Diagnosing and representing model error in strong constraint 4DVAR

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Contents

- Model errors
- Development of a combined model error and observation error covariance matrix for use in 4DVar
- Estimation of the combined matrix with diagnostics
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Random model error

Models are **best representations** of **true** dynamical **systems**

$$\begin{aligned} \mathbf{x}_i^t &= \mathbf{M}_{\{i-1\}\to i}\mathbf{x}_{i-1}^t \\ &= \widetilde{\mathbf{M}}_{\{i-1\}\to i}\mathbf{x}^t{}_{i-1} + \boldsymbol{\eta}_i \qquad i = 1, 2, ..., \end{aligned}$$

where the model error $\boldsymbol{\eta}_i \sim \mathcal{N}(\mathbf{0}, \mathbf{Q}_i)$.

Four dimensional variational data assimilation (4DVar)

$$\mathcal{J}(\mathbf{x}_0) = \frac{1}{2}(\mathbf{x}_0 - \mathbf{x}^b)^T \mathbf{B}^{-1}(\mathbf{x}_0 - \mathbf{x}^b) + \frac{1}{2}(\hat{\mathbf{y}} - \hat{\mathbf{H}}\mathbf{x}_0)^T \hat{\mathbf{R}}^{-1}(\hat{\mathbf{y}} - \hat{\mathbf{H}}\mathbf{x}_0),$$

$$\hat{\mathbf{y}} = \begin{pmatrix} \mathbf{y}_0 \\ \mathbf{y}_1 \\ \vdots \\ \vdots \\ \vdots \\ \mathbf{y}_N \end{pmatrix} \quad \hat{\mathbf{H}} = \begin{pmatrix} \mathbf{H}_0 \\ \mathbf{H}_1\mathbf{M}_{0\to 1} \\ \vdots \\ \vdots \\ \vdots \\ \mathbf{H}_N\mathbf{M}_{0\to N} \end{pmatrix} \text{ and } \hat{\mathbf{R}} = \begin{pmatrix} \mathbf{R}_0 & 0 & \cdots & \cdots & 0 \\ 0 & \mathbf{R}_1 & 0 & \cdots & 0 \\ \vdots & 0 & 0 & \vdots & \vdots \\ \vdots & \vdots & \cdots & \ddots & 0 \\ 0 & \cdots & \cdots & 0 & \mathbf{R}_N \end{pmatrix}.$$

- $\epsilon_b = \mathbf{x}^b - \mathbf{x}^t{}_0$ with $\epsilon_b \sim \mathcal{N}(\mathbf{0}, \mathbf{B})$,
- $\epsilon_{ob} = \hat{\mathbf{y}} - \hat{\mathbf{H}}\mathbf{x}^t{}_0$ with $\epsilon_{ob} \sim \mathcal{N}(\mathbf{0}, \hat{\mathbf{R}})$.

4DVar with erroneous model

$$\mathcal{J}(\mathbf{x}_0) \quad = \quad \frac{1}{2}(\mathbf{x}_0 - \mathbf{x}^b)^T \mathbf{B}^{-1}(\mathbf{x}_0 - \mathbf{x}^b) + \frac{1}{2}(\hat{\mathbf{y}} - \widetilde{\mathbf{H}}\mathbf{x}_0)^T \mathbf{R}^{*-1}(\hat{\mathbf{y}} - \widetilde{\mathbf{H}}\mathbf{x}_0),$$

$$\hat{\mathbf{y}} = \begin{pmatrix} \mathbf{y}_0 \\ \mathbf{y}_1 \\ \vdots \\ \vdots \\ \vdots \\ \mathbf{y}_N \end{pmatrix} \qquad \widetilde{\mathbf{H}} = \begin{pmatrix} \mathbf{H}_0 \\ \mathbf{H}_1 \color{red}{\widetilde{\mathbf{M}}_{0\rightarrow 1}} \\ \vdots \\ \vdots \\ \vdots \\ \mathbf{H}_N \color{red}{\widetilde{\mathbf{M}}_{0\rightarrow N}} \end{pmatrix}$$

$$\boxed{\epsilon^*_{ob} = \hat{\mathbf{y}} - \widetilde{\mathbf{H}}\mathbf{x}^t{}_0 \text{ with } \epsilon^*_{ob} \sim \mathcal{N}(?,?)}$$

Combined model error and observation error

$$\begin{aligned} \epsilon_{obi} &= \mathbf{y}_i - \mathbf{H}_i \mathbf{M}_{0\to i} \mathbf{x}^t{}_0, & \epsilon_{obi} &\sim \mathcal{N}(\mathbf{0}, \mathbf{R}_i) & (1) \\ \epsilon^*_{obi} &= \mathbf{y}_i - \mathbf{H}_i \widetilde{\mathbf{M}}_{0\to i} \mathbf{x}^t{}_0, & \epsilon^*_{obi} &\sim \mathcal{N}(?, ?) & (2) \end{aligned}$$

Combined model error and observation error

$$
\begin{aligned}
\epsilon_{ob\,i} &= \mathbf{y}_i - \mathbf{H}_i \mathbf{M}_{0\to i} {\mathbf{x}^t}_0, \qquad \epsilon_{ob\,i} \sim \mathcal{N}(\mathbf{0}, \mathbf{R}_i) \qquad (1) \\
\epsilon^*_{ob\,i} &= \mathbf{y}_i - \mathbf{H}_i \widetilde{\mathbf{M}}_{0\to i} {\mathbf{x}^t}_0, \qquad \epsilon^*_{ob\,i} \sim \mathcal{N}(?, ?) \qquad (2)
\end{aligned}
$$

Substracting (1) from (2) and rearranging,

$$
\begin{aligned}
\epsilon^*_{ob\,i} &= \epsilon_{ob\,i} + \mathbf{H}_i (\mathbf{M}_{0\to i} {\mathbf{x}^t}_0 - \widetilde{\mathbf{M}}_{0\to i} {\mathbf{x}^t}_0), \\
&= \epsilon_{ob\,i} + \mathbf{H}_i \sum_{j=1}^{i} \widetilde{\mathbf{M}}_{j\to i} \eta_j,
\end{aligned}
$$

Combined model error and observation error

$$\begin{aligned} \epsilon_{obi} &= \mathbf{y}_i - \mathbf{H}_i \mathbf{M}_{0\rightarrow i} \mathbf{x}^t{}_0, \qquad \epsilon_{obi} \sim \mathcal{N}(\mathbf{0}, \mathbf{R}_i) \quad (1) \\ \epsilon^*_{obi} &= \mathbf{y}_i - \mathbf{H}_i \widetilde{\mathbf{M}}_{0\rightarrow i} \mathbf{x}^t{}_0, \qquad \epsilon^*_{obi} \sim \mathcal{N}(?, ?) \quad (2) \end{aligned}$$

Substracting (1) from (2) and rearranging,

$$\begin{aligned} \epsilon^*_{obi} &= \epsilon_{obi} + \mathbf{H}_i (\mathbf{M}_{0\rightarrow i} \mathbf{x}^t{}_0 - \widetilde{\mathbf{M}}_{0\rightarrow i} \mathbf{x}^t{}_0), \\ &= \epsilon_{obi} + \mathbf{H}_i \sum_{j=1}^{i} \widetilde{\mathbf{M}}_{j\rightarrow i} \eta_j, \\ < \epsilon^*_{obi} > &= \mathbf{0}. \end{aligned}$$

Combined model error and observation error covariance

Let,

$$\mathbf{R}^*{}_{(i,k)} = < \boldsymbol{\epsilon}^*_{ob\,i} (\boldsymbol{\epsilon}^*_{ob\,k})^T > .$$

Combined model error and observation error covariance

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Then,

$$\mathbf{R}^*{}_{(i,k)} = \begin{cases} \mathbf{R}_0 & \text{for i=k=0} \\ \mathbf{R}_i + \mathbf{H}_i \left[\sum_{j=1}^{min(i,k)} \widetilde{\mathbf{M}}_{j\to i} \mathbf{Q}_j \widetilde{\mathbf{M}}_{j\to k}{}^T \right] \mathbf{H}_k{}^T & \text{for i=k} \\ \mathbf{H}_i \left[\sum_{j=1}^{min(i,k)} \widetilde{\mathbf{M}}_{j\to i} \mathbf{Q}_j \widetilde{\mathbf{M}}_{j\to k}{}^T \right] \mathbf{H}_k{}^T & \text{otherwise.} \end{cases}$$

Combined model error and observation error covariance

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$$\mathbf{R}^*{}_{(i,k)} =< \boldsymbol{\epsilon}^*_{ob\,i}(\boldsymbol{\epsilon}^*_{ob\,k})^T > .$$

Then,

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Let $\mathbf{Q}^*{}_{(i,k)} = \mathbf{H}_i \left[\sum_{j=1}^{min(i,k)} \widetilde{\mathbf{M}}_{j \to i} \mathbf{Q}_j \widetilde{\mathbf{M}}_{j \to k}{}^T \right] \mathbf{H}_k{}^T$.

Combined model error and observation error covariance matrix

Then,

$$\mathbf{R}^* = \begin{pmatrix} \mathbf{R}_0 & 0 & & \cdots & 0 \\ 0 & \mathbf{R}_1 + \mathbf{Q}^*{}_{(1,1)} & \mathbf{Q}^*{}_{(1,2)} & \cdots & \mathbf{Q}^*{}_{(1,N)} \\ \vdots & \mathbf{Q}^*{}_{(2,1)} & \mathbf{R}_2 + \mathbf{Q}^*{}_{(2,2)} & \vdots & \vdots \\ \vdots & \vdots & \cdots & \ddots & \vdots \\ 0 & \mathbf{Q}^*{}_{(N,1)} & \cdots & \cdots & \mathbf{R}_N + \mathbf{Q}^*{}_{(N,N)} \end{pmatrix}.$$

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- An increase in block diagonal terms. This is an accumulation of the model error over the assimilation time window.

Combined model error and observation error covariance matrix

Then,

$$
\mathbf{R}^* = \begin{pmatrix}
\mathbf{R}_0 & 0 & & \cdots & 0 \\
0 & \mathbf{R}_1 + \mathbf{Q}^*{}_{(1,1)} & \mathbf{Q}^*{}_{(1,2)} & \cdots & \mathbf{Q}^*{}_{(1,N)} \\
\vdots & \mathbf{Q}^*{}_{(2,1)} & \mathbf{R}_2 + \mathbf{Q}^*{}_{(2,2)} & \vdots & \vdots \\
\vdots & \vdots & \cdots & \ddots & \vdots \\
0 & \mathbf{Q}^*{}_{(N,1)} & \cdots & \cdots & \mathbf{R}_N + \mathbf{Q}^*{}_{(N,N)}
\end{pmatrix}.
$$

- An increase in block diagonal terms. This is an accumulation of the model error over the assimilation time window.
- The formation of off diagonal block model error covariance terms. This is the presence of time correlations caused by the error in the model.

Increase in analysis accuracy

Erroneous model $\mathbf{x}_i = \widetilde{\mathbf{M}}_{\{i-1\}\rightarrow i}\mathbf{x}_{i-1}$ used within the strong constraint 4DVar cost function.

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Erroneous model $\mathbf{x}_i = \widetilde{\mathbf{M}}_{\{i-1\}\to i}\mathbf{x}_{i-1}$ used within the strong constraint 4DVar cost function.

Error in the model not accounted for (use of $\hat{\mathbf{R}}$)	Error in the model accounted for (use of $\hat{\mathbf{R}}^*$)
$\mathbf{x}^a{}_0 = \mathbf{x}^b + \hat{\mathbf{K}}(\hat{\mathbf{y}} - \widetilde{\mathbf{H}}\mathbf{x}^b)$	$\mathbf{x}^a{}_0{}^* = \mathbf{x}^b + \hat{\mathbf{K}}^*(\hat{\mathbf{y}} - \widetilde{\mathbf{H}}\mathbf{x}^b)$

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$\mathbf{A} = (\mathbf{I} - \hat{\mathbf{K}}\widetilde{\mathbf{H}})\mathbf{B} + \hat{\mathbf{K}}\hat{\mathbf{Q}}^*\hat{\mathbf{K}}^T$	$\mathbf{A}^* = (\mathbf{I} - \hat{\mathbf{K}}^*\widetilde{\mathbf{H}})\mathbf{B}$

Table : Analysis error covariance matrices where $\hat{\mathbf{Q}}^* = \hat{\mathbf{R}}^* - \hat{\mathbf{R}}$

Increase in analysis accuracy

Error in the model not accounted for (use of $\hat{\mathbf{R}}$)	Error in the model accounted for (use of $\hat{\mathbf{R}}^*$)
$\mathbf{A} = (\mathbf{I} - \hat{\mathbf{K}}\widetilde{\mathbf{H}})\mathbf{B} + \hat{\mathbf{K}}\hat{\mathbf{Q}}^*\hat{\mathbf{K}}^T$	$\mathbf{A}^* = (\mathbf{I} - \hat{\mathbf{K}}^*\widetilde{\mathbf{H}})\mathbf{B}$

unbounded

bounded by **B**

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$\mathbf{A} = (\mathbf{I} - \hat{\mathbf{K}}\widetilde{\mathbf{H}})\mathbf{B} + \hat{\mathbf{K}}\hat{\mathbf{Q}}^*\hat{\mathbf{K}}^T$	$\mathbf{A}^* = (\mathbf{I} - \hat{\mathbf{K}}^*\widetilde{\mathbf{H}})\mathbf{B}$
unbounded	bounded by $\mathbf{B}$

- No model error is present: Best Linear Unbiased Estimate (BLUE) has $\mathbf{A} = (\mathbf{I} - \hat{\mathbf{K}}\hat{\mathbf{H}})\mathbf{B}$ with $\hat{\mathbf{K}} = \mathbf{B}\hat{\mathbf{H}}^T(\hat{\mathbf{H}}\mathbf{B}\hat{\mathbf{H}}^T + \hat{\mathbf{R}})^{-1}$.

Increase in analysis accuracy

Error in the model not accounted for (use of $\hat{\mathbf{R}}$)	Error in the model accounted for (use of $\hat{\mathbf{R}}^*$)
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- Model error is present: replacement of $\hat{\mathbf{R}}$ with $\hat{\mathbf{R}}^*$ leads to $\mathbf{A}^*$ having the same form $\Rightarrow$ analysis ${\mathbf{x}^a}_0{}^*$ is more statistically accurate than the analysis ${\mathbf{x}^a}_0$.

Increase in analysis accuracy: Scalar case

- Erroneous model $x_i = \widetilde{\beta} x_{i-1}$,
- true model state $x^t{}_i = \beta x^t{}_{i-1} = \widetilde{\beta} x^t{}_{i-1} + \eta_i$,
- direct observations at time t_1 with operator $h_1 = 1$,
- ${\sigma_{ob}}^{*2} = {\sigma_{ob}}^2 + {\sigma_q}^2$

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- direct observations at time t_1 with operator $h_1 = 1$,
- ${\sigma_{ob}}^{*2} = {\sigma_{ob}}^2 + {\sigma_q}^2$

Let $r = \frac{{\sigma_b}^2}{{\sigma_{ob}}^2}$, then the difference in the analysis error variance,

$$ {\sigma_a}^2 - {\sigma_a}^{*2} = \frac{{\sigma_q}^4 r^2 \widetilde{\beta}^2}{({\sigma_b}^2 + {\sigma_{ob}}^2 + {\sigma_q}^2)(\widetilde{\beta}^2 r + 1)^2} \geq 0. \quad (3) $$

Increase in analysis accuracy: Scalar case

Increase in analysis accuracy more significant,

- increase in: model error, observation accuracy,
- decrease in: background accuracy

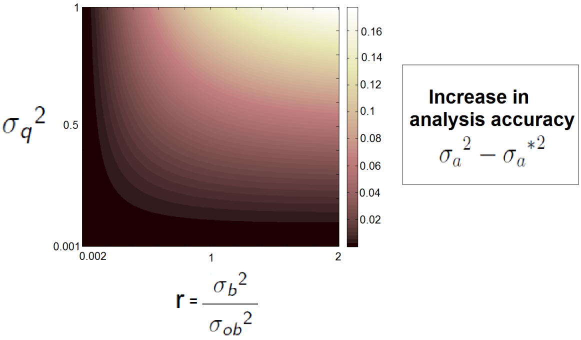

Figure : Increase in analysis accuracy for scalar case $\widetilde{\beta} = 1$, $\sigma_{ob}{}^2 = 10^{-3}$

How do we specify the model error statistics?

$$
\mathbf{R^*}_{(i,k)} = \begin{cases} \mathbf{R}_0 & \text{for i=k=0} \\ \mathbf{R}_i + \mathbf{H}_i \left[\sum_{j=1}^{min(i,k)} \widetilde{\mathbf{M}}_{j\to i} \mathbf{Q}_j \widetilde{\mathbf{M}}_{j\to k}{}^T \right] \mathbf{H}_k{}^T & \text{for i=k} \\ \mathbf{H}_i \left[\sum_{j=1}^{min(i,k)} \widetilde{\mathbf{M}}_{j\to i} \mathbf{Q}_j \widetilde{\mathbf{M}}_{j\to k}{}^T \right] \mathbf{H}_k{}^T & \text{otherwise,} \end{cases}
$$

How can we specify $\mathbf{Q}_j$?

Estimation of combined error covariance matrix

We have developed a method to estimate $\mathbf{R}^*_{(i,k)}$. Let,

- $(\mathbf{d}^o{}_b)_i = \mathbf{y}_i - \mathbf{H}_i \widetilde{\mathbf{M}}_{0\to i} \mathbf{x}^b$,
- $(\mathbf{d}^o{}_b)_k = \mathbf{y}_k - \mathbf{H}_k \widetilde{\mathbf{M}}_{0\to k} \mathbf{x}^b$.

[1] E. Andersson: Modelling the temporal evolution of innovation statistics *Proceedings of Workshop on recent developments in data assimilation for atmosphere and ocean, ECMWF, Reading*, 2003, pp. 153-164.

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Then,

$$\boxed{\mathbf{R}^*{}_{(i,k)} = E[(\mathbf{d}^o{}_b)_i(\mathbf{d}^o{}_b)_k{}^T] - \mathbf{H}_i\widetilde{\mathbf{M}}_{0\to i}\mathbf{B}\widetilde{\mathbf{M}}_{0\to k}{}^T\mathbf{H}_k{}^T. \qquad (4)}$$

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Note the diagonal elements of $\mathbf{H}_i \widetilde{\mathbf{M}}_{0\to i} \mathbf{B} \widetilde{\mathbf{M}}_{0\to i}{}^T \mathbf{H}_i{}^T$ can be estimated for a very large system using the randomisation method [1].

[1] E. Andersson: Modelling the temporal evolution of innovation statistics *Proceedings of Workshop on recent developments in data assimilation for atmosphere and ocean, ECMWF, Reading*, 2003, pp. 153-164.

Obtaining a sample of innovation vectors

For estimation of $\mathbf{R}^*{}_{(i,k)}$ we need to evaluate $E[(\mathbf{d}^o{}_b)_i(\mathbf{d}^o{}_b)_k{}^T]$ where,

$$\boxed{(\mathbf{d}^o{}_b)_i = \mathbf{y}_i - \mathbf{H}_i\widetilde{\mathbf{M}}_{0\to i}\mathbf{x}^b.}$$

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Require:

- sample of **background** vectors, **observation** vectors and **erroneous models**.

Idealized coupled nonlinear model

Couples the Lorenz 63 system and 2 linear equations (Molteni et al. [2]),

$$
\begin{aligned}
\dot{x} &= -\sigma x + \sigma y + \alpha v, \\
\dot{y} &= -xz + rx - y + \alpha w, \\
\dot{z} &= xy - bz, \\
\dot{w} &= -\Omega v - k(w - w^*) - \alpha y, \\
\dot{v} &= \Omega(w - w^*) - kv - \alpha x,
\end{aligned}
\qquad (5)
$$

where $\sigma = 10$, $r = 30$, $b = \frac{8}{3}$, $k = 0.1$, $\Omega = \frac{\pi}{10}$ and $w^* = 2$.

[2] F. Molteni, L. Ferranti, T.N. Palmer, P. Viterbo: A dynamical interpretation of the global response to equatorial Pacific SST anomalies *Journal of climate*, **vol.6**, 1993, pp. 777-795.

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\dot{v} &= \Omega(w - w^*) - kv - \alpha x,
\end{aligned} \tag{5}$$

where $\sigma = 10$, $r = 30$, $b = \frac{8}{3}$, $k = 0.1$, $\Omega = \frac{\pi}{10}$ and $w^* = 2$.

- Runge-Kutta 2nd order method with fixed time step $\Delta t = 0.01$ used to approximate solution of coupled ODE's.

[2] F. Molteni, L. Ferranti, T.N. Palmer, P. Viterbo: A dynamical interpretation of the global response to equatorial Pacific SST anomalies *Journal of climate*, **vol.6**, 1993, pp. 777-795.

True idealized coupled nonlinear model

- True initial conditions on the coupled model attractor:
  $\mathbf{x}^t{}_0 = (-3.4866, -5.7699, 18.341, -10.7175, -7.1902)$.

We add random forcing at each time-step to obtain the true model state at the next time-step,

$$\mathbf{x}_i^t \quad = \quad \widetilde{\mathcal{M}}_{\{i-1\}\to i}(\mathbf{x}^t{}_{i-1}) + \boldsymbol{\eta}_i, \qquad\qquad i = 1, 2, ...50,$$

- where the model error covariance matrix $\mathbf{Q}_i$ $(i = 1, 2, ..., 50)$ is diagonal with variances set to 0.02, 0.02, 0.2, 0.01, 0.01.

Numerical experiments: design

- Assimilation window length of 50 time-steps.
- Background error covariance matrix $\mathbf{B}$ with standard deviations approximately 10% of the true initial conditions.
- Direct observations every 10 time-steps with diagonal error covariance matrix $\mathbf{R}_i$ in which the standard deviations are approximately 2% of the maximum absolute value of each respective variable,
- Perturb the true model states using $\mathbf{B}$ and $\mathbf{R}_i$ respectively to produce background model state $\mathbf{x}^b$ and observations $\mathbf{y}_i$.

Numerical experiments: results

Twin experiment: Compare 4DVar analysis accuracy using $\mathbf{R}^*$ as opposed to $\hat{\mathbf{R}}$.

Estimate diagonal entries of $\mathbf{R}^*$ at observation times:

- Evaluate sample size of $1,000$ innovations $(\mathbf{d}^o{}_b)_i = \mathbf{y}_i - \mathbf{H}_i \widetilde{\mathbf{M}}_{0\to i}\mathbf{x}^b$ (i=10,20,30,40,50).
- Estimate diagonal entries of $E[(\mathbf{d}^o{}_b)_i (\mathbf{d}^o{}_b)_i{}^T]$.
- Estimate combined model error and observation error variances using:
  - $\mathbf{R}^*{}_{(i,i)} = E[(\mathbf{d}^o{}_b)_i (\mathbf{d}^o{}_b)_i{}^T] - \mathbf{H}_i \widetilde{\mathbf{M}}_{0\to i} \mathbf{B} \widetilde{\mathbf{M}}_{0\to i}{}^T \mathbf{H}_i{}^T$.

Numerical experiments: results

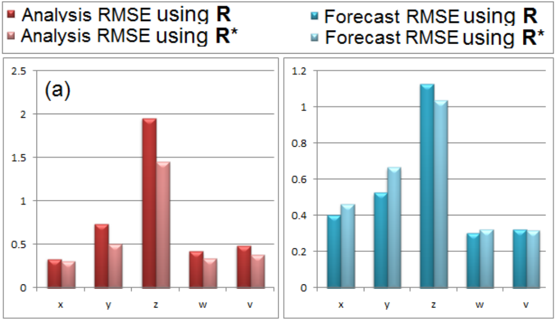

Figure : Analysis RMSE and the subsequent RMSE of the analysis trajectories over the assimilation window over a sample of 100 data assimilation runs.

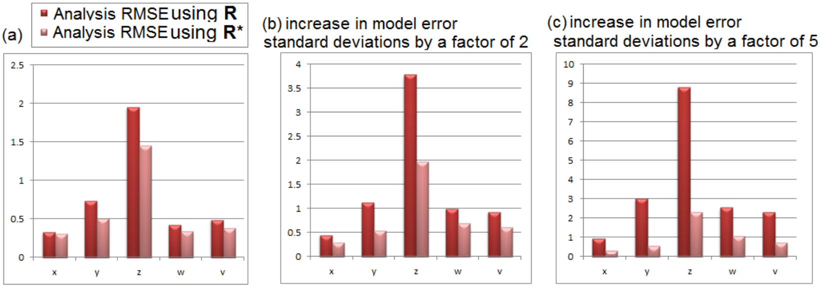

Figure : Results from a sample of 100 data assimilation runs in each of (a), (b) and (c).

Numerical experiments: results

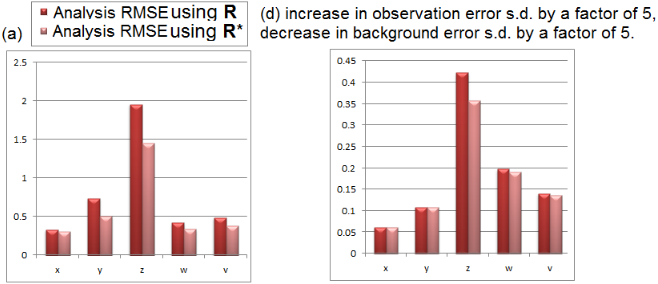

Figure : Results from a sample of 100 data assimilation runs in each of (a) and (d).

When the model used in 4DVar is erroneous, using $\mathbf{R}^*$ as opposed to $\hat{\mathbf{R}}$ increases the analysis accuracy at the initial time.

Experimental results have shown the increase is most significant when,

- the model error is large,
- the observations are very accurate,
- the background is very inaccurate.

Obtaining a sample of innovation vectors operationally

We know:

- Previously samples of innovation vectors have been collected (in areas where frequent observations were available) [1].
- The observational data was collected over short time period, for example in hourly bins [1].

[1] E. Andersson: Modelling the temporal evolution of innovation statistics *Proceedings of Workshop on recent developments in data assimilation for atmosphere and ocean, ECMWF, Reading*, 2003, pp. 153-164. [3] J.M. Brankart et al.: A generic approach to explicit simulation of uncertainty in the NEMO model *Geoscientific Model Development*, **vol.8**, 2015, pp. 1285-1297.

Obtaining a sample of innovation vectors operationally

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We also know:

- Ensemble prediction systems represent random error in a model forecast using stochastic physics [3].

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Considerations:

- What are the implications of using observations accross a short time period? Estimation of a time-averaged $\mathbf{R}^*$.
- Do the stochastic physics used to run an ensemble of forecasts account for all random error in the model?

Summary

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- Developed a method to estimate this combined matrix using diagnostics.
- We have shown using the combined model error and observation error covariance matrix, as opposed to only the observation error covariance matrix, increases the analysis accuracy.
- Application of the method suited to reanalysis, where the objective is to best estimate the analysis at the initial time and start of an assimilation window (not beneficially applicable to long term forecasts).

Questions

Thank you for listening

Any questions?