Accounting for an imperfect model in 4D-Var

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• Introduction: Incremental 4D-Var
• Model Error in 4D-Var
• Weak constraint 4D-Var
Introduction to 4D-Var
4D Variational Data Assimilation

- Model: \( M \),
- Observations: \( y \),
- Background: \( x_b \),
- Observation operator: \( H \),
- Cost function to minimise:

\[
J(x) = \frac{1}{2} (x - x_b)^T B^{-1} (x - x_b) + \frac{1}{2} [y - H(x)]^T R^{-1} [y - H(x)] + J_c
\]

- In discrete form:

\[
J(x) = \frac{1}{2} (x - x_b)^T B^{-1} (x - x_b) + \frac{1}{2} \sum_{i=0}^{n} [y_i - H_i(M_i(x))]^T R_i^{-1} [y_i - H_i(M_i(x))] + J_c
\]

- The control variable is the initial condition \( x_0 \).
Imperfect model in 4D-Var

Incremental 4D-Var

- The cost function is expressed in terms of increments with respect to the background state $\delta x = x - x_b$.
- $\mathcal{H}$ and $\mathcal{M}$ are linearised around $x_i = \mathcal{M}_i(x_0)$.

$$J(\delta x) = \frac{1}{2} \delta x^T B^{-1} \delta x + \frac{1}{2} \sum_{i=0}^{n} (H_i M_i \delta x - d_i)^T R_i^{-1} (H_i M_i \delta x - d_i)$$

where
- $H_i$ and $M_i$ are the linearised observation operator and model,
- $d_i = y_i - \mathcal{H}_i(\mathcal{M}_i(x_b))$ are the innovations.

- The innovations, which are the primary input to the assimilation, are always computed using the full observation operator and model, at full resolution, to ensure the highest possible accuracy.
Imperfect model in 4D-Var

Incremental 4D-Var

- One complex problem is replaced by a series of (slightly) easier problems.
- Gauss-Newton algorithm.
The Outer Iterations

After each minimisation at inner level:

- $x_0$ is updated: $x_0^j = x_b + \delta x_j$,
- $H_i$ and $M_i$ are re-linearised around $x_i = M_i(x_0^j)$,
- Innovations are re-calculated using the full nonlinear observation operator $H$ and model $M$:

$$d_i^j = y_i - H_i(M_i(x_0^j))$$

- Superscript $j$ represents the outer iteration.
- The nonlinear model $M$ remains at the highest resolution throughout.
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The Inner Iterations

- Tangent Linear approximation:

\[ \mathcal{M}(x + \delta x) \approx \mathcal{M}(x) + M\delta x \quad \text{and} \quad \mathcal{H}(x + \delta x) \approx \mathcal{H}(x) + H\delta x \]

- Approximations to reduce cost: the tangent linear model (and its adjoint) is degraded with respect to the full model \( \mathcal{M} \):
  - Lower resolution T95/T159/T255 (\( \approx 200/120/80 \) km) instead of T799 (\( \approx 25 \) km),
  - Simplified physics (some processes are ignored),
  - Simpler dynamics (spectral instead of grid-point humidity).

- The results in shorter control vector and cheaper TL and AD models during the minimisation.
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Incremental 4D-Var

\[ x_0 = x_b \]

\[ x_i \]

\[ S(x_{i,0}) \]

Departures \[ d = y - H(x_i) \]

\[ J \]

\[ \nabla J \]

\[ x_{i+1} = x_i + S^{-1}(\delta x_i) \]

\[ x_a \]

High resolution nonlinear trajectory

Trajectory

Low resolution linear model

Low resolution adjoint model

Iterative minimisation algorithm

High resolution nonlinear forecast

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Imperfect model in 4D-Var

Operational 4D-Var

- The assimilation window is 12 hours.
- Number of observations: $3.3 \times 10^6$
- Size of control variable: $30 \times 10^6$
- Computational cost:

<table>
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<th>Threads</th>
<th>CPUs</th>
<th>Time</th>
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<td>8</td>
<td>768</td>
<td>1h25min</td>
</tr>
<tr>
<td>10 day forecast</td>
<td>96</td>
<td>8</td>
<td>768</td>
<td>1h15min</td>
</tr>
</tbody>
</table>

(on IBM SP)
Imperfect model in 4D-Var

Model Error in 4D-Var
Imperfect model in 4D-Var

Weak constraint 4D-Var

- The model $\mathcal{M}$ is verified exactly although it is not perfect...
- The model can be imposed as a constraint in the cost function, in the same way as other sources of information:

$$\mathcal{F}_i(x) = x_i - \mathcal{M}_i(x_{i-1})$$

- Model error $\eta$ is defined as: $\eta_i = x_i - \mathcal{M}_i(x_{i-1})$
- The cost function becomes:

$$J(x) = \frac{1}{2} \sum_{i=0}^{n} [\mathcal{H}(x_i) - y_i]^T R_i^{-1} [\mathcal{H}(x_i) - y_i]$$

$$+ \frac{1}{2} (x_0 - x_b)^T B^{-1} (x_0 - x_b) + \frac{1}{2} \sum_{i=1}^{n} \sum_{j=1}^{n} \eta_i^T Q_{i,j}^{-1} \eta_j$$

- Model error covariance matrix $Q$ has to be defined.
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**4D-Var with Model Error Forcing**

- The cost function is written as a function of $(x_0, \eta)$:

$$J(x_0, \eta) = \frac{1}{2} \sum_{i=0}^{n} [\mathcal{H}(x_i) - y_i]^T R_i^{-1} [\mathcal{H}(x_i) - y_i]$$

$$+ \frac{1}{2} (x_0 - x_b)^T B^{-1} (x_0 - x_b) + \eta^T Q^{-1} \eta$$

with $x_i = \mathcal{M}_i(x_{i-1}) + \eta_i$.

- The *usual* model error term in 4D-Var.
- $\eta_i$ is a 3D atmospheric state,
- $\eta_i$ represents the instantaneous model error,
- $\eta$ is constrained by the fact that it is propagated by the model.
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4D-Var with Model Error Forcing

- TL and AD models can be used with little modification,
- Information is propagated between observations and IC control variable by TL and AD models.
- Practical implementation: $\eta$ constant by intervals.
Imperfect model in 4D-Var

Model Error Covariance Matrix
Model error covariance matrix

• The usual choice is $Q = \alpha B$.

• Linearisation in incremental formulation gives:

$$\delta x_n = M_n \ldots M_1 \delta x_0 + \sum_{i=1}^{n} M_n \ldots M_{i+1} \eta_i$$

• $\delta x_0$ can be identified with $\eta_0$.

• The solution of the analysis equation satisfies:

$$\delta x_0 = BH^T (R + HBH^T)^{-1} (y - \mathcal{H}(x_b))$$

$$\eta = QH^T (R + HQH^T)^{-1} (y - \mathcal{H}(x_b))$$

• If $Q$ and $B$ are proportional, $\delta x_0$ and $\eta$ are constrained in the same directions, may be with different relative amplitudes.

• They both predominantly retrieve the same information: $Q = \alpha B$ is too limiting.
Generating a Model Error Covariance Matrix

- $B$ is 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.
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Model Error Covariance Matrix

- Run forecasts from 4D-Var ensemble (T319),
- Save tendencies after 12h, 18h, 24h, 30h,
- Normalise tendencies to 1 hour time-steps,
- 10 members, one month (26 days),
- 936 realisations of model errors,
- Run statistical model.
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Average Temperature Vertical Correlations

Background Error

Model Error
Imperfect model in 4D-Var

**Temperature Horizontal Correlations**

**Background Error**

**Model Error**

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Imperfect model in 4D-Var

Average Standard Deviation Profiles

Q has narrower correlations and smaller amplitudes than B
Results: Constant Model Error Forcing
Results: Fit to observations

AMprofiler-windspeed Std Dev N.Amer

Background Departure

Analysis Departure

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

Zonal Mean Temperature
July 2004

M.E. Forcing $\rightarrow$
M.E. Mean Increment
Control Mean Increment

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**Mean Model Error Forcing**

Temperature
Model level 11 (≈5hPa)

Mean M.E. Forcing $\rightarrow$

M.E. Mean Increment $\downarrow$

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

Min = -1.60, Max = 1.15, RMS Global=0.55, N.hem=0.51, S.hem=0.41, Tropics=0.69

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AMSU-A Departures

STATISTICS FOR RADIANCES FROM NOAA-16 / AMSU-A - 13
MEAN FIRST GUESS DEPARTURE (OBS-FG) (BCORR.) (CLEAR)
DATA PERIOD = 2004070200 - 2004073118 , HOUR = ALL
EXP = ENRC
Min: -1.9618  Max: 2.7  Mean: -0.169506

EXP = ENRC
DATA PERIOD = 2004070100 - 2004073118 , HOUR = ALL
MEAN FIRST GUESS DEPARTURE (OBS-FG) (BCORR.) (CLEAR)
STATISTICS FOR RADIANCES FROM NOAA-16 / AMSU-A - 14
DATA PERIOD = 2004070200 - 2004073118 , HOUR = ALL
EXP = ENRC
Min: -3.3564  Max: 5.46  Mean: 0.006309

EXP = EPTG
DATA PERIOD = 2004070100 - 2004073118 , HOUR = ALL
MEAN FIRST GUESS DEPARTURE (OBS-FG) (BCORR.) (CLEAR)
STATISTICS FOR RADIANCES FROM NOAA-16 / AMSU-A - 14
DATA PERIOD = 2004070200 - 2004073118 , HOUR = ALL
EXP = EPTG
Min: -2.6  Max: 2.16  Mean: -0.111883

Control
Model Error
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AMSU-A Statistics

- Bias is more uniform,
- BG std. dev. is reduced in SH,
- More data is used.

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Temperature Analysis Profile

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Temperature Increments Profile

Increment - Temperature (K)

Forcing - Temperature (K/h)

Weak Q
Weak B
Strong

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Fit to radiosonde data

- Oscillations in bias are reduced,
- Std. deviation is reduced above 50 hPa (bg and an).

One source of model error was corrected by the forcing term.
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Low Level Mean Model Error Forcing

Friday 30 April 2004 21UTC ©ECMWF Mean Model Error (ej6a)
Temperature, Model Level 60
Min = -0.10, Max = 0.05, RMS Global=0.00, N.hem=0.01, S.hem=0.00, Tropics=0.00
Imperfect model in 4D-Var

Low Level Mean Model Error Forcing

Friday 30 April 2004 21UTC ©ECMWF Mean Model Error (ej6a)
Temperature, Model Level 60
Min = -0.10, Max = 0.05, RMS Global=0.00, N.hem=0.01, S.hem=0.00, Tropics=0.00

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Fit to Observation with Model Error

exp:ej6a Model Error 2004050100-2004050712(6)  
AIREP-T MyBox  
used T

STD.DEV

BIAS

- The only significant source of data in the box is aircraft data (Denver airport).
- The bias for aircraft low level temperature observations was reduced.
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Low Level Mean Model Error Forcing

Friday 30 April 2004 21UTC ©ECMWF Mean Model Error (ej8k)
Temperature, Model Level 60
Min = -0.07, Max = 0.06, RMS Global=0.00, N.hem=0.01, S.hem=0.00, Tropics=0.00

Removing aircraft data in the box eliminates the spurious forcing.

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Aircraft Temperature Bias

USA ACARS and TEMP 00z temperature biases
Monthly averages for asc, desc and cruise level

Observations are biased.

Figure from Lars Isaksen
Imperfect model in 4D-Var

12 Observations Experiment

Systematic model error captures stationary errors (model or observations).
Model Bias Control Variable
Imperfect model in 4D-Var

Model Bias Control Variable

- The cost function was written as a function of \((x_0, \eta)\) where model error \(\eta\) is defined by: 
  \[ x_i = M_i(x_{i-1}) + \eta_i. \]

- This is the usual change of variable used when accounting for model error in 4D-Var but other control variables can be used.

- The cost function can be written as a function of \((x_0, \beta)\) where model bias \(\beta\) is defined by: 
  \[ x_i = M_i(x_0) + \beta_i. \]
Imperfect model in 4D-Var

\[ J(x_0, \beta) = \frac{1}{2} \sum_{i=0}^{n} [\mathcal{H}(x^m_i + \beta_i) - y_i]^T R_i^{-1} [\mathcal{H}(x^m_i + \beta_i) - y_i] \]

\[ + \frac{1}{2} (x_0 - x_b)^T B^{-1} (x_0 - x_b) + \beta^T Q_\beta^{-1} \beta \]

with \( x^m_i = M_{i,0}(x_0) \).

- \( \beta_i \) is a 3D atmospheric state,
- The model is not perturbed,
- \( \beta \) sees global (model – all observations) bias,
- Does not correct for bias of one subset of observations against another subset of observations.
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4D-Var with Model Bias

- Bias added to forecast at post-processing stage,
- Makes sense if $\beta$ is slowly varying or constant ($\beta_i = \beta$),
- Information is propagated between observations and IC control variable by TL and AD models (not modified),
- Model bias is represented by additional parameters, without entering the model equations,
- Optimisation problem is very similar to strong constraint 4D-Var.
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Model Bias: Fit to Observations

Jo/n Cost Function

Model Bias (0529) - Control (0528)

Fit to analysis and background is improved.

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Model Bias

Average Model Bias - Temperature (K) - July 1989

Bias is large!

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Mean Model Bias

Temperature
Model level 4 ($\approx 1$ hPa)
June 1989

Mean Bias $\rightarrow$
Mean Increment with Bias
Control Mean Increment

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Seasonal Variation of Model Bias

Model Bias
- 60N-20N - Temperature - Model Level 7

Mean 1124 - Avg = 0.6
Std. dev. 1124 - Avg = 4.5

Increments
- 60N-20N - Temperature - Model Level 7

Mean 1124 - Avg = -0.011
Mean 1112 - Avg = -0.028
Std. dev. 1124 - Avg = 0.98
Std. dev. 1112 - Avg = 1

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Weak Constraint 4D-Var
Imperfect model in 4D-Var

\section*{Model State Control Variable}

\begin{equation}
J(x) = \frac{1}{2} (x_0 - x_b)^T B^{-1} (x_0 - x_b) + \frac{1}{2} \sum_{i=0}^{n} \left[ H(x_i) - y_i \right]^T R_i^{-1} \left[ H(x_i) - y_i \right] \\
+ \frac{1}{2} \sum_{i=1}^{n} \left[ x_i - M_i(x_{i-1}) \right]^T Q_i^{-1} \left[ x_i - M_i(x_{i-1}) \right]
\end{equation}

- Use \( \{x_i\}_{i=0,\ldots,n} \) as the control variable.

- Incremental cost function:

\begin{equation}
J(\delta x) = \frac{1}{2} (\delta x_0 - b)^T B^{-1} (\delta x_0 - b) + \frac{1}{2} \sum_{i=0}^{n} (H\delta x_i - d_i)^T R_i^{-1} (H\delta x_i - d_i) \\
+ \frac{1}{2} \sum_{i=1}^{n} (q_i + M_{i-1}\delta x_{i-1} - \delta x_i)^T Q_i^{-1} (q_i + M_{i-1}\delta x_{i-1} - \delta x_i)
\end{equation}

where \( b = x^g - x_b, \quad d_i = H(x_i^g) - y_i \) and \( q_i = M_{i-1}(x_{i-1}^g) - x_i^g \).

- The model does not appear in the \( J_o \) term,

- In practice \( x_i \) is defined at regular intervals within the assimilation window.
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Model State Control Variable

Forcing 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 (in theory...).

- Tangent linear and adjoint models:
  - can be used without modification,
  - propagate information between observations and control variable within each sub-window.

- Information is propagated across sub-windows by $J_q$ term.
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**Weak Constraint 4D-Var: Examples**

- 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,
  - It makes more sense to use $Q = \alpha B$ in that case.

- One 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.
Imperfect model in 4D-Var

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 constraint 4D-Var with an assimilation window that extends indefinitely in the past...
- ...which is equivalent to a Kalman smoother that has been running indefinitely.

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Comments

- The difference between the $\eta$, $\beta$ or $x$ formulations of weak constraint 4D-Var is only a change of variable,

- These three problems are equivalent,

- They would lead to the same solution if we could solve exactly these full nonlinear problems.

- As soon as approximations are introduced (size of control variable, model for model error, linearisation), the problems become different.

- The formulation with $x$ as the control variable is the closest to the original problem: it is the only one that does not directly propagate information through the model over the full length of the assimilation window.

- It can be interpreted as coupling several cycles of assimilation (3D-Var or 4D-Var).
Conclusions
Imperfect model in 4D-Var

Control Variable in 4D-Var

The general 4D-Var cost function is:

\[
J(x) = \frac{1}{2} (x_0 - x_b)^T B^{-1} (x_0 - x_b) + \frac{1}{2} \sum_{i=0}^{n} [\mathcal{H}(x_i) - y_i]^T R_i^{-1} [\mathcal{H}(x_i) - y_i] \\
+ \frac{1}{2} \sum_{i=1}^{n} [x_i - \mathcal{M}_i(x_{i-1})]^T Q_i^{-1} [x_i - \mathcal{M}_i(x_{i-1})]
\]

Some possible changes of variable are:

<table>
<thead>
<tr>
<th>4D-Var</th>
<th>4D-Var_x</th>
<th>4D-Var_\eta</th>
<th>4D-Var_\beta</th>
</tr>
</thead>
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<td>(x_0)</td>
<td>(x)</td>
<td>(x_0, \eta)</td>
<td>(x_0, \beta)</td>
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<td>(x_i = \mathcal{M}<em>i(x</em>{i-1}))</td>
<td>(x_i \approx \mathcal{M}<em>i(x</em>{i-1}))</td>
<td>(x_i = \mathcal{M}<em>i(x</em>{i-1}) + \eta_i)</td>
<td>(x_i = \mathcal{M}_{i,0}(x_0) + \beta_i)</td>
</tr>
<tr>
<td>(\Downarrow)</td>
<td>(\Downarrow)</td>
<td>(\Downarrow)</td>
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</tr>
<tr>
<td>3D Initial Condition</td>
<td>4D Atmospheric State</td>
<td>3D I.C. + Model Error Forcing</td>
<td>3D I.C. + Model Bias</td>
</tr>
</tbody>
</table>

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Model Error and Model Bias

• First results show:
  – Improved fit to observations,
  – Reduced oscillations in the winter stratosphere,
  – Both capture a part of observation bias.

• Possibilities:
  – Bias is an additional product requested by some users, particularly in reanalysis,
  – Prevent large departures in the stratosphere and mesosphere from propagating downwards,
  – Remove bias (systematic error) first, then random error,
  – Better knowledge of model error should help to improve the model.

• Difficulties:
  – Choice of model for model error (constant 3D state?),
  – Determine appropriate error statistics (Q),
  – Interaction with Observation VarBC.
Imperfect model in 4D-Var

Model State Weak Constraint 4D-Var

• Possibilities:
  – Takes into account the fact that the model is imperfect without directly estimating model error.
  – Long window weak constraint 4D-Var (=KS) can produce long and consistent 4D pictures of the atmosphere,
  – Could be implemented in addition to a model bias term,
  – Applies to operational analysis and reanalysis (long window),
  – Model error can be indirectly estimated,
  – Better knowledge of model error should help to improve the model.

• Difficulties:
  – Determine appropriate error statistics ($Q$),
  – Conditioning, optimisation algorithm,
  – Interaction with Observation VarBC.