Weak Constraints 4D-Var for the Stratosphere

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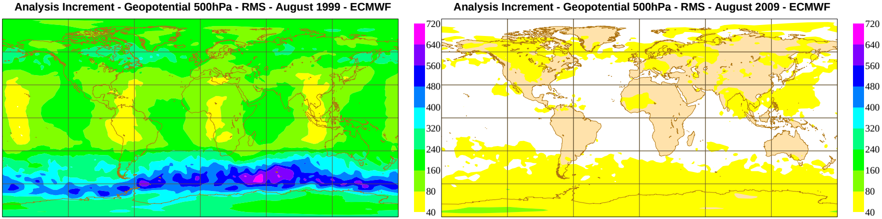
Errors in 4D-Var

$$J(\mathbf{x}) = \frac{1}{2}[\mathcal{H}(\mathbf{x}) - \mathbf{y}]^T \mathbf{R}^{-1}[\mathcal{H}(\mathbf{x}) - \mathbf{y}] + \frac{1}{2}(\mathbf{x}_0 - \mathbf{x}_b)^T \mathbf{B}^{-1}(\mathbf{x}_0 - \mathbf{x}_b) + J_c + \ldots$$



The 4D-Var analysis increments today are one order of magnitude smaller than they were 10 years ago.

Outline

Outline

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

- 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.

4D-Var with Model Error Forcing

- We define the model error as:

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

- The cost function becomes:

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

- η_i has the dimension of a 3D state,
- η_i represents the instantaneous model error,
- η_i is propagated by the model: $\mathbf{x}_i = \mathcal{M}_i(\mathbf{x}_{i-1}) + \eta_i$.
- All results shown later are for constant forcing over the length of one assimilation window, i.e. for correlated model error.

Outline

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.

- **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*.
- **Q** can be estimated by applying the statistical model used for **B** to tendencies instead of analysis increments.
- **Q** has narrower correlations and smaller amplitudes than **B**.

Model Error Covariance Matrix

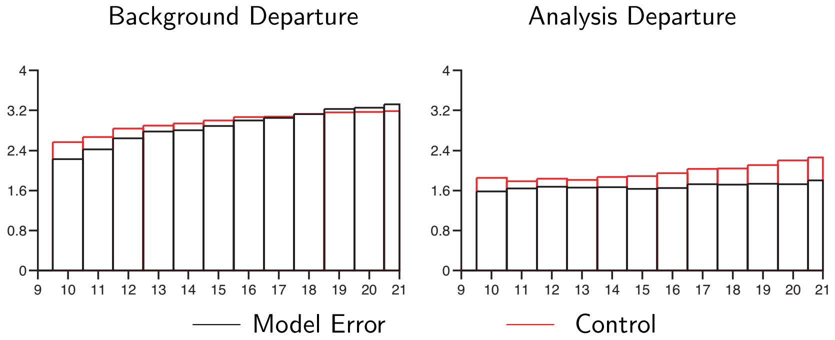
- Currently, tendency differences between integrations of the members of an ensemble are used as a proxy for samples of model error.
- Use results from stochastic representation of uncertainties in EPS.
- Compare the covariances of η produced by the current system with the matrix $\mathbf{Q}$ being used.
- 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).
- Is it possible to extract model error information using the relation $\mathbf{P}^f = \mathbf{MP}^a\mathbf{M}^T + \mathbf{Q}$?
- Model error is correlated in time: $\mathbf{Q}$ should account for time correlations.
- Can model drift (5-10 days) give information about systematic model error?

Outline

Outline

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

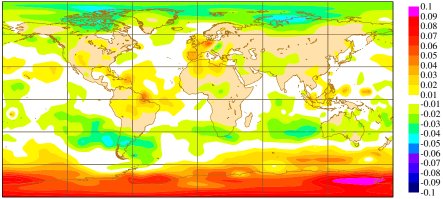
Temperature
Model level 11 (≈5hPa)
July 2004

Mean M.E. Forcing ⟶

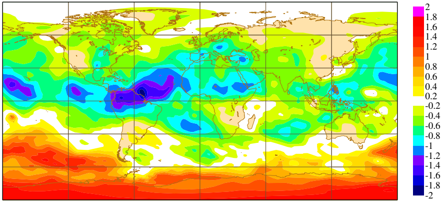
M.E. Mean Increment ↘

Control Mean Increment ↓

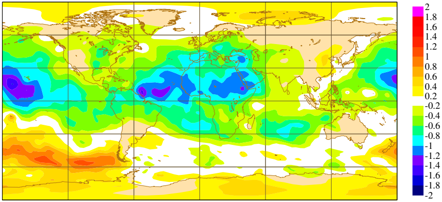
Wednesday 30 June 2004 21UTC ©ECMWF Mean Model Error Forcing (eptg)
Temperature, Model Level 11
Min = -0.05, Max = 0.10, RMS Global=0.02, N.hem=0.01, S.hem=0.03, Tropics=0.01



Monday 5 July 2004 00UTC ©ECMWF Mean Increment (enrc)
Temperature, Model Level 11
Min = -1.97, Max = 1.61, RMS Global=0.66, N.hem=0.54, S.hem=0.65, Tropics=0.77



Monday 5 July 2004 00UTC ©ECMWF Mean Increment (eptg)
Temperature, Model Level 11
Min = -1.60, Max = 1.15, RMS Global=0.55, N.hem=0.51, S.hem=0.41, Tropics=0.69



Outline

Weak Constraints 4D-Var with Cycling Term

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

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

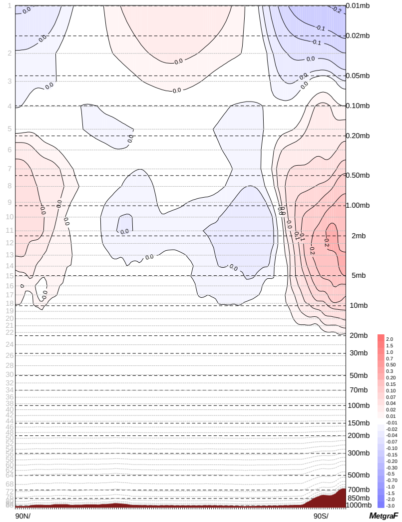
- For systematic model error, we might consider:

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

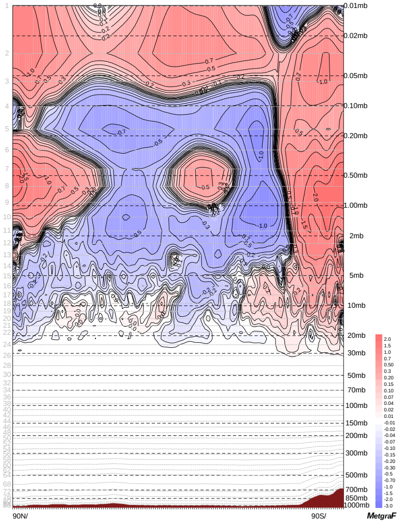
- Test case: can we address the model bias in the stratosphere?

Weak Constraints 4D-Var with Cycling Term

No Cycling Term



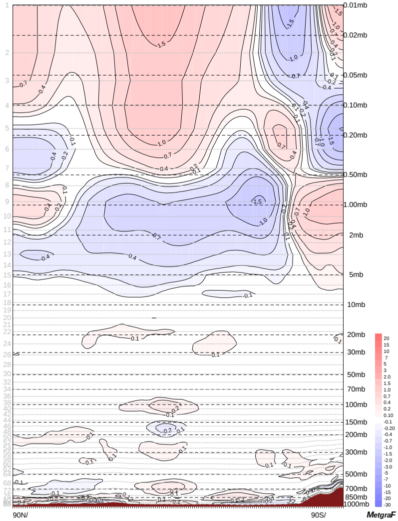
With Cycling Term



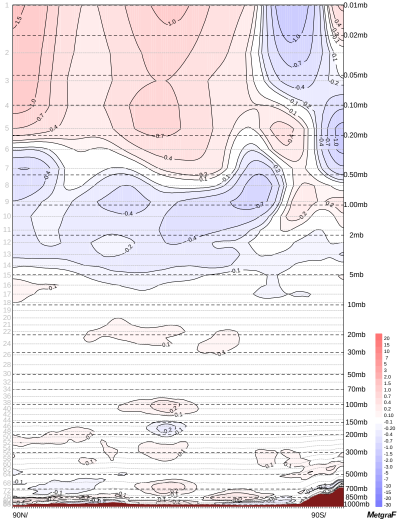
Monthly Mean Model Error (Temperature (K/12h), July 2008)

Weak Constraints 4D-Var with Cycling Term

No Cycling Term



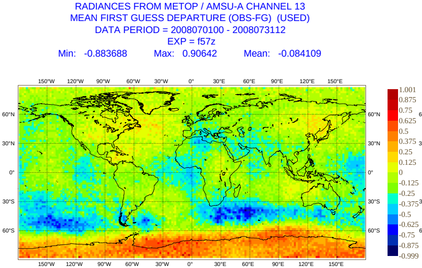
With Cycling Term

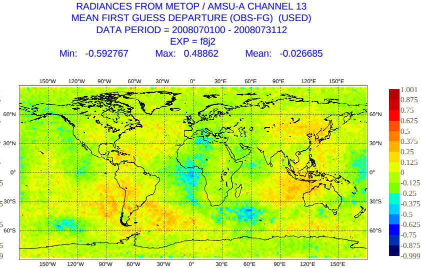


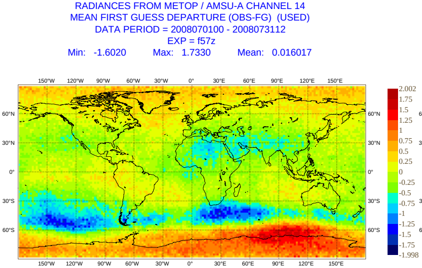
Monthly Mean Analysis Increment (Temperature (K), July 2008)

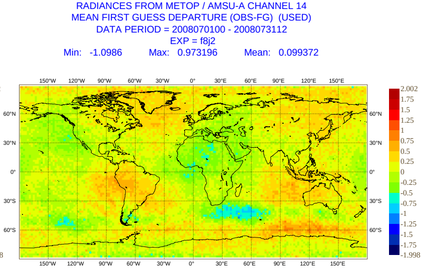
Weak Constraints 4D-Var with Cycling Term

AMSU-A Background departures, Channels 13 and 14









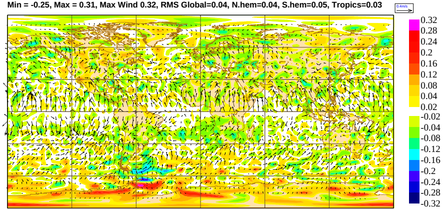
Control

Model Error

Weak Constraints 4D-Var with Cycling Term

Monthly Means
Model level 14 (≈5hPa)
July 2008

Mean Model Error (f8j2), 2008070100-2008073112
Temperature, Model Level 14
Min = -0.25, Max = 0.31, Max Wind 0.32, RMS Global=0.04, N.hem=0.04, S.hem=0.05, Tropics=0.03

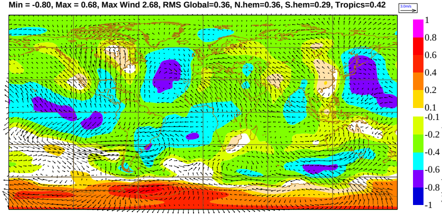


Model Error ⟶

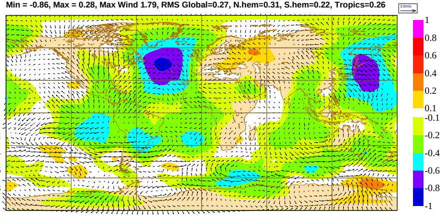
Analysis Increment with M.E. ↘

Increment without Model Error
↓

Mean Increment, CY35R2 Control (f5qs), 2008070100-2008073112
Temperature, Model Level 14
Min = -0.80, Max = 0.68, Max Wind 2.68, RMS Global=0.36, N.hem=0.36, S.hem=0.29, Tropics=0.42

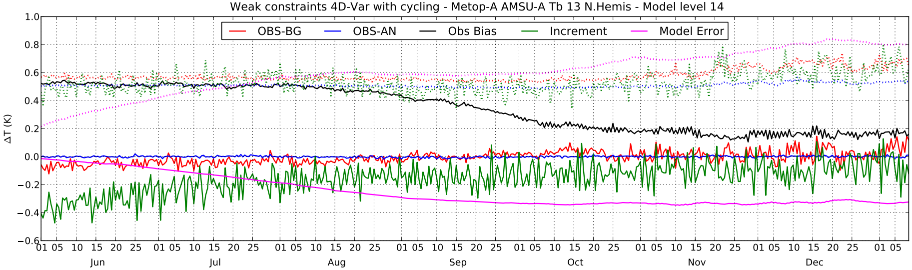


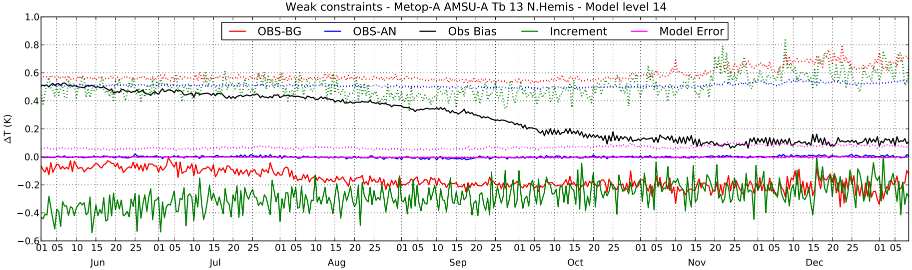
Weak Constraints 4D-Var Mean Increment (f8j2), 2008070100-2008073112
Temperature, Model Level 14
Min = -0.86, Max = 0.28, Max Wind 1.79, RMS Global=0.27, N.hem=0.31, S.hem=0.22, Tropics=0.26



The analysis increment is reduced in most areas.

Weak Constraints 4D-Var with Cycling Term

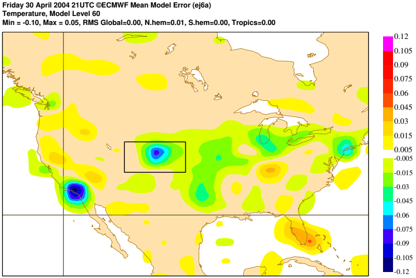


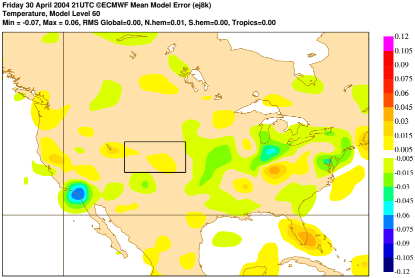


The short term forecast is improved with the model error cycling.
Weak constraints 4D-Var can correct for seasonal bias (partially).

Outline

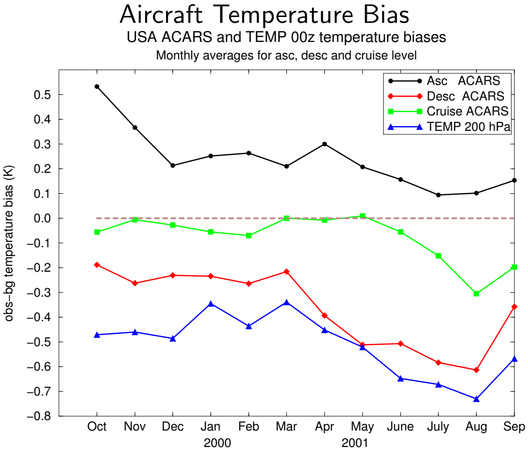
Model Error or Observation Error?





- 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?

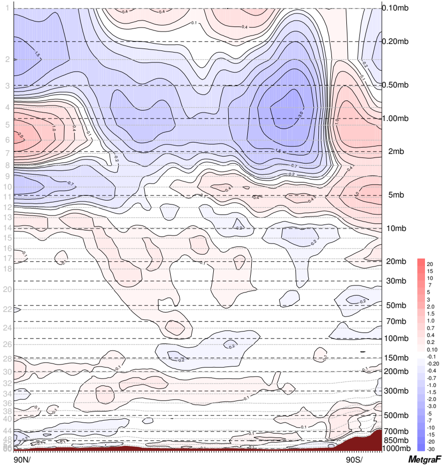


Observations are biased.

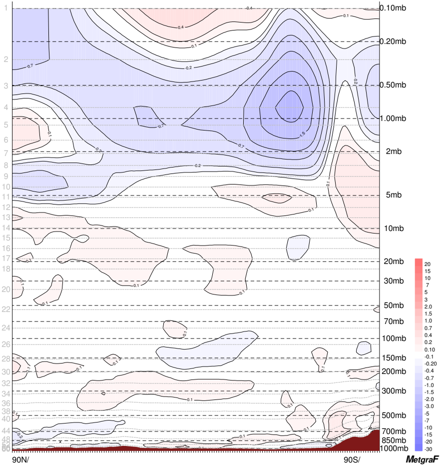
Figure from Lars Isaksen.

Is it model error?

ERA interim



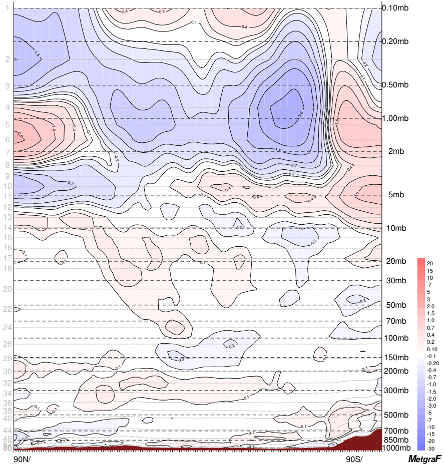
Weak Constraint



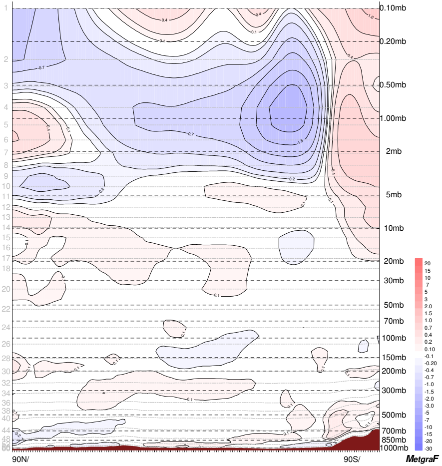
Monthly Mean Analysis Increment (Temperature, June 1993)

Impact of Balance Operators

ERA interim



Without Balance Operators



Monthly Mean Analysis Increment (Temperature, June 1993)

Forecast scores and fit to observations are unchanged.

Background Errors

- In the troposphere, 4D-Var seems insensitive to the balance operators.
  - 4D-Var is able to extract balance information from the observations: for a sufficiently well observed system, a solution that includes significant amplitudes of gravity waves is not compatible with the observations.
  - This ability depends on having a sufficiently well observed system. In the current system, with 10×10^6 observations over 12 hours, balance is largely observed.
  - Today's analysis increment are very small. Even if unbalanced, they add little to the model's natural level of gravity wave noise.

- In the stratosphere:
  - The regression found a strong correlation between temperature and divergence.
  - The regression coefficients are very noisy.
  - This may reflect the true nature of background errors in the stratosphere or a shortcoming in the way the analysis ensemble was generated.
  - It can be improved (restart cycling of statistics, wavelet formulation).

- Balance is important. 4D-Var can, in part, extract it from observations.

Observation Error or Model Error?

Observation error bias correction can compensate for model error.

Outline

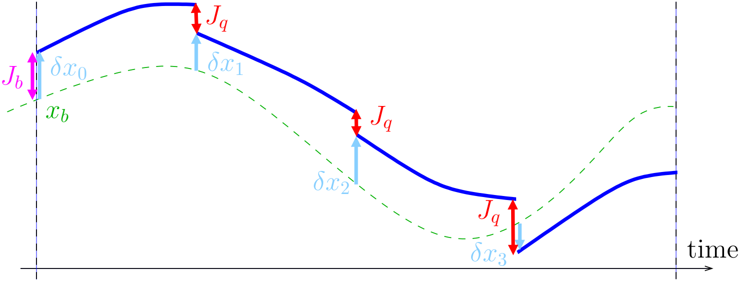
4D State Control Variable

- Use $\mathbf{x} = \{\mathbf{x}_i\}_{i=0,\dots,n}$ as the control variable.

- The nonlinear cost function is:

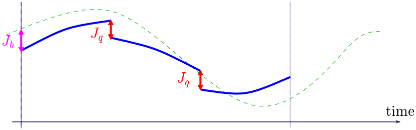
$$
\begin{aligned}
J(\mathbf{x}) &= \frac{1}{2}(\mathbf{x}_0 - \mathbf{x}_b)^T \mathbf{B}^{-1}(\mathbf{x}_0 - \mathbf{x}_b) \\
&+ \frac{1}{2}\sum_{i=0}^{n}[\mathcal{H}(\mathbf{x}_i) - \mathbf{y}_i]^T \mathbf{R}_i^{-1}[\mathcal{H}(\mathbf{x}_i) - \mathbf{y}_i] \\
&+ \frac{1}{2}\sum_{i=1}^{n}[\mathcal{M}(\mathbf{x}_{i-1})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

4D State Control Variable



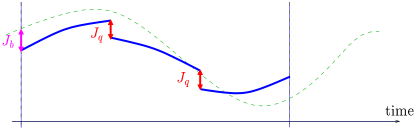
- Model integrations within each time-step (or sub-window) are independent:
  - Information is not propagated across sub-windows by TL/AD models,
  - Natural parallel implementation.
- Tangent linear and adjoint models:
  - Can be used without modification,
  - Propagate information between observations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

Weak Constraint 4D-Var: Sliding Window

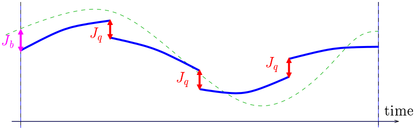


(1) Weak constraint 4D-Var

Weak Constraint 4D-Var: Sliding Window

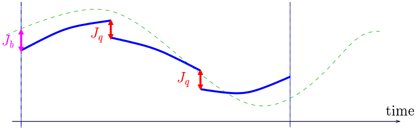


(1) Weak constraint 4D-Var

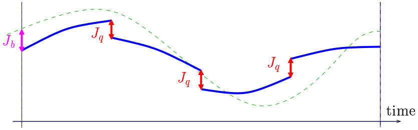


(2) Extended window

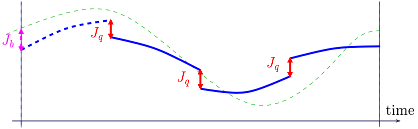
Weak Constraint 4D-Var: Sliding Window



(1) Weak constraint 4D-Var

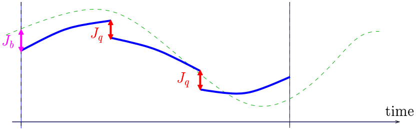


(2) Extended window

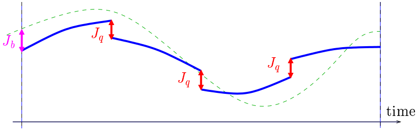


(3) Initial term has converged

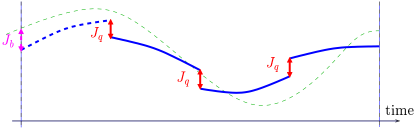
Weak Constraint 4D-Var: Sliding Window



(1) Weak constraint 4D-Var



(2) Extended window



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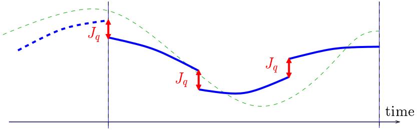
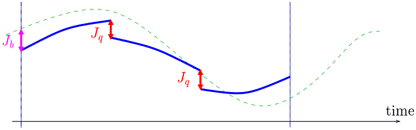
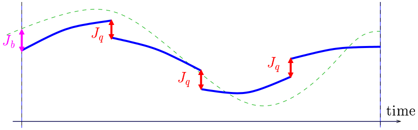


(4) Assimilation window is moved forward

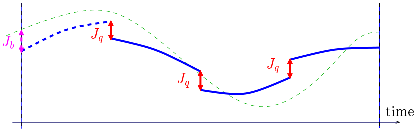
Weak Constraint 4D-Var: Sliding Window



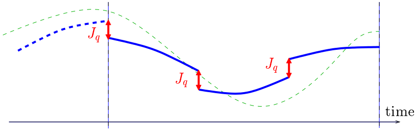
(1) Weak constraint 4D-Var



(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.

4D State Control Variable: Questions

- Condition number:
  - The maximum eigenvalue of the minimisation problem is approximately the same as the strong constraint 4D-Var problems for the sub-windows.
  - The smallest eigenvalue is roughly in $1/n^2$.
  - The condition number is larger than for strong constraint 4D-Var,
  - Increases with the number of sub-windows (it takes n iterations to propagate information).
- Simplified Hessian of the cost function is close to a Laplacian operator: small eigenvalues are obtained for constant perturbations which might be well observed and project onto eigenvectors of J_o" associated with large eigenvalues.
- Using the square root of this tri-diagonal matrix to precondition the minimisation is equivalent to using the initial state and forcing formulation.
- Can we combine the benefits of treating sub-windows in parallel with efficient minimization?

Outline

Weak Constraints 4D-Var: Summary

- In strong constraint 4D-Var, we can use the constraints to reduce the minimization problem to an initial value problem.
- Weak constraint 4D-Var with a model error forcing term is very similar to an initial value problem with parameter estimation (parameters happen to represent model error).
- Weak constraint 4D-Var has already taught us about observation bias and errors in the balance operators.
- Weak constraint 4D-Var with constant model error forcing in the stratosphere became operational in September 2009.
- Weak constraint 4D-Var with a 4D state control variable is a fully four dimensional problem where J_q acts as a coupling term between sub-windows.

Developments in Weak Constraints 4D-Var

- In the current formulation of weak constraints 4D-Var (model error forcing):
  - Cycling 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),
  - Address systematic model error.
- 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?
  - Address random model error?
- The two weak constraint 4D-Var approaches are mathematically equivalent (for linear problems) but lead to very different minimization problems.
  - 4D-Var scales well up to 1,000s of processors, it has to scale to 10,000s of processors in the future.
  - Can we combine the benefits of treating sub-windows in parallel with efficient preconditioning?

Weak Constraints 4D-Var: Open Questions

- Weak Constraints 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 Constraints 4D-Var requires knowledge of the statistical properties of model error (covariance matrix).
  - How can we access realistic samples of model error? How can observations be used? Can model drift 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 forecast model is such an important component of the data assimilation system. It is surprising how little we know about its error characteristics.

- The statistical description of model error is one of the main current challenges in data assimilation.