Weak Constraint 4D-Var

Yannick Trémolet

ECMWF Training Course - Data Assimilation

March 14, 2014

Outline

1. Introduction
2. Theoretical Maximum Likelihood Formulation
3. Practical 4D Variational Data Assimilation
   - Model Error Forcing Control Variable
   - 4D State Control Variable
4. Covariance Matrix
5. Results
   - Constant Model Error Forcing
   - Systematic Model Error
   - Is it model error?
6. Towards a long assimilation window
7. Summary and Discussion

Outline

1. Introduction
2. Theoretical Maximum Likelihood Formulation
3. Practical 4D Variational Data Assimilation
   - Model Error Forcing Control Variable
   - 4D State Control Variable
4. Covariance Matrix
5. Results
   - Constant Model Error Forcing
   - Systematic Model Error
   - Is it model error?
6. Towards a long assimilation window
7. Summary and Discussion

4D Variational Data Assimilation

4D-Var comprises the minimisation of:

$$
\begin{aligned}
J(\mathbf{x}) &= \frac{1}{2}[\mathcal{H}(\mathbf{x})-\mathbf{y}]^T\mathbf{R}^{-1}[\mathcal{H}(\mathbf{x})-\mathbf{y}] \\
&+ \frac{1}{2}(\mathbf{x}_0-\mathbf{x}_b)^T\mathbf{B}^{-1}(\mathbf{x}_0-\mathbf{x}_b)+\frac{1}{2}\mathcal{F}(\mathbf{x})^T\mathbf{C}^{-1}\mathcal{F}(\mathbf{x})
\end{aligned}
$$

- $\mathbf{x}$ is the 4D state of the atmosphere over the assimilation window.
- $\mathcal{H}$ is a 4D observation operator, accounting for the time dimension.
- $\mathcal{F}$ represents the remaining theoretical knowledge after background information has been accounted for (balance, DFI...).
- Control variable reduces to $\mathbf{x}_0$ using the hypothesis: $\mathbf{x}_i = \mathcal{M}_i(\mathbf{x}_{i-1})$.
- The solution is a trajectory of the model $\mathcal{M}$ even though it is not perfect...

Weak Constraint 4D-Var

- A typical assumption in data assimilation is to ignore model error (bias and random).
- The perfect model assumption limits the length of the analysis window that can be used to roughly 12 hours.
- Model bias can affect assimilation of some observations (radiance data in the stratosphere).
- In weak constraint 4D-Var, we define the model error as

$$\eta_i = \mathbf{x}_i^t - \mathcal{M}_i(\mathbf{x}_{i-1}^t) \quad \text{for } i = 1, \ldots, n$$

  and we allow it to be non-zero.
- Note: $\mathbf{x}^t$ represents the true atmospheric state which is of course not known.

Outline

1. Introduction
2. Theoretical Maximum Likelihood Formulation
3. Practical 4D Variational Data Assimilation
   - Model Error Forcing Control Variable
   - 4D State Control Variable
4. Covariance Matrix
5. Results
   - Constant Model Error Forcing
   - Systematic Model Error
   - Is it model error?
6. Towards a long assimilation window
7. Summary and Discussion

Weak Constraint 4D-Var

- We can derive the weak constraint cost function using Bayes' rule:

$$p(\mathbf{x}_0 \cdots \mathbf{x}_n | \mathbf{x}_b; \mathbf{y}_0 \cdots \mathbf{y}_n) = \frac{p(\mathbf{x}_b; \mathbf{y}_0 \cdots \mathbf{y}_n | \mathbf{x}_0 \cdots \mathbf{x}_n) p(\mathbf{x}_0 \cdots \mathbf{x}_n)}{p(\mathbf{x}_b; \mathbf{y}_0 \cdots \mathbf{y}_n)}$$

- The denominator is independent of $\mathbf{x}_0 \cdots \mathbf{x}_n$.
- The term $p(\mathbf{x}_b; \mathbf{y}_0 \cdots \mathbf{y}_n | \mathbf{x}_0 \cdots \mathbf{x}_n)$ simplifies to:

$$p(\mathbf{x}_b | \mathbf{x}_0) \prod_{i=0}^{n} p(\mathbf{y}_i | \mathbf{x}_i)$$

- Hence

$$p(\mathbf{x}_0 \cdots \mathbf{x}_n | \mathbf{x}_b; \mathbf{y}_0 \cdots \mathbf{y}_n) \propto p(\mathbf{x}_b | \mathbf{x}_0) \left[\prod_{i=0}^{n} p(\mathbf{y}_i | \mathbf{x}_i) \right] p(\mathbf{x}_0 \cdots \mathbf{x}_n)$$

Weak Constraint 4D-Var

$$p(\mathbf{x}_0 \cdots \mathbf{x}_n | \mathbf{x}_b; \mathbf{y}_0 \cdots \mathbf{y}_n) \propto p(\mathbf{x}_b | \mathbf{x}_0) \left[\prod_{i=0}^{n} p(\mathbf{y}_i | \mathbf{x}_i) \right] p(\mathbf{x}_0 \cdots \mathbf{x}_n)$$

- Taking minus the logarithm gives the cost function:

$$J(\mathbf{x}_0 \cdots \mathbf{x}_n) = -\log p(\mathbf{x}_b | \mathbf{x}_0) - \sum_{i=0}^{n} \log p(\mathbf{y}_i | \mathbf{x}_i) - \log p(\mathbf{x}_0 \cdots \mathbf{x}_n)$$

- The terms involving $\mathbf{x}_b$ and $\mathbf{y}_i$ are the background and observation terms of the strong constraint cost function.
- The final term is new. It represents the *a priori* probability of the sequence of states $\mathbf{x}_0 \cdots \mathbf{x}_n$.

Weak Constraint 4D-Var

- Given the sequence of states $\mathbf{x}_0 \cdots \mathbf{x}_n$, we can calculate the corresponding model errors:

$$\eta_i = \mathbf{x}_i - \mathcal{M}_i(\mathbf{x}_{i-1}) \text{ for } i = 1, \ldots, n$$

- We can use our knowledge of the statistics of model error to define

$$p(\mathbf{x}_0 \cdots \mathbf{x}_n) \equiv p(\mathbf{x}_0; \eta_1 \cdots \eta_n)$$

- One possibility is to assume that model error is uncorrelated in time. In this case:

$$p(\mathbf{x}_0 \cdots \mathbf{x}_n) \equiv p(\mathbf{x}_0)p(\eta_1) \cdots p(\eta_n)$$

- If we take $p(\mathbf{x}_0) = const.$ (all states equally likely), and $p(\eta_i)$ as Gaussian with covariance matrix $\mathbf{Q}_i$, weak constraint 4D-Var adds the following term to the cost function:

$$\frac{1}{2} \sum_{i=1}^{n} \eta_i^T \mathbf{Q}_i^{-1} \eta_i$$

Weak Constraint 4D-Var

- For Gaussian, temporally-uncorrelated model error, the weak constraint 4D-Var cost function is:

$$
\begin{aligned}
J(\mathbf{x}) &= \frac{1}{2}(\mathbf{x}_0 - \mathbf{x}_b)^T \mathbf{B}^{-1}(\mathbf{x}_0 - \mathbf{x}_b) \\
&+ \frac{1}{2}\sum_{i=0}^{n}[\mathcal{H}_i(\mathbf{x}_i) - \mathbf{y}_i]^T \mathbf{R}_i^{-1}[\mathcal{H}_i(\mathbf{x}_i) - \mathbf{y}_i] \\
&+ \frac{1}{2}\sum_{i=1}^{n}[\mathbf{x}_i - \mathcal{M}_i(\mathbf{x}_{i-1})]^T \mathbf{Q}_i^{-1}[\mathbf{x}_i - \mathcal{M}_i(\mathbf{x}_{i-1})]
\end{aligned}
$$

- Do not reduce the control variable using the model and retain the 4D nature of the control variable.
- Account for the fact that the model contains some information but is not exact by adding a model error term to the cost function.
- The model $\mathcal{M}$ is not verified exactly: it is a weak constraint.
- If model error is correlated in time, the model error term contains additional cross-correlation blocks.

Outline

1. Introduction
2. Theoretical Maximum Likelihood Formulation
3. Practical 4D Variational Data Assimilation
   - Model Error Forcing Control Variable
   - 4D State Control Variable
4. Covariance Matrix
5. Results
   - Constant Model Error Forcing
   - Systematic Model Error
   - Is it model error?
6. Towards a long assimilation window
7. Summary and Discussion

Outline

1. Introduction
2. Theoretical Maximum Likelihood Formulation
3. Practical 4D Variational Data Assimilation
   - Model Error Forcing Control Variable
   - 4D State Control Variable
4. Covariance Matrix
5. Results
   - Constant Model Error Forcing
   - Systematic Model Error
   - Is it model error?
6. Towards a long assimilation window
7. Summary and Discussion

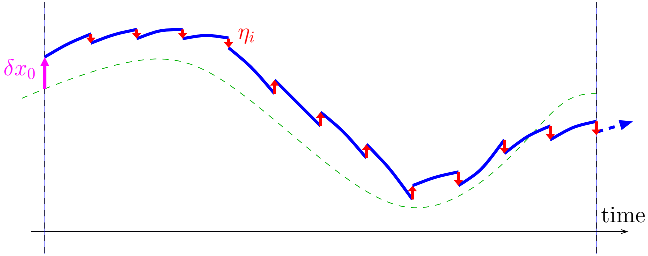
4D-Var with Model Error Forcing

$$
\begin{aligned}
J(\mathbf{x}_0, \eta) &= \frac{1}{2}\sum_{i=0}^{n}[\mathcal{H}(\mathbf{x}_i) - \mathbf{y}_i]^T \mathbf{R}_i^{-1}[\mathcal{H}(\mathbf{x}_i) - \mathbf{y}_i] \\
&+ \frac{1}{2}(\mathbf{x}_0 - \mathbf{x}_b)^T \mathbf{B}^{-1}(\mathbf{x}_0 - \mathbf{x}_b) + \frac{1}{2}\eta^T \mathbf{Q}^{-1}\eta
\end{aligned}
$$

$$
\text{with } \mathbf{x}_i = \mathcal{M}_i(\mathbf{x}_{i-1}) + \eta_i .
$$

- η_i has the dimension of a 3D state,
- η_i represents the instantaneous model error,
- η_i is propagated by the model.
- All results shown later are for constant forcing over the length of one assimilation window, i.e. for correlated model error.

4D-Var with Model Error Forcing



- TL and AD models can be used with little modification,
- Information is propagated between observations and initial condition control variable by TL and AD models.

Outline

1 Introduction

2 Theoretical Maximum Likelihood Formulation

3 Practical 4D Variational Data Assimilation
- Model Error Forcing Control Variable
- 4D State Control Variable

4 Covariance Matrix

5 Results
- Constant Model Error Forcing
- Systematic Model Error
- Is it model error?

6 Towards a long assimilation window

7 Summary and Discussion

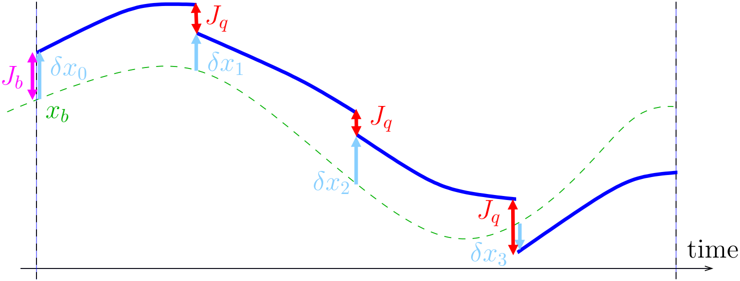
4D State Control Variable

- Use $\mathbf{x} = \{\mathbf{x}_i\}_{i=0,\ldots,n}$ as the control variable.
- Nonlinear cost function:

$$
\begin{aligned}
J(\mathbf{x}) &= \frac{1}{2}(\mathbf{x}_0 - \mathbf{x}_b)^T \mathbf{B}^{-1}(\mathbf{x}_0 - \mathbf{x}_b) \\
&+ \frac{1}{2}\sum_{i=0}^{n}[\mathcal{H}(\mathbf{x}_i) - \mathbf{y}_i]^T \mathbf{R}_i^{-1}[\mathcal{H}(\mathbf{x}_i) - \mathbf{y}_i] \\
&+ \frac{1}{2}\sum_{i=1}^{n}[\mathcal{M}(\mathbf{x}_{i-1}) - \mathbf{x}_i]^T \mathbf{Q}_i^{-1}[\mathcal{M}(\mathbf{x}_{i-1}) - \mathbf{x}_i]
\end{aligned}
$$

- In principle, the model is not needed to compute the J_o term.
- In practice, the control variable will be defined at regular intervals in the assimilation window and the model used to fill the gaps.

4D State Control Variable



- Model integrations within each time-step (or sub-window) are independent:
  - Information is not propagated across sub-windows by TL/AD models,
  - Natural parallel implementation.
- Tangent linear and adjoint models:
  - Can be used without modification,
  - Propagate information between observations and control variable within each sub-window.
- Several 4D-Var cycles are coupled and optimised together.

Outline

1. Introduction
2. Theoretical Maximum Likelihood Formulation
3. Practical 4D Variational Data Assimilation
   - Model Error Forcing Control Variable
   - 4D State Control Variable
4. Covariance Matrix
5. Results
   - Constant Model Error Forcing
   - Systematic Model Error
   - Is it model error?
6. Towards a long assimilation window
7. Summary and Discussion

Model Error Covariance Matrix

- An easy choice is $\mathbf{Q} = \alpha\mathbf{B}$.
- If $\mathbf{Q}$ and $\mathbf{B}$ are proportional, $\delta\mathbf{x}_0$ and η are constrained in the same directions, may be with different relative amplitudes.
- They both predominantly retrieve the same information.

- $\mathbf{B}$ can be estimated from an ensemble of 4D-Var assimilations.
- Considering the forecasts run from the 4D-Var members:
  - At a given step, each model state is supposed to represent the same *true* atmospheric state,
  - The tendencies from each of these model states should represent possible evolutions of the atmosphere from that same *true* atmospheric state,
  - The differences between these tendencies can be interpreted as possible uncertainties in the model or realisations of *model error*.
- $\mathbf{Q}$ can be estimated by applying the statistical model used for $\mathbf{B}$ to tendencies instead of analysis increments.
- $\mathbf{Q}$ has narrower correlations and smaller amplitudes than $\mathbf{B}$.

Model Error Covariance Matrix

- Most of the techniques developped to model **B** can be re-used to model **Q** (spectral technique, wavelets, filtering...).
- Obtaining samples of model error is much more difficult:
  - Currently, tendency differences between integrations of the members of an ensemble are used as a proxy for samples of model error.
  - Use results from stochastic representation of uncertainties in EPS.
  - Compare the covariances of η produced by the current system with the matrix **Q** being used.
- It is possible to derive an estimate of $\mathbf{HQH}^T$ from cross-covariances between observation departures produced from pairs of analyses with different length windows (R. Todling).
  - This produces a projection of **Q** on a fixed observing network, not in the full matrix.
- Characterising the statistical properties of model error is one of the main current problems in data assimilation and ensemble forecasting.

Outline

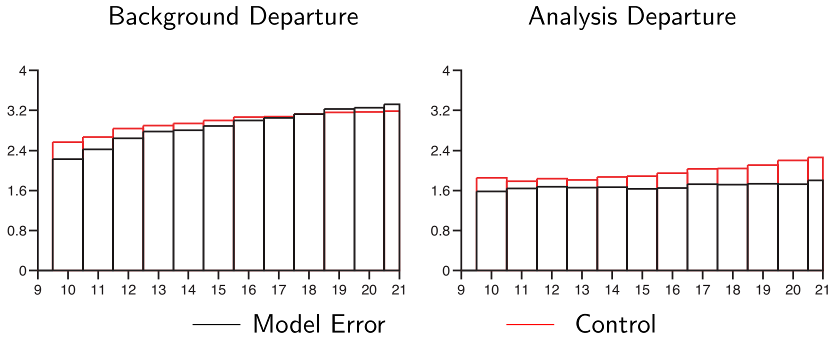
1. Introduction
2. Theoretical Maximum Likelihood Formulation
3. Practical 4D Variational Data Assimilation
   - Model Error Forcing Control Variable
   - 4D State Control Variable
4. Covariance Matrix
5. Results
   - Constant Model Error Forcing
   - Systematic Model Error
   - Is it model error?
6. Towards a long assimilation window
7. Summary and Discussion

Outline

1. Introduction
2. Theoretical Maximum Likelihood Formulation
3. Practical 4D Variational Data Assimilation
   - Model Error Forcing Control Variable
   - 4D State Control Variable
4. Covariance Matrix
5. Results
   - Constant Model Error Forcing
   - Systematic Model Error
   - Is it model error?
6. Towards a long assimilation window
7. Summary and Discussion

Results: Fit to observations

AMprofiler-windspeed Std Dev N.Amer

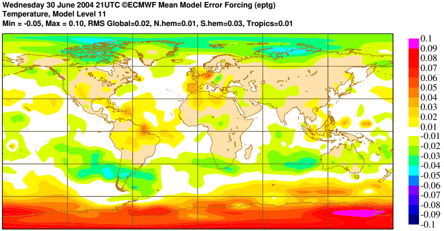


- Fit to observations is more uniform over the assimilation window.
- Background fit improved only at the start: error varies in time ?

Mean Model Error Forcing

Temperature
Model level 11 ($\approx$5hPa)
July 2004

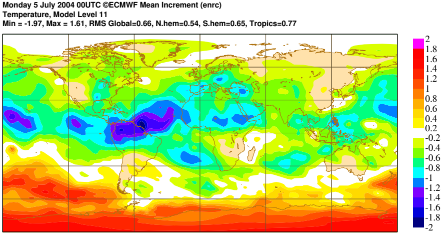
Mean M.E. Forcing $\longrightarrow$

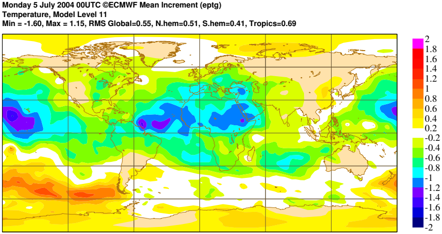


M.E. Mean Increment $\searrow$

Control Mean Increment

$\downarrow$





Outline

1. Introduction
2. Theoretical Maximum Likelihood Formulation
3. Practical 4D Variational Data Assimilation
   - Model Error Forcing Control Variable
   - 4D State Control Variable
4. Covariance Matrix
5. Results
   - Constant Model Error Forcing
   - Systematic Model Error
   - Is it model error?
6. Towards a long assimilation window
7. Summary and Discussion

Weak Constraint 4D-Var with Cycling Term

- Model error is not only random: there are biases.
- For random model error, the 4D-Var cost function is:

$$\begin{aligned} J(\mathbf{x}_0, \eta) &= \frac{1}{2}\sum_{i=0}^{n}[\mathcal{H}(\mathbf{x}_i) - \mathbf{y}_i]^T \mathbf{R}_i^{-1}[\mathcal{H}(\mathbf{x}_i) - \mathbf{y}_i] \\ &+ \frac{1}{2}(\mathbf{x}_0 - \mathbf{x}_b)^T \mathbf{B}^{-1}(\mathbf{x}_0 - \mathbf{x}_b) + \frac{1}{2}\eta^T \mathbf{Q}^{-1}\eta \end{aligned}$$

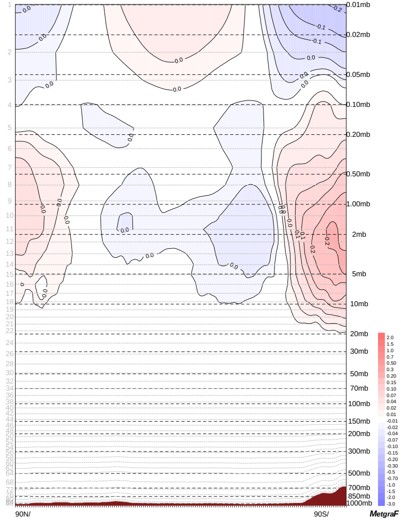
- For systematic model error, we might consider:

$$\begin{aligned} J(\mathbf{x}_0, \eta) &= \frac{1}{2}\sum_{i=0}^{n}[\mathcal{H}(\mathbf{x}_i) - \mathbf{y}_i]^T \mathbf{R}_i^{-1}[\mathcal{H}(\mathbf{x}_i) - \mathbf{y}_i] \\ &+ \frac{1}{2}(\mathbf{x}_0 - \mathbf{x}_b)^T \mathbf{B}^{-1}(\mathbf{x}_0 - \mathbf{x}_b) + \frac{1}{2}(\eta - \eta_b)^T \mathbf{Q}^{-1}(\eta - \eta_b) \end{aligned}$$

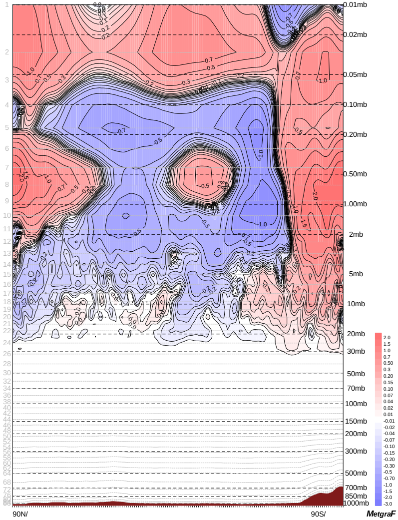
- Test case: can we address the model bias in the stratosphere?

Weak Constraint 4D-Var with Cycling Term

No Cycling Term



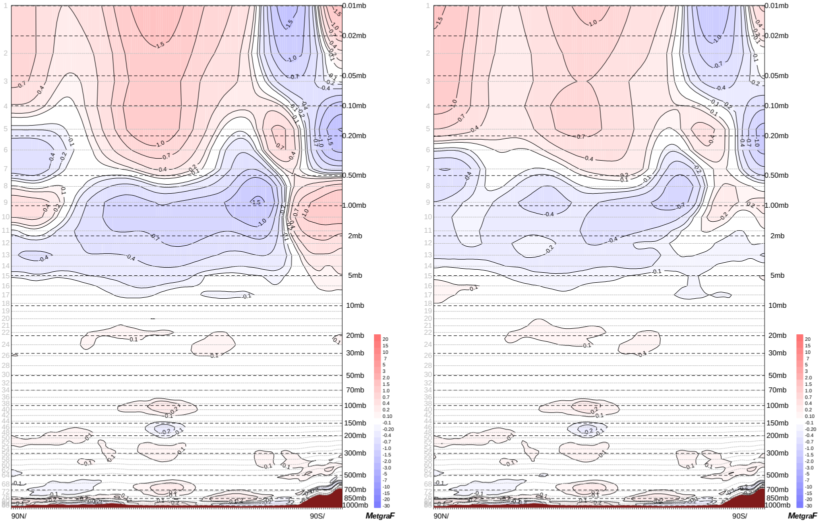
With Cycling Term



Monthly Mean Model Error (Temperature (K/12h), July 2008)

Weak Constraint 4D-Var with Cycling Term

No Cycling Term | With Cycling Term

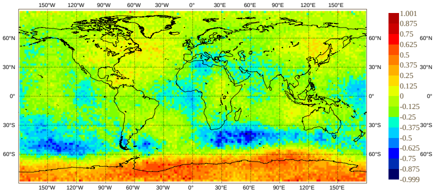


Monthly Mean Analysis Increment (Temperature (K), July 2008)

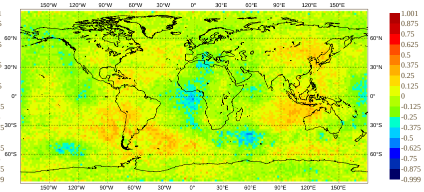
Weak Constraint 4D-Var with Cycling Term

AMSU-A Background departures, Channels 13 and 14

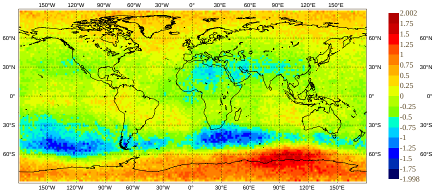
RADIANCES FROM METOP / AMSU-A CHANNEL 13
MEAN FIRST GUESS DEPARTURE (OBS-FG) (USED)
DATA PERIOD = 2008070100 - 2008073112
EXP = f57z
Min: -0.883688 Max: 0.90642 Mean: -0.084109



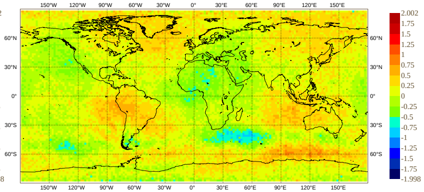
RADIANCES FROM METOP / AMSU-A CHANNEL 13
MEAN FIRST GUESS DEPARTURE (OBS-FG) (USED)
DATA PERIOD = 2008070100 - 2008073112
EXP = f8j2
Min: -0.592767 Max: 0.48862 Mean: -0.026685



RADIANCES FROM METOP / AMSU-A CHANNEL 14
MEAN FIRST GUESS DEPARTURE (OBS-FG) (USED)
DATA PERIOD = 2008070100 - 2008073112
EXP = f57z
Min: -1.6020 Max: 1.7330 Mean: 0.016017



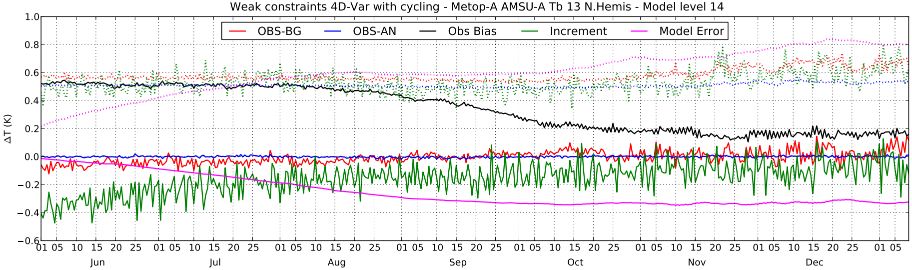
RADIANCES FROM METOP / AMSU-A CHANNEL 14
MEAN FIRST GUESS DEPARTURE (OBS-FG) (USED)
DATA PERIOD = 2008070100 - 2008073112
EXP = f8j2
Min: -1.0986 Max: 0.973196 Mean: 0.099372

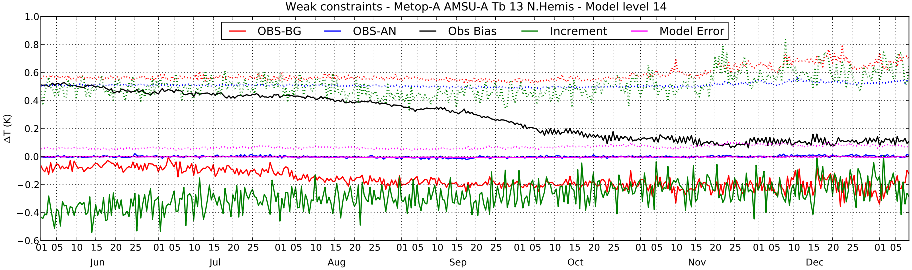


Control

Model Error

Weak Constraint 4D-Var with Cycling Term



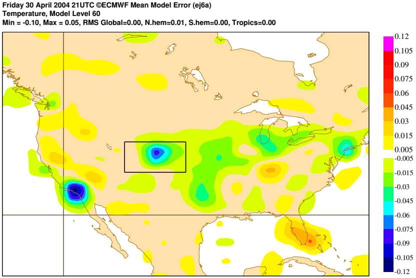


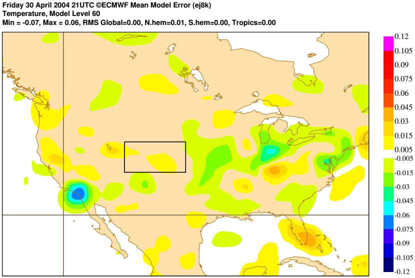
The short term forecast is improved with the model error cycling.
Weak constraint 4D-Var can correct for seasonal bias (partially).

Outline

1. Introduction
2. Theoretical Maximum Likelihood Formulation
3. Practical 4D Variational Data Assimilation
   - Model Error Forcing Control Variable
   - 4D State Control Variable
4. Covariance Matrix
5. Results
   - Constant Model Error Forcing
   - Systematic Model Error
   - Is it model error?
6. Towards a long assimilation window
7. Summary and Discussion

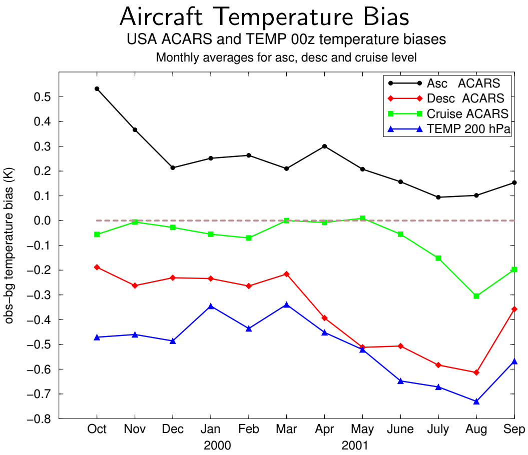
Model Error or Observation Error?





- The only significant source of observations in the box is aircraft data (Denver airport).
- Removing aircraft data in the box eliminates the spurious forcing.

Model Error or Observation Error?

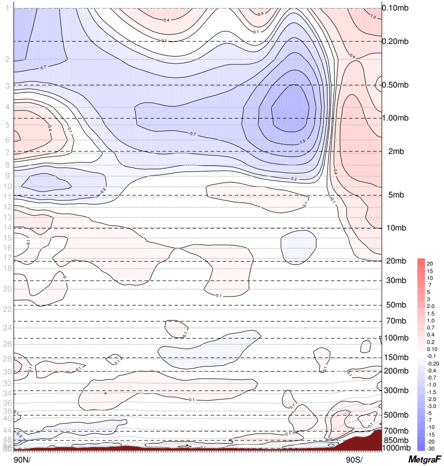


Observations are biased.

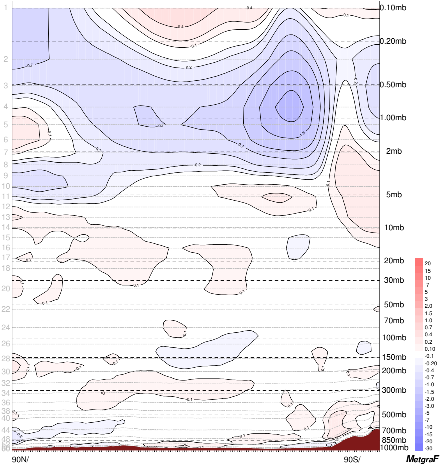
Figure from Lars Isaksen

Is it model error?

Strong Constraint



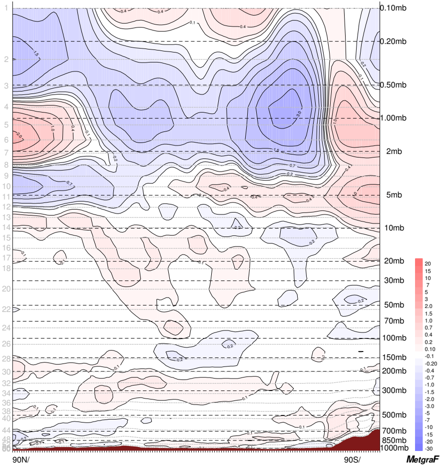
Weak Constraint



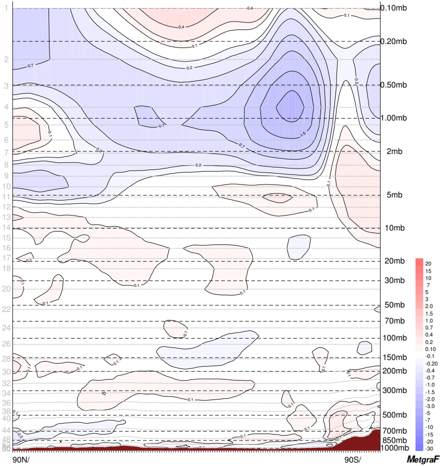
The mean temperature increment is smaller with weak constraint 4D-Var (Stratosphere only, June 1993).

Is it model error?

ERA interim

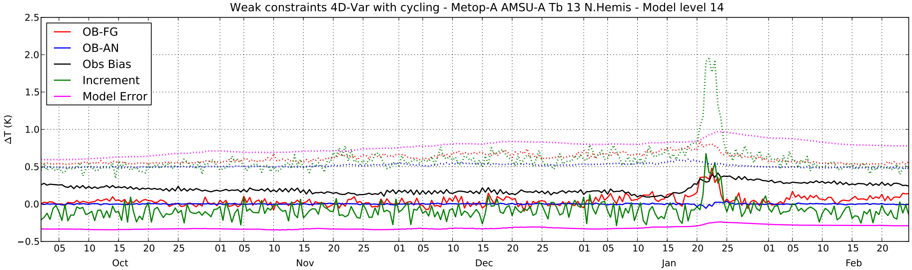


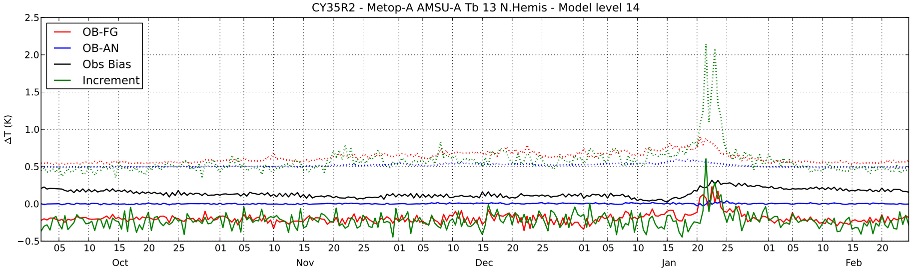
Weak Constraint



The work on model error has helped identify other sources of error in the system (balance term).

Observation Error or Model Error?





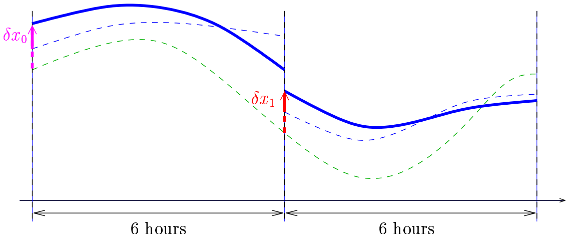
Observation error bias correction can compensate for model error.

Outline

1. Introduction
2. Theoretical Maximum Likelihood Formulation
3. Practical 4D Variational Data Assimilation
   - Model Error Forcing Control Variable
   - 4D State Control Variable
4. Covariance Matrix
5. Results
   - Constant Model Error Forcing
   - Systematic Model Error
   - Is it model error?
6. Towards a long assimilation window
7. Summary and Discussion

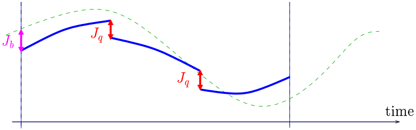
Weak Constraint 4D-Var Configurations

- 6-hour sub-windows:



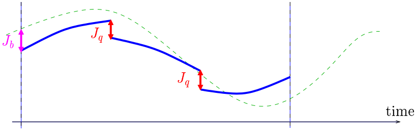
  - Better than 6-hour 4D-Var: two cycles are coupled through J_q,
  - Better than 12-hour 4D-Var: more information (imperfect model), more control.
- Single time-step sub-windows:
  - Each assimilation problem is instantaneous = 3D-Var,
  - Equivalent to a string of 3D-Var problems coupled together and solved as a single minimisation problem,
  - Approximation can be extended to non instantaneous sub-windows.

Weak Constraint 4D-Var: Sliding Window

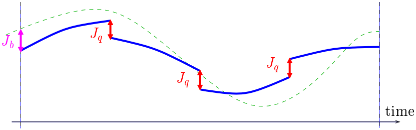


(1) Weak constraint 4D-Var

Weak Constraint 4D-Var: Sliding Window

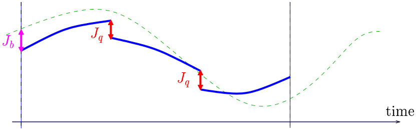


(1) Weak constraint 4D-Var

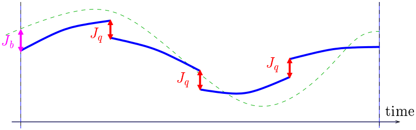


(2) Extended window

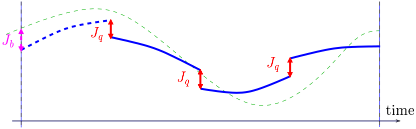
Weak Constraint 4D-Var: Sliding Window



(1) Weak constraint 4D-Var

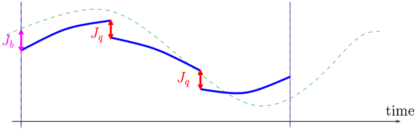


(2) Extended window

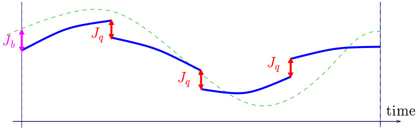


(3) Initial term has converged

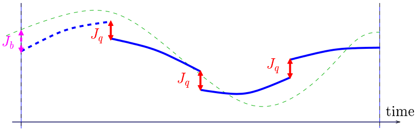
Weak Constraint 4D-Var: Sliding Window



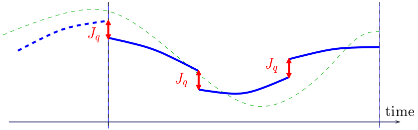
(1) Weak constraint 4D-Var



(2) Extended window

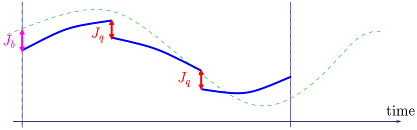


(3) Initial term has converged

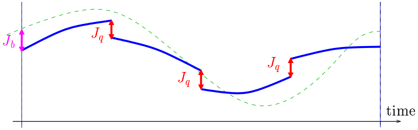


(4) Assimilation window is moved forward

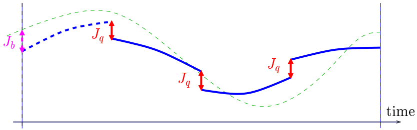
Weak Constraint 4D-Var: Sliding Window



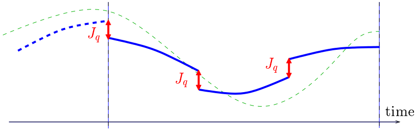
(1) Weak constraint 4D-Var



(2) Extended window



(3) Initial term has converged



(4) Assimilation window is moved forward

- This implementation is an approximation of weak contraint 4D-Var with an assimilation window that extends indefinitely in the past...
- ...which is equivalent to a Kalman smoother that has been running indefinitely.

Outline

1. Introduction
2. Theoretical Maximum Likelihood Formulation
3. Practical 4D Variational Data Assimilation
   - Model Error Forcing Control Variable
   - 4D State Control Variable
4. Covariance Matrix
5. Results
   - Constant Model Error Forcing
   - Systematic Model Error
   - Is it model error?
6. Towards a long assimilation window
7. Summary and Discussion

Weak Constraint 4D-Var: Summary and Questions

- In the forcing formulation of weak constraint 4D-Var:
  - Background term to address systematic error,
  - Interactions with variational observation bias correction,
  - 24h assimilation window,
  - Extend model error to the troposphere and to other variables (humidity).
- Weak constraint 4D-Var with a 4D state control variable:
  - Four dimensional problem with a coupling term between sub-windows and can be interpreted as a smoother over assimilation cycles.
  - Can we extend the incremental formulation?
- The two weak constraint 4D-Var approaches are mathematically equivalent (for linear problems) but lead to very different minimization problems.
  - Can we combine the benefits of treating sub-windows in parallel with efficient minimization?
  - 4D-Var scales well up to 1,000s of processors, can it scale to 100,000s of processors in the future?

Weak Constraint 4D-Var: Open Questions

- Weak Constraint 4D-Var allows the perfect model assumption to be removed and the use of longer assimilation windows.
  - How much benefit can we expect from long window 4D-Var?
- Weak Constraint 4D-Var requires knowledge of the statistical properties of model error (covariance matrix).
  - The forecast model is such an important component of the data assimilation system. It is surprising how little we know about its error characteristics.
  - How can we access realistic samples of model error? How can observations be used?
  - 4D-Var can handle time-correlated model error. What type of correlation model should be used?
  - Can we distinguish model error from observation bias or other errors? Is there a need to anchor the system?
- The statistical description of model error is one of the main current challenges in data assimilation.