}A$ in equation (3)), the adjoint sensitivity with respect to temperature at 850 hPa, and the projection of the perturbation onto the adjoint sensitivity field. It is this projection field which sums to form the single ensemble sensitivity value. Since the largest ensemble sensitivity values exist outside of the significant adjoint sensitivity field, the statistically-spread perturbation originating at locations with large ensemble sensitivity must have larger projections onto the adjoint sensitivity field than do statistically-spread perturbations originating within regions of significant adjoint sensitivity.

B. Interpretation of Variance Reduction Fields

Ensemble sensitivity alone does not determine response function variance reduction, as the ensemble variance of both the initial-time model state variable and the observation are included in the formulation of the variance reduction due to hypothetical observations. Comparing the ensemble sensitivity field to the initial-time variance field fosters a more complete understanding of the variance reduction field due to observations. Figure 2 shows the ensemble variance of initial-time temperature at sigma level 22 (850 hPa), as well as the ensemble sensitivity with respect to temperature and the response function variance reduction due to a single temperature observation. The maximum in each of these fields occupies a different location, although the maximum in the ensemble variance and the variance reduction are relatively close to each other.
The largest ensemble variance in Figure 2a is seen near the domain boundaries, away from large ensemble sensitivity values. Such large variance near the boundaries is likely the consequence of the variance given to the boundary conditions needed to force a limited-area EnKF (Torn et al. 2006). Over the ocean where significant ensemble sensitivity values exist, there is little ensemble variance, except for over a narrow region which extends southwestward from southwestern Canada. It was shown in AH2007 that for zero observation variance, the response function variance reduction due to an observation at a single point is equivalent to \( \partial J_e / \partial Y_T \), where the subscript T indicates temperature. Variance reductions in Figure 2c were calculated with an observation variance of 0.5 K², but it is clear that the region of largest variance reduction near 42°N, 138°W is due to the influence of relatively large ensemble variance in this region. At the point of maximum variance reduction, 93% of the net projection field at this level (a single row of \( D^{-1} A \) multiplied by the adjoint sensitivity field in equation (3)), which is the contribution from this level to the ensemble sensitivity value, results from the region of significant adjoint sensitivity. This supports the finding of AH2007 that the majority of an ensemble sensitivity value is due to regions of significant adjoint sensitivity. Thus, even though ensemble sensitivities are weighted differently across the domain by the ensemble variance in producing response function variance reduction, their dependence on regions of large adjoint sensitivity suggests that such regions of adjoint sensitivity are important for observation targeting.
C. Observation Targeting guided by Adjoint and Ensemble Sensitivities

Figure 2 also depicts the adjoint sensitivity with respect to initial-time temperature at sigma level 22 (850 hPa). It is apparent from Figures 2c and 2d that the maximum in response function variance guided by the ensemble sensitivities is displaced southwest from the significant adjoint sensitivity field. In turn, regions for targeting temperature observations at the 850-hPa level are different based on the ensemble and adjoint sensitivity methods. In order to compare the response function variance reductions from targeted observations in both regions, a hypothetical adaptive aircraft is considered which is able to measure temperature along a flight track including 5 adjacent grid points at 850 hPa at the initial time. For a given field, the five grid points along which a flight track is selected are chosen by first identifying the maximum magnitude of the field, and then choosing five adjacent grid points, including that grid point, that have the have the largest average magnitude.

For observations along a single flight track, the extrema in both adjoint sensitivity and variance reduction fields are considered. Although choosing the flight track from the variance reduction field guided by ensemble sensitivity is obvious, the adjoint sensitivity field contains two clear local maxima in magnitude, and both these regions will be considered independently. Table 1 shows the response function variance reduction (original response function variance is 4.80 mb²) associated with observations along a single flight track centered on the maximum value in the variance reduction field, as well as observations along a single flight track centered on the two extrema of the adjoint sensitivity field. A 1.70 mb² reduction in response function variance results from
observations along a flight track through the maximum in the variance reduction field, compared to 1.25 mb$^2$ for observations at the minimum in the adjoint sensitivity field, and 0.77 mb$^2$ for observations at the maximum in the adjoint sensitivity field.

It is possible that two unmanned aircraft would be available to gather two separate flight tracks of observations. In this case, the obvious choice for flight tracks using adjoint sensitivity guidance would be to observe both extrema in the adjoint sensitivity field that were previously considered independently. Selecting a second flight track using the variance reduction field requires calculating the response function variance reduction from an observation conditioned on the simultaneous assimilation of the observations along the flight track through the maximum variance reduction values in Figure 2c. Figure 3a shows the response function variance reduction that would be realized from such a sixth 850-hPa temperature observation. The second flight track is selected to include observations at the local maxima near 42°N, 152°W in Figure 3a. Note that the variance reduction values resulting from a sixth observation conditioned on the simultaneous assimilation of the five observations along the first flight track selected are relatively small compared to the variance reduction values due to a single observation in Figure 2c.

Table 1 includes the response function variance reduction from observations along two flight tracks using guidance from both the adjoint sensitivity and variance reduction fields. The variance reduction from observations along two flight tracks guided by the variance reduction field is 2.28 mb$^2$, 80% more than the variance reduction of 1.27 mb$^2$ using adjoint sensitivity guidance. Furthermore, assimilating observations along a second flight track using the variance reduction field still significantly reduces the
response function variance, something that is not achieved using adjoint sensitivity guidance. In fact, the entire region of significant adjoint sensitivity must be observed, which amounts to about 200 grid points, to achieve a similar variance reduction realized from the 10 grid points observed in the two flight tracks using the variance reduction field.

Lastly, Figure 3 shows the response function variance reduction which would be realized from an eleventh observation if the ten observations along the first two flight tracks guided by the variance reduction field were simultaneously assimilated. Maxima in this field are in regions of local maxima after selecting the first flight track (figure 3a), although values are very small in the region of the second flight track. Assimilating temperature observations along a third flight track at the local maximum in central British Columbia near 55°N, 105°W further reduces the response function variance 0.24 mb² for a total variance reduction of 2.52 mb². Table 1 includes this variance reduction from observations along a third flight track, and summarizes the diminishing returns of response function variance reduction from observations along each subsequent flight track. Observations along three flight tracks guided by the variance reduction field, which amount to 15 grid points, reduce the original response function variance by 53%.

V. Summary and Conclusions

Ensemble sensitivity is a quantity that combines adjoint sensitivity and the statistics of the initial state provided by an ensemble. Adjoint sensitivity at a single point
estimates the change in a forecast response function due to a perturbation at that point, whereas ensemble sensitivity at a single point represents the change in a forecast response function due to a perturbation at that point, spread throughout the domain by the initial-time ensemble statistics. This fundamental difference between adjoint and ensemble sensitivities results in the structures of these types of sensitivities being very different in terms of scale, location, and magnitude.

Ensemble sensitivities can be combined with initial-time state variance and observation variance to produce forecast response function variance reduction fields due to observations. For a low-level pressure response function at 24-hr forecast time for a typical wintertime flow situation, the maximum variance reduction values shifted to the east of extrema in the ensemble sensitivity field, because of larger initial-time variance in that region. Maxima in the variance reduction field existed to the northeast of local maxima in the variance field, however, resulting in different locations of extrema in each of the adjoint sensitivity, ensemble sensitivity, variance, and variance reduction fields.

Both ensemble and adjoint sensitivity was used to identify regions where targeted observations could be taken to improve the forecast. Observations beyond the routine observational network were considered which would significantly reduce the variance of the low-level pressure 24-hr forecast response function within an EnKF. Temperature observations along flight tracks at 850 hPa including 5 adjacent model grid points were considered to compare response function variance reduction guided by adjoint sensitivity and variance reduction fields. For observations along a single flight track, targeting guided by the variance reduction field was 36% larger than that using adjoint sensitivity guidance. The difference was more pronounced considering observations along two
flight tracks, with a variance reduction 80% larger using the variance reduction field than that using adjoint sensitivity guidance. Observing the entire region of significant adjoint sensitivity produced a similar variance reduction to that considering observations along only two flight tracks under guidance from the variance reduction field, but ten times as many model grid points had to be observed to achieve this equivalence. Observations along a third flight track determined from the variance reduction field further reduced the variance to over half the original forecast response function variance. In all cases considered, diminishing returns to the response function variance reduction were realized with observations along each subsequent flight track.

Practical implementation of targeting observations to reduce response function variance clearly favors ensemble guidance through the variance reduction field for 850-hPa temperature observations for the case considered here. It is not clear whether this result holds when considering the full depth of the troposphere, as well as other observations such as winds, pressure, and mixing ratio. Furthermore, these results are based on the assumption of a good tangent-linear approximation to perturbation evolution, and need to be tested with the assimilation of actual observations into an EnKF to determine the accuracy of the predicted variance reductions, and how such predictability compares with other data assimilation systems. These aspects will be investigated in future work in the development of ensemble sensitivity for adaptive data assimilation strategies.
References


Figure and Table Captions

Figure 1.  500-hPa geopotential height (solid lines, contour interval is 40 m) in the left column, and sea-level pressure (solid lines, contour interval is 3 hPa) in the right column forecast at 00 hr, 12 hr, and 24 hr initialized from the ensemble mean initial condition at 1200 UTC 3 February 2005.

Figure 2.  A) Variance in temperature, contour interval is 0.5 K², b) ensemble sensitivity of the response function with respect to temperature, contour interval is 40 Pa/K, c) reduction in forecast response function variance from the assimilation of a single temperature observation, contour interval is 0.3 mb², and d) adjoint sensitivity of the response function with respect to temperature, contour interval is 0.15 Pa/K at sigma level 22 (850 hPa) at 1200 UTC 3 February 2005. Solid lines denote positive values, dashed lines denote negative values.

Figure 3.  Reduction in forecast response function variance from the assimilation of a single temperature observation at 1200 UTC 3 February 2005 at sigma level 22 (850 hPa) given a) the simultaneous assimilation of observations along a single flight track centered on the maximum variance reduction in Figure 2c near 42°N, 138°W, contour interval is 0.08 mb², and b) the simultaneous assimilation of observations along both the first flight track from Figure 2c and the flight track centered on the local maximum variance reduction in panel (a) near 42°N, 152°W, contour interval is 0.06 mb².
Table 1. Response function variance reduction from temperature observations along various flight tracks and selected grid points at sigma level 22 (850 hPa).
Figure 1 - 500-hPa geopotential height (solid lines, contour interval is 40 m) in the left column, and sea-level pressure (solid lines, contour interval is 3 hPa) in the right column forecast at 00 hr, 12 hr, and 24 hr initialized from the ensemble mean initial condition at 1200 UTC 3 February 2005.
Figure 2 - A) Variance in temperature, contour interval is 0.5 K$^2$, b) ensemble sensitivity of the response function with respect to temperature, contour interval is 400 Pa/K, c) reduction in forecast response function variance from the assimilation of a single temperature observation, contour interval is 0.15 mb$^2$, and d) adjoint sensitivity of the response function with respect to temperature, contour interval is 0.15 Pa/K, at sigma level 22 (850 hPa) at 1200 UTC 3 February 2005. Solid lines denote positive values, dashed lines denote negative values.
Figure 3 - Reduction in forecast response function variance from the assimilation of a single temperature observation at 1200 UTC 3 February 2005 at sigma level 22 (850 hPa) given a) the simultaneous assimilation of observations along a single flight track centered on the maximum variance reduction in Figure 2c near 42°N, 138°W, contour interval is 0.08 mb², and b) the simultaneous assimilation of observations along both the first flight track from Figure 2c and the flight track centered on the local maximum variance reduction in panel (a) near 42°N, 152°W, contour interval is 0.06 mb².
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Table 1 - Response function variance reduction from temperature observations along various flight tracks and selected grid points at sigma level 22 (850 hPa).