Recent developments in the use and understanding of adjoint-derived estimates of observation impact

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Background / Outline for this Talk

• Adjoint-based estimates of observation impact have become increasingly popular as an alternative/complement to traditional observing system experiments (OSEs)

✓ Used at several centers for experimentation or routine monitoring

✓ Inter-comparison project between centers in progress

• For linear analysis problems, observation impact is closely related to (is an extension of) observation sensitivity ...see Baker and Daley (2000)

- This talk touches on:
 - \checkmark Initial comparison of results for two centers
 - ✓ Need for, implications of >1st order estimates of impact
 - ✓ Extension to nonlinear analysis problems
 - ✓ Comparison, complementarity with OSEs

The Data Assimilation System

• Consider a forecast model: $\mathbf{x}^{f} = \mathbf{m}(\mathbf{x}_{0})$

and atmospheric analysis: $\mathbf{x}_{a} = \mathbf{x}_{b} + \mathbf{K}[\mathbf{y} - H(\mathbf{x})]$

where \mathbf{x}_b is a background state, \mathbf{y} are observations, H is a (possibly nonlinear) observation operator and \mathbf{K} determines the weight, or gain, given to each observation

...the difference $\delta \mathbf{y} = \mathbf{y} - H(\mathbf{x})$ is the innovation vector

• Assume, for now, that H is either <u>linear</u> or only a function of $\mathbf{x}_{\rm b}$, and define the analysis increment:

$$\delta \mathbf{x}_0 = \mathbf{x}_a - \mathbf{x}_b = \mathbf{K} \delta \mathbf{y} \tag{1}$$

Note that (1) may be viewed as a transformation between a perturbation δx_0 in *state space* and a perturbation δy in *observation space*

Estimating the Impact of Observations on Forecasts

Langland and Baker (2004) showed that the adjoint of a data assimilation system could be used effectively to measure the impact of observations on forecast skill



• Consider forecasts from an analysis x_a and background state x_b , and energy-based measure of forecast error $e = (\mathbf{x}^f - \mathbf{x}^t)^T \mathbf{C} (\mathbf{x}^f - \mathbf{x}^t)$ where x^t is a verification analysis state

• The difference $\delta e = e_a^f - e_b^f$ measures the combined impact of all obs assimilated at t = 0...

...it can be estimated as a sum of contributions from <u>individual</u> obs using information from the model and analysis adjoints

LB04 Observation Impact Estimate

$$\delta e \approx (\delta \mathbf{y})^{\mathrm{T}} \mathbf{K}^{\mathrm{T}} [\mathbf{M}_{b}^{\mathrm{T}} \mathbf{C} (\mathbf{x}_{b}^{f} - \mathbf{x}^{t}) + \mathbf{M}_{a}^{\mathrm{T}} \mathbf{C} (\mathbf{x}_{a}^{f} - \mathbf{x}^{t})]$$
analysis adjoint model adjoint

• The impact of arbitrary subsets of observations can be estimated by summing only terms involving the desired elements of δy

• The vector $\mathbf{K}^{T}[...]$ is computed only once and involves the **entire set** of observations

...removing or changing the properties of one observation changes the scalar measure of all other observations

- Application is subject to assumptions and simplifications in \mathbf{M}^{T}

 $\delta e < 0$...the observation **improves** the forecast $\delta e > 0$...the observation **degrades** the forecast

Impacts of Major Observing Systems in GEOS-5

24h Error Norm (Globe, NH, SH, Tropics) - July 2005 00UTC Totals



Gelaro and Zhu (2009)

Assessing Impacts of Hyper-Spectral Instruments

GEOS-5 Adjoint Data Assimilation System



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Comparison of Observation Impacts in Two Systems

24h Global Error Norm - Baseline Obs - Jan 2007 00+06 UTC

NASA GEOS-5

Navy NOGAPS



Overall impacts similar in NASA and Navy systems despite differences in algorithms, RT models, observation counts...

...notable differences in Satwinds, SSMI speeds

Impact of NOAA-18 AMSU-A Ch. 7 (binned by obs location)

Observations that produce large forecast error reductions

Observations that produce forecast error increases in **both models**

Land or ice surface contamination of radiance data?

24h Global Error Norm Baseline Obs Jan 2007 00+06 UTC



Scatter of Observation Impact vs Innovation

24h Global Error Norm - Baseline Obs - 21Jan 2007 00UTC

NASA GEOS-5

Navy NOGAPS



Orders of Approximation of δe

Errico (2007) placed the LB04 measure in the context of variousorder Taylor series approximations of δe in terms of δy

$$\delta \mathbf{x}_0 = \mathbf{K} \delta \mathbf{y} \implies (\delta \mathbf{x}_0)^{\mathrm{T}} \mathbf{g} = (\delta \mathbf{y})^{\mathrm{T}} \tilde{\mathbf{g}}$$

1st order:

$$\delta e_1 = \delta \mathbf{y}^{\mathrm{T}} \underbrace{2 \mathbf{K}^{\mathrm{T}} \mathbf{M}_{\mathrm{b}}^{\mathrm{T}} \mathbf{C} (\mathbf{x}_{\mathrm{b}}^{f} - \mathbf{x}^{t})}_{\tilde{\mathbf{g}}_1}$$

3rd order (LB04):

$$\delta e_3 = \delta \mathbf{y}^T \mathbf{K}^T [\mathbf{M}_b^T \mathbf{C} (\mathbf{x}_b^f - \mathbf{x}^t) + \mathbf{M}_a^T \mathbf{C} (\mathbf{x}_a^f - \mathbf{x}^t)] + a \text{ higher order term}$$

$$\widetilde{\mathbf{g}}_3$$

Note that $\tilde{\mathbf{g}}_1$ is a gradient and independent of $\delta \mathbf{y}$, but $\tilde{\mathbf{g}}_3$ is a weight that depends on all δy through \mathbf{x}_a

First- vs. Higher-Order Approximations of δe



A Caveat with Higher-Order Approximations

Terms beyond first-order in the approximation δe_3 have the form:

$$\delta e_3 - \delta e_1 \approx (\delta \mathbf{y})^{\mathrm{T}} \mathbf{K}^{\mathrm{T}} \mathbf{M}^{\mathrm{T}} \mathbf{C} \mathbf{M} \mathbf{K} (\delta \mathbf{y})$$

Errico (2007) noted that the nonlinear dependence of these terms on δy means partial sums of δe_3 involve **cross terms** with other observations, which may render results **ambiguous**

Gelaro et al. (2007) found this effect to be small when measuring impacts of the major observing systems ...smaller subsets?

3rd order



1st order

Order of approximation affects the magnitudes of the impact estimate... ...but 'not' their relative contributions

Nonlinear Analysis Problems



Observation Impact in Incremental Variational Data Assim.

Trémolet (2008) examined observation impact in a variational data assimilation system, accounting for j = 1,...,m outer loops

• Increment is not: $\mathbf{x}_{a} - \mathbf{x}_{b} = \mathbf{K} \delta \mathbf{y}$

It is, after loop *j*:
$$\mathbf{x}_j - \mathbf{x}_b = \mathbf{K}_j \mathbf{d}_j + \mathbf{K}_j \mathbf{H}_j (\mathbf{x}_{j-1} - \mathbf{x}_b)$$

or $\mathbf{x}_a - \mathbf{x}_b = \sum_{j=1}^m \mathbf{L}_j \mathbf{K}_j \mathbf{d}_j$
where $\mathbf{d}_j = \mathbf{y} - H(\mathbf{x}_{j-1}), \ \mathbf{L}_j = \mathbf{K}_m \mathbf{H}_m \dots \mathbf{K}_{j+1} \mathbf{H}_{j+1}$ and $\mathbf{L}_m = \mathbf{I}$

Then observation impact is:

$$I = \sum_{j=1}^{m} \left\langle \mathbf{K}_{j}^{\mathrm{T}} \mathbf{L}_{j}^{\mathrm{T}} \mathbf{g}, \mathbf{d}_{j} \right\rangle$$

where \boldsymbol{g} is a gradient or weight in model space

• For example, with m=2 outer loops: $I = \langle \mathbf{K}_1^T \mathbf{H}_2^T \mathbf{K}_2^T \mathbf{g}, \mathbf{d}_1 \rangle + \langle \mathbf{K}_2^T \mathbf{g}, \mathbf{d}_2 \rangle$

Observation Impact with Outer Loops



Impact per observation type on the analysis increment with 1, 2, and 3 outer loop iterations

- Outer loop (nonlinear) effects are larger in 4D-Var
- Overall observation impact is smaller in 4D-Var

Trémolet (2008)

Observing System Experiments (OSEs)

- Subsets of observations are **removed** from the assimilation system and forecasts are compared against a control system that includes all observations
- Because of expense, usually involve a relatively small number of independent experiments, each considering a relatively large subset of observations



Gelaro and Zhu (2009)

Comparison and Interpretation of ADJ and OSE Results ...a few things to keep in mind...

ADJ: measures the impacts of observations in the context of all other observations present in the assimilation system

OSE: removal of observations changes or degrades the system... \mathbf{K} differs for each member

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ADJ: measures the impact of observations in each analysis cycle separately and against the control background

OSE: measures the impact of removing information from both the background and analysis in a cumulative manner

ADJ: measures the response of a single forecast metric to all perturbations of the observing system

OSE: measures the effect of a single perturbation on all forecast metrics

Quantitative Comparison of ADJ and OSE Results



- Strictly speaking, quantitative comparison is limited to the forecast range and metric for which the ADJ results are valid on the one hand (e.g. 24h SH *e*-norm) and to the selected observing systems removed in the OSEs on the other hand
- Even then, comparisons between the ADJ and OSE results are complicated by the fact that values/changes in *e* measured in the OSE context are not directly comparable to values of δe measured in the ADJ context

Quantitative Comparison of ADJ and OSE Results

OSE: $e = (\mathbf{x}_0^f - \mathbf{x}^t)^{\mathrm{T}} \mathbf{C} (\mathbf{x}_0^f - \mathbf{x}^t)$

ADJ:
$$\delta e = (\delta \mathbf{y})^{\mathrm{T}} \mathbf{K}^{\mathrm{T}} [\mathbf{M}_{\mathrm{b}}^{\mathrm{T}} \mathbf{C} (\mathbf{x}_{\mathrm{b}}^{f} - \mathbf{x}^{t}) + \mathbf{M}_{\mathrm{a}}^{\mathrm{T}} \mathbf{C} (\mathbf{x}_{\mathrm{a}}^{f} - \mathbf{x}^{t})]$$

Gelaro and Zhu (2009) defined a fractional impact F_j of observing system j for each approach:

$$F_j(ADJ) = \delta e_j / \delta e$$

• Measures the % **decrease** in error due to the **presence** of obs system *j* with respect to the background forecast

•
$$\sum_{j} F_{j}(ADJ) = 1$$

$$F_j(\text{OSE}) = (e_{\text{no}_j} - e_{\text{ctl}})/e_{\text{ctl}}$$

• Measures the % **increase** in error due to the **removal** of obs system *j* with respect to the control forecast

• $\sum_{j} F_{j}(\text{OSE}) \neq 1$

% Contributions to 24hr Forecast Error Reduction January 2006



Gelaro and Zhu (2009)

% Contributions to 24hr Forecast Error Reduction July 2005



OSE Time Series of SH 24-hr Forecast Error Norm



Skill collapses when <u>all</u> AMSUA removed during SH winter...OSE and ADJ results become difficult to compare

Normalized % Contributions to 24hr Forecast Error Reduction

July 2005 January 2006 Jan2006 00z Tropical Error Norm Jul2005 00z Tropical Error Norm 25 35 ADI AD Fractional Impact (%) Fractional Impact (%) OSE 30 OSE 20 25 15 20 15 10 10 5 5 0 0 ANSUA1 ANSLA2 AMSUA3 Ofscar | ANSUA1 AMSUA2 | ANSUA3 alircraft Ofscar 1 Saturino aircraft Saturina 90₈₁ AIRS AIRS ! 90E,

...ADJ and OSE responses differ in magnitude in the tropics, but assign similar relative 'value' to the various observing systems

Digging deeper into the 'mix of observations'

• Both OSEs and ADJ measure the <u>net</u> effect of observations on the forecast

• We are also interested in dependencies and redundancies between observing systems as observations are added or removed ...inform current data selection, future data needs

• Such information is implicitly available in an OSE in terms of the responses of the <u>remaining</u> observing systems when a given set of observations is removed

• These responses can be measured through the **combined use of OSEs and ADJs**, by applying the ADJ to the perturbed (vs. only the control) members of an OSE

Combined Use of ADJ and OSEs

ADJ applied to perturbed OSE members to examine how changing the mix of observations influences their impacts



- Removal of AMSUA results in large increase in AIRS (and other) impacts
- Removal of AIRS results in significant increase in AMSUA impact
- Removal of raobs results in significant increase in AMSUA, aircraft and other impacts (but not AIRS)

Combined Use of ADJ and OSEs

ADJ applied to perturbed OSE members to examine how changing the mix of observations influences their impacts



- Removal of AMSUA results in large increase in AIRS impact in tropics
- Removal of wind observations results in significant decrease in AIRS impact in tropics (in fact, AIRS degrades forecast without satwinds!)

Conclusions on the Complementarity of ADJ and OSE

• Despite fundamental differences in how impact is measured, ADJ and OSE methods provide comparable estimates of the overall 'value' of most observing systems

• Differences in OSE and ADJ results should be expected and do not necessarily point to shortcomings in either:

✓ different treatment of background information

 ✓ removal of whole observing systems that contribute disproportionately to analysis quality (AMSU-A)

- Information gleaned from OSEs and ADJs should be viewed as complementary; ADJ extends, not replaces, OSEs:
 - ✓ applicable forecast range, metrics differ
 - ✓ ADJ well suited for routine monitoring

• The combined use of ADJs and OSEs illuminates the complex, complementary nature of how observations are used by the assimilation system

Calibration of Observing System Simulation Experiments (OSSEs) Using an Adjoint DAS



OSSE Requirements:

1. A self-consistent, realistic simulation of nature (ECMWF)

2. Simulation of all presentlyutilized observations, derived from the 'nature run'

3. A validated baseline assimilation with the simulated data that produces various relevant statistics similar to corresponding ones in the real DAS

See poster by Errico and Yang

References Cited in this Talk

- Baker, N. and Daley, R. 2000. Observation and background adjoint sensitivity in the adaptive observation-targeting problem. *Quart. J. R. Meteorol. Soc.* **126,** 1431–1454.
- Errico, R. M. 2007. Interpretation of an adjoint-derived observational impact measure. *Tellus* **59A**, 273–276.
- Gelaro, R. and Zhu Y. 2009. Examination of observation impacts derived from observing system experiments (OSEs) and adjoint models. *Tellus* **61A**, 179–193.
- Gelaro, R., Zhu,Y. and Errico, R.M. 2007. Examination of various-order adjoint-based approximations of observation impact. *Meteorologische Zeitschrift* **16**, 685–692.
- Langland, R. H. and Baker, N. 2004. Estimation of observation impact using the NRL atmospheric variational data assimilation adjoint system. *Tellus* **56A**, 189–201.
- Trémolet, Y. 2008. Computation of observation sensitivity and observation impact in incremental variational data assimilation. *Tellus* **60A**, 964–978.
- Trémolet, Y. 2007. First-order and higher-order approximations of observation impact. *Meteorologische Zeitschrift* **16**, 693–694.