Rapid update cycling with overlapping windows

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Workshop on Meteorological Sensitivity Analysis and Data Assimilation
Roanoke, Tuesday 2nd June 2015

Main benefits of frequent analysis updates

(i) Hourly update for global analysis enables timely BCs for possible/likely future hourly running of UKV and other LAMs

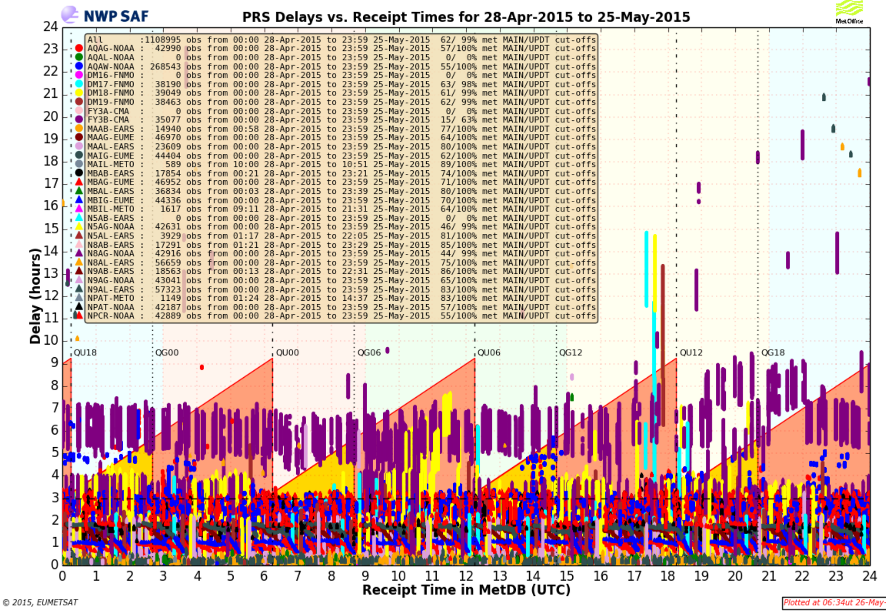
(ii) Error in linear approximation to smooth function declines quadratically with increment size

$$\phi(\mathbf{x}+\delta\mathbf{x}) = \phi(\mathbf{x}) + \phi'(\mathbf{x})\delta\mathbf{x} + \frac{1}{2}\phi''(\mathbf{x})(\delta\mathbf{x},\delta\mathbf{x}) + ...$$

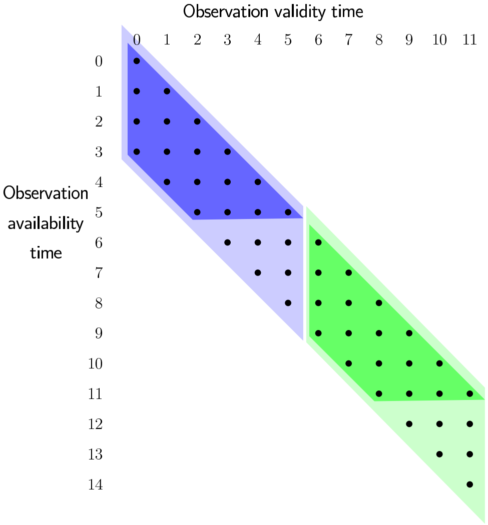
hourly update $\rightarrow$ smaller increment $\rightarrow$ (hopefully) improved PF Model performance

(iii) Potentially, improved affordability

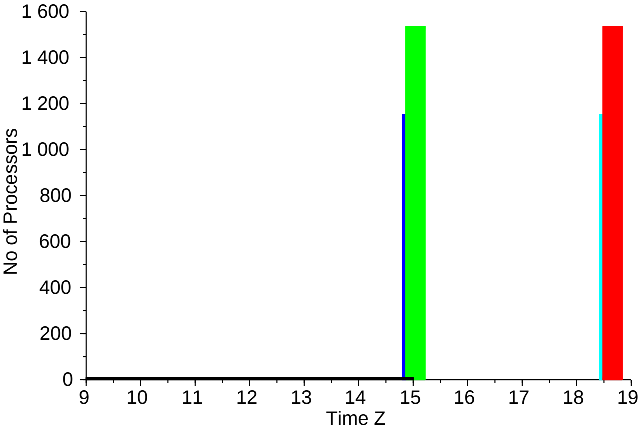
More on these later.

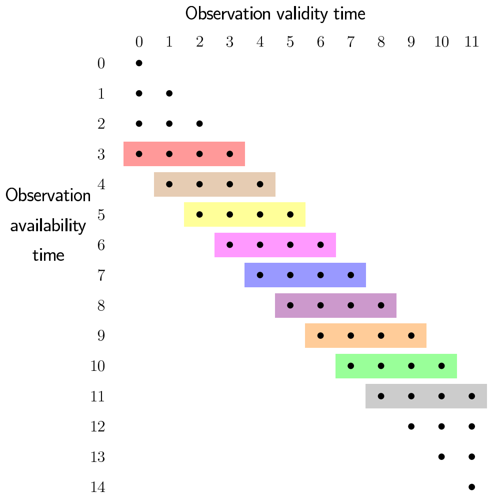

NWP SAF
PRS Delays vs. Receipt Times for 28-Apr-2015 to 25-May-2015
Met Office
All :1108995 obs from 00:00 28-Apr-2015 to 23:59 25-May-2015 62/ 99% met MAIN/UPDT cut-offs
AQAG-NOAA : 42990 obs from 00:00 28-Apr-2015 to 23:59 25-May-2015 57/100% met MAIN/UPDT cut-offs
AQAL-NOAA : 0 obs from 00:00 28-Apr-2015 to 23:59 25-May-2015 0/ 0% met MAIN/UPDT cut-offs
AQAW-NOAA : 268543 obs from 00:00 28-Apr-2015 to 23:59 25-May-2015 55/100% met MAIN/UPDT cut-offs
DM16-FNMO : 0 obs from 00:00 28-Apr-2015 to 23:59 25-May-2015 0/ 0% met MAIN/UPDT cut-offs
DM17-FNMO : 38190 obs from 00:00 28-Apr-2015 to 23:59 25-May-2015 63/ 98% met MAIN/UPDT cut-offs
DM18-FNMO : 39049 obs from 00:00 28-Apr-2015 to 23:59 25-May-2015 61/ 99% met MAIN/UPDT cut-offs
DM19-FNMO : 38463 obs from 00:00 28-Apr-2015 to 23:59 25-May-2015 62/ 99% met MAIN/UPDT cut-offs
FY3A-CMA : 0 obs from 00:00 28-Apr-2015 to 23:59 25-May-2015 0/ 0% met MAIN/UPDT cut-offs
FY3B-CMA : 35077 obs from 00:00 28-Apr-2015 to 23:59 25-May-2015 15/ 63% met MAIN/UPDT cut-offs
MAAB-EARS : 14940 obs from 00:58 28-Apr-2015 to 23:59 25-May-2015 77/100% met MAIN/UPDT cut-offs
MAAG-EUME : 46970 obs from 00:00 28-Apr-2015 to 23:59 25-May-2015 64/100% met MAIN/UPDT cut-offs
MAAL-EARS : 23609 obs from 00:00 28-Apr-2015 to 23:59 25-May-2015 80/100% met MAIN/UPDT cut-offs
MAIG-EUME : 44404 obs from 00:00 28-Apr-2015 to 23:59 25-May-2015 62/100% met MAIN/UPDT cut-offs
MAIL-METO : 589 obs from 10:00 28-Apr-2015 to 10:51 25-May-2015 89/100% met MAIN/UPDT cut-offs
MBAB-EARS : 17854 obs from 00:21 28-Apr-2015 to 23:21 25-May-2015 74/100% met MAIN/UPDT cut-offs
MBAG-EUME : 46952 obs from 00:00 28-Apr-2015 to 23:59 25-May-2015 71/100% met MAIN/UPDT cut-offs
MBAL-EARS : 36834 obs from 00:03 28-Apr-2015 to 23:39 25-May-2015 80/100% met MAIN/UPDT cut-offs
MBIG-EUME : 44336 obs from 00:00 28-Apr-2015 to 23:59 25-May-2015 70/100% met MAIN/UPDT cut-offs
MBIL-METO : 1617 obs from 09:11 28-Apr-2015 to 21:31 25-May-2015 64/100% met MAIN/UPDT cut-offs
N5AB-EARS : 0 obs from 00:00 28-Apr-2015 to 23:59 25-May-2015 0/ 0% met MAIN/UPDT cut-offs
N5AG-NOAA : 42631 obs from 00:00 28-Apr-2015 to 23:59 25-May-2015 46/ 99% met MAIN/UPDT cut-offs
N5AL-EARS : 3929 obs from 01:17 28-Apr-2015 to 22:05 25-May-2015 81/100% met MAIN/UPDT cut-offs
N8AB-EARS : 17291 obs from 01:21 28-Apr-2015 to 23:29 25-May-2015 85/100% met MAIN/UPDT cut-offs
N8AG-NOAA : 42916 obs from 00:00 28-Apr-2015 to 23:59 25-May-2015 44/ 99% met MAIN/UPDT cut-offs
N8AL-EARS : 56659 obs from 00:00 28-Apr-2015 to 23:59 25-May-2015 75/100% met MAIN/UPDT cut-offs
N9AB-EARS : 18563 obs from 00:13 28-Apr-2015 to 22:31 25-May-2015 86/100% met MAIN/UPDT cut-offs
N9AG-NOAA : 43041 obs from 00:00 28-Apr-2015 to 23:59 25-May-2015 65/100% met MAIN/UPDT cut-offs
N9AL-EARS : 57323 obs from 00:00 28-Apr-2015 to 23:59 25-May-2015 83/100% met MAIN/UPDT cut-offs
NPAT-METO : 1149 obs from 01:24 28-Apr-2015 to 14:37 25-May-2015 83/100% met MAIN/UPDT cut-offs
NPAT-NOAA : 42187 obs from 00:00 28-Apr-2015 to 23:59 25-May-2015 57/100% met MAIN/UPDT cut-offs
NPCR-NOAA : 42889 obs from 00:00 28-Apr-2015 to 23:59 25-May-2015 55/100% met MAIN/UPDT cut-offs
QU18
QG00
QU00
QG06
QU06
QG12
QU12
QG18
Delay (hours)
Receipt Time in MetDB (UTC)
© 2015, EUMETSAT
Plotted at 06:34ut 26-May-

Scheduling of global main and update runs



HPC resources used for global 4D-Var




Observation validity time
0 1 2 3 4 5 6 7 8 9 10 11
Observation availability time
0
1
2
3
4
5
6
7
8
9
10
11
12
13
14

Need optimal (Bayesian) estimation theory for overlapping windows.

Suppose that we at time k the following vectors of observations have just become available:

$\mathbf{y}_k^{(k)}$ valid at time k
$\mathbf{y}_{k-1}^{(k)}$ valid at time $k-1$
.
.
$\mathbf{y}_{k-L}^{(k)}$ valid at time $k-L$

Superscripts denote when the obs are available and subscripts their validity time, the longest time interval to availability being L time steps.

		Observation validity time			
		$k-2$	$k-1$	k	$k+1$
	$(k-2)$	$\mathbf{y}_{k-2}^{(k-2)}$			
Obs	$(k-1)$	$\mathbf{y}_{k-2}^{(k-1)}$	$\mathbf{y}_{k-1}^{(k-1)}$		
availability	(k)	$\mathbf{y}_{k-2}^{(k)}$	$\mathbf{y}_{k-1}^{(k)}$	$\mathbf{y}_{k}^{(k)}$	
time	$(k+1)$		$\mathbf{y}_{k-1}^{(k+1)}$	$\mathbf{y}_{k}^{(k+1)}$	$\mathbf{y}_{k+1}^{(k+1)}$
	$(k+2)$			$\mathbf{y}_{k}^{(k+2)}$	$\mathbf{y}_{k+1}^{(k+2)}$

Table: Notation for observation validity and availability times

Define $\underline{\mathbf{y}}_k$ to be the obs just available and therefore used at time k, so

$$\underline{\mathbf{y}}_k = \begin{pmatrix} \mathbf{y}_k^{(k)} \\ \mathbf{y}_{k-1}^{(k)} \\ \cdot \\ \cdot \\ \mathbf{y}_{k-L}^{(k)} \end{pmatrix} \tag{1}$$

Supposing

$$\mathbf{x}_{i+1} = \mathbf{f}(\mathbf{x}_i) + \boldsymbol{\omega}_i \text{ where } \boldsymbol{\omega}_i \sim N(\mathbf{0}, Q_i)$$

set

$$\underline{\mathbf{x}}_k = \begin{pmatrix} \mathbf{x}_k \\ \mathbf{x}_{k-1} \\ \vdots \\ \mathbf{x}_{k-L} \end{pmatrix}, \ \underline{\mathbf{f}}(\underline{\mathbf{x}}_k) = \begin{pmatrix} \mathbf{f}(\mathbf{x}_k) \\ \mathbf{x}_k \\ \vdots \\ \mathbf{x}_{k-L+1} \end{pmatrix}, \ \underline{\boldsymbol{\omega}}_k = \begin{pmatrix} \boldsymbol{\omega}_k \\ \mathbf{0} \\ \vdots \\ \mathbf{0} \end{pmatrix} \tag{2}$$

so

$$\underline{\mathbf{x}}_{k+1} = \underline{\mathbf{f}}(\underline{\mathbf{x}}_k) + \underline{\boldsymbol{\omega}}_k$$

Supposing also that

$$\mathbf{y}_i^{(k)} = H_i^{(k)}\mathbf{x}_i + \boldsymbol{\nu}_i^{(k)} \text{ where } \boldsymbol{\nu}_i^{(k)} \sim N(\mathbf{0}, R_i^{(k)})$$

and setting

$$\underline{\boldsymbol{\nu}}_k = \begin{pmatrix} \boldsymbol{\nu}_k^{(k)} \\ \boldsymbol{\nu}_{k-1}^{(k)} \\ \vdots \\ \boldsymbol{\nu}_{k-L}^{(k)} \end{pmatrix}$$

$$\underline{H}_k = \begin{pmatrix} H_k^{(k)} & & & \\ & H_{k-1}^{(k)} & & \\ & & \ddots & \\ & & & H_{k-L}^{(k)} \end{pmatrix}, \; \underline{Q}_k = \begin{pmatrix} Q_k & & & \\ & 0 & & \\ & & \ddots & \\ & & & 0 \end{pmatrix}$$

etc

Thus our system can be written

$$\underline{\mathbf{x}}_{k+1} = \underline{\mathbf{f}}(\underline{\mathbf{x}}_k) + \underline{\boldsymbol{\omega}}_k$$
$$\underline{\mathbf{y}}_k = \underline{H}_k \underline{\mathbf{x}}_k + \underline{\boldsymbol{\nu}}_k$$

for

$$\underline{\boldsymbol{\nu}}_k \sim N(\mathbf{0}, \underline{R}_k)$$
$$\underline{\boldsymbol{\omega}}_k \sim N(\mathbf{0}, \underline{Q}_k)$$

and our problem is to find

$$E[\underline{\mathbf{x}}_k | \underline{\mathbf{y}}_0, \underline{\mathbf{y}}_1, .., \underline{\mathbf{y}}_k]$$

This is now in a form to which we can apply standard filtering theory.

Eg, consider case where $\mathbf{f}$ is linearisable.

We have

$$\underline{\mathbf{f}}'(\underline{\mathbf{x}}_k) = \begin{pmatrix} \mathbf{f}'(\mathbf{x}_k) & 0 & 0 & 0 & 0 \\ I & 0 & 0 & 0 & 0 \\ 0 & I & 0 & 0 & 0 \\ \cdot & \cdot & \cdot & \cdot & \cdot \\ 0 & 0 & 0 & 0 & 0 \end{pmatrix}$$

and overlapping window problem is solved by applying Extended Kalman Filter to extended states/operators:

Given first guesses $\underline{\hat{\mathbf{x}}}_{L|L-1}, \underline{P}_{L|L-1}$

For $k = L, L+1, L+2, ..$

Assimilate:

$$\begin{aligned} \underline{K} &= \underline{P}_{k|k-1}\underline{H}_k^T(\underline{R}_k + \underline{H}_k\underline{P}_{k|k-1}\underline{H}_k^T)^{-1} \\ \underline{\hat{\mathbf{x}}}_{k|k} &= \underline{\hat{\mathbf{x}}}_{k|k-1} + \underline{K}(\underline{\mathbf{y}}_k - \underline{H}_k\underline{\hat{\mathbf{x}}}_{k|k-1}) \\ \underline{P}_{k|k} &= (\underline{I} - \underline{KH}_k)\underline{P}_{k|k-1} \end{aligned}$$

Predict:

$$\begin{aligned} \underline{\hat{\mathbf{x}}}_{k+1|k} &= \underline{\mathbf{f}}(\underline{\hat{\mathbf{x}}}_{k|k}) \\ \underline{P}_{k+1|k} &= \underline{\mathbf{f}}'(\underline{\hat{\mathbf{x}}}_{k|k})\underline{P}_{k|k}\underline{\mathbf{f}}'(\underline{\hat{\mathbf{x}}}_{k|k})^T + \underline{Q}_k \end{aligned}$$

End for $k = L, L+1, L+2, ..$

Remarks

• Above is EKF solution, but can equally well use unscented KF, ensemble SRF, etc

• It is a sequential solution which is equivalent to assimilating all obs up to that time simultaneously

• Full solution only involves model (or PF model) integration over last time slot, however

• the solution involves carrying $nL \times 1$ state vectors and $nL \times nL$ covariance matrices (more on this later)

• If all new obs occur only in last time slot simplifies to EKS

• Solution is equivalent to a modified version of 4D-Var, as shown on next slide:

Suppose $L = 2$ and the analysis error covariance at the end of previous window $\{i-2, i-1, i\}$ is

$$\underline{A}_i = \begin{pmatrix} A_{i,i} & A_{i,i-1} & A_{i,i-2} \\ A_{i-1,i} & A_{i-1,i-1} & A_{i-1,i-2} \\ A_{i-2,i} & A_{i-2,i-1} & A_{i-2,i-2} \end{pmatrix}$$

The optimal solution derived above for window $\{i-1, i, i+1\}$ is equivalent to the extended 4D-Var problem: minimise

$$\frac{1}{2}\begin{pmatrix} \boldsymbol{\delta}_i \\ \boldsymbol{\delta}_{i-1} \end{pmatrix}^T \begin{pmatrix} A_{i,i} & A_{i,i-1} \\ A_{i-1,i} & A_{i-1,i-1} \end{pmatrix}^{-1} \begin{pmatrix} \boldsymbol{\delta}_i \\ \boldsymbol{\delta}_{i-1} \end{pmatrix} +$$

$$\frac{1}{2}\sum_{i-1}^{i+1}(\mathbf{y}_j^{(i+1)} - (\mathbf{x}_j^g + \boldsymbol{\delta}_j))^T R^{-1}(\mathbf{y}_j^{(i+1)} - (\mathbf{x}_j^g + \boldsymbol{\delta}_j)) +$$

$$\frac{1}{2}(\boldsymbol{\delta}_{i+1} - M_i^{i+1}\boldsymbol{\delta}_i)^T Q^{-1}(\boldsymbol{\delta}_{i+1} - M_i^{i+1}\boldsymbol{\delta}_i)$$

First issue: size of states and covariances.

The state vectors are $nL \times 1$ and covariance matrices $nL \times nL$, ie, enormous!

Several approximations possible, eg

Retain from the previous analysis stage merely $\mathbf{x}^a_{i-L+1}$ and its $n \times n$ error covariance $A_{i-L+1,i-L+1}$, which will be used as the background state and its covariance at the beginning of the new sliding window, to be performed by weak constraint 4D-Var.

Optimal solution:

$$\begin{pmatrix} \mathbf{x}_{i+1}^g \\ \mathbf{x}_i^g \\ \mathbf{x}_{i-1}^g \end{pmatrix} = \begin{pmatrix} \mathbf{f}_i^{i+1}(\mathbf{x}_i^a) \\ \mathbf{x}_i^a \\ \mathbf{x}_{i-1}^a \end{pmatrix}$$

Then minimise

$$\frac{1}{2} \begin{pmatrix} \boldsymbol{\delta}_i \\ \boldsymbol{\delta}_{i-1} \end{pmatrix}^T \begin{pmatrix} A_{i,i} & A_{i,i-1} \\ A_{i-1,i} & A_{i-1,i-1} \end{pmatrix}^{-1} \begin{pmatrix} \boldsymbol{\delta}_i \\ \boldsymbol{\delta}_{i-1} \end{pmatrix} +$$

$$\frac{1}{2} \sum_{i-1}^{i+1} (\mathbf{y}_j^{(i+1)} - (\mathbf{x}_j^g + \boldsymbol{\delta}_j))^T R^{-1} (\mathbf{y}_j^{(i+1)} - (\mathbf{x}_j^g + \boldsymbol{\delta}_j)) +$$

$$\frac{1}{2} (\boldsymbol{\delta}_{i+1} - M_i^{i+1} \boldsymbol{\delta}_i)^T Q^{-1} (\boldsymbol{\delta}_{i+1} - M_i^{i+1} \boldsymbol{\delta}_i)$$

Then

$$\begin{pmatrix} \mathbf{x}_{i+1}^a \\ \mathbf{x}_i^a \\ \mathbf{x}_{i-1}^a \end{pmatrix} = \begin{pmatrix} \mathbf{x}_{i+1}^g \\ \mathbf{x}_i^g \\ \mathbf{x}_{i-1}^g \end{pmatrix} + \begin{pmatrix} \boldsymbol{\delta}_{i+1} \\ \boldsymbol{\delta}_i \\ \boldsymbol{\delta}_{i-1} \end{pmatrix}$$

Approximation:

$$\begin{pmatrix} \mathbf{x}^g_{i+1} \\ \mathbf{x}^g_i \\ \mathbf{x}^g_{i-1} \end{pmatrix} = \begin{pmatrix} \mathbf{f}^{i+1}_{i-1}(\mathbf{x}^a_{i-1}) \\ \mathbf{f}^{i}_{i-1}(\mathbf{x}^a_{i-1}) \\ \mathbf{x}^a_{i-1} \end{pmatrix}$$

Then minimise

$$\frac{1}{2}\boldsymbol{\delta}^T_{i-1}\left(A_{i-1,i-1} \right)^{-1}\boldsymbol{\delta}_{i-1} +$$

$$\frac{1}{2}\sum_{i-1}^{i+1}(\mathbf{y}_j^{(i+1)} - (\mathbf{x}^g_j + \boldsymbol{\delta}_j))^T R^{-1}(\mathbf{y}_j^{(i+1)} - (\mathbf{x}^g_j + \boldsymbol{\delta}_j)) +$$

$$\frac{1}{2}(\boldsymbol{\delta}_i - M^i_{i-1}\boldsymbol{\delta}_{i-1})^T Q^{-1}(\boldsymbol{\delta}_i - M^i_{i-1}\boldsymbol{\delta}_{i-1}) +$$

$$\frac{1}{2}(\boldsymbol{\delta}_{i+1} - M^{i+1}_i\boldsymbol{\delta}_i)^T Q^{-1}(\boldsymbol{\delta}_{i+1} - M^{i+1}_i\boldsymbol{\delta}_i)$$

Then

$$\begin{pmatrix} \mathbf{x}^a_{i+1} \\ \mathbf{x}^a_i \\ \mathbf{x}^a_{i-1} \end{pmatrix} = \begin{pmatrix} \mathbf{x}^g_{i+1} \\ \mathbf{x}^g_i \\ \mathbf{x}^g_{i-1} \end{pmatrix} + \begin{pmatrix} \boldsymbol{\delta}_{i+1} \\ \boldsymbol{\delta}_i \\ \boldsymbol{\delta}_{i-1} \end{pmatrix}$$

Several other approximations possible, all sharing property that they converge to optimal solution as model error $Q \to 0$.

Practically, Issue 1 is likely to be tractable.

Maybe more significant is

Second Issue, cycling of error covariances

Currently, the background error covariances used for large scale DA are largely climatological. Overcoming this by use of longer window is still one option, though costly if performing analyses hourly.

Use of longer windows in RUC as one way to overcome shortcomings of fixed B.

Tiny example for illustrative purposes:

Suppose for each validity time i two obs eventually become available, $y_i^{(i)}$ at time i and $y_i^{(i+1)}$ at time $i+1$.

Model is

$$x_{i+1} = r_i x_i$$

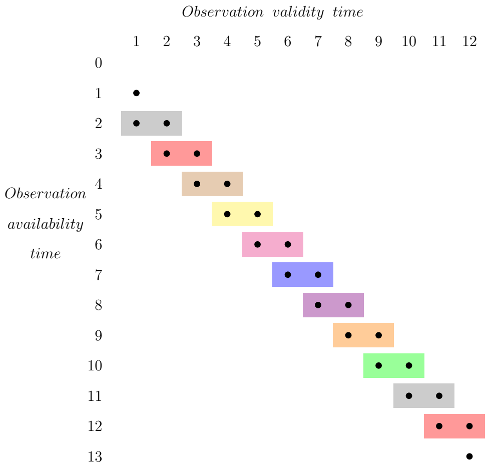
where r_i is randomly drawn from $U[1,2]$.

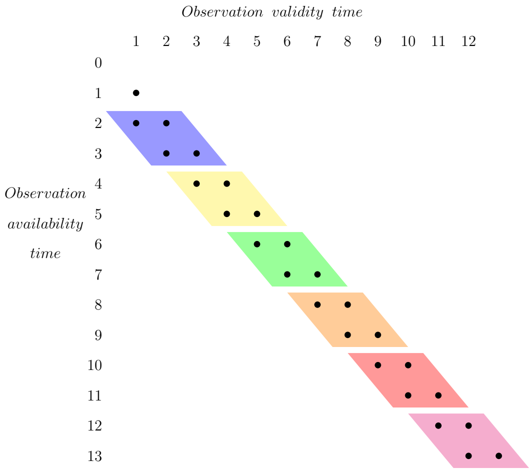
At time i we assimilate (with fixed B) either

(1) $y_{i-1}^{(i)}$ and $y_i^{(i)}$;

(2) $y_{i-2}^{(i-1)}$, $y_{i-1}^{(i-1)}$, $y_{i-1}^{(i)}$ and $y_i^{(i)}$;

(3) $y_{i-4}^{(i-3)}$, $y_{i-3}^{(i-3)}$, $y_{i-3}^{(i-2)}$, $y_{i-2}^{(i-2)}$, $y_{i-2}^{(i-1)}$, $y_{i-1}^{(i-1)}$, $y_{i-1}^{(i)}$ and $y_i^{(i)}$;


Observation validity time
1 2 3 4 5 6 7 8 9 10 11 12
Observation availability time
0 1 2 3 4 5 6 7 8 9 10 11 12 13


Observation validity time
1 2 3 4 5 6 7 8 9 10 11 12
Observation availability time
0
1
2
3
4
5
6
7
8
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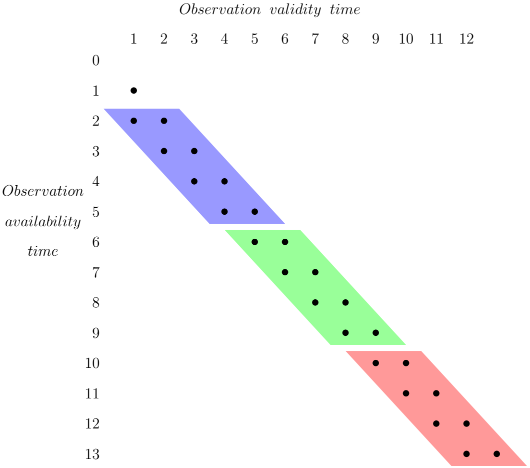
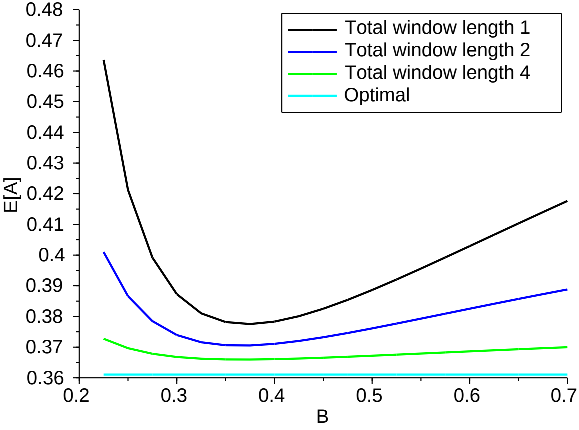
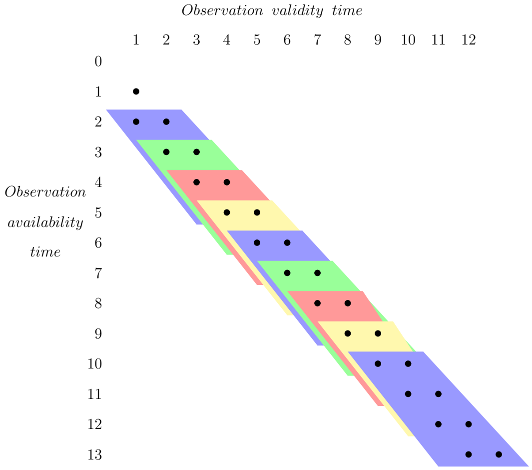
10
11
12
13


Observation validity time
1 2 3 4 5 6 7 8 9 10 11 12
0 1 2 3 4 5 6 7 8 9 10 11 12 13
Observation availability time

Mean square analysis error at end of window (so all methods have seen same obs) can be calculated in closed form.



So for hourly analyses we could do something like this ...



Alternatively we can go back to the optimal solution and attempt to cycle covariances (approximately) correctly.

Several possibilities:

(a) Estimate posterior covariance from Var Hessian using limited memory quasi-Newton (‘LM Q-N’) machinery, and evolve to next time level by solving auxiliary (also LM Q-N) minimisation problem (cf ‘VKF’);

(b) As (a) but use CG/Lanczos (cf ‘EVIL’)

(c) Use ensemble square root filter (cf current hybrid)

Cycling of covariances by LM Q-N

Exploit following facts:

- Analysis error covariance A in principle equals inverse of Hessian H of J
- With LM Q-N methods such as BFGS, at each iteration the estimate of H^{-1}

$$H_{est}^{-1} \leftarrow H_{est}^{-1} \; + \; rank\ 2\ matrix$$

- Given (a low rank estimate of) A the inverse Hessian of

$$\mathbf{x}^T(MAM^T + Q)\mathbf{x}$$

is B^{-1}, the inverse of the background error covariance required at the next cycle.

Remarks

To get good approx to H_{est}^{-1} need to reformulate problem so that H is pert to identity

Can achieve this by preconditioning by U where

$$UU^T = diag(B, Q, Q, ..)$$

Then in limit of zero-sized subspace, method collapses to 4D-Var with non-cycled climatological B.

The estimation of the analysis covariance is effectively zero cost.

Can increase rank of covariance approximations by

• Accumulating vector pairs over many cycles (LM Q-N well suited to this)

(also, may be scope for parallelism in computation of vector pairs)

• Exploiting structure of problem ('partial separability')

Estimation of covariances by ensemble SRF

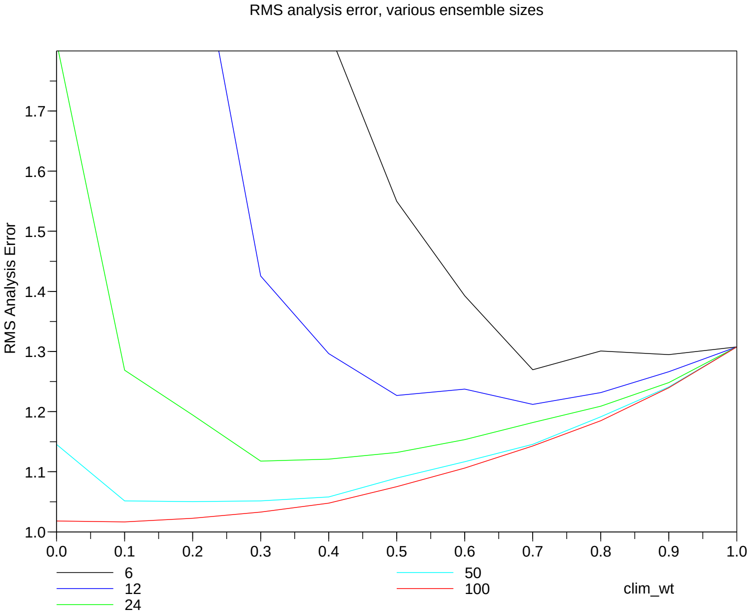
More than one way to use ensemble SRF for covariances

One way is based directly on optimal strategy, where basic objects are $nL \times 1$ vectors and $nL \times nL$ covariance matrices

Estimate climatological $\underline{B}_{clim}$ by bootstrapping, then

Run optimal strategy in its variational form (for the analysis) and ensemble SRF (for the adaptive part of the covariances) in tandem, using for the prior covariance $\underline{\mathrm{B}}$ a convex combination of $\underline{B}_{clim}$ and the ensemble SRF estimate $\underline{B}_{ens}$

In this case the ensemble is only run for one time slot, from $i-1$ to i.


RMS analysis error, various ensemble sizes
RMS Analysis Error
1.0
1.1
1.2
1.3
1.4
1.5
1.6
1.7
0.0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1.0
6
12
24
50
100
clim_wt

Concluding Remarks

There are several potential benefits from frequent update cycling, including timely boundary conditions for LAMs, and potentially better performance and affordability.

For frequent analyses the assimilation windows will normally overlap. An optimal Bayesian solution to this problem is readily obtained.

In the presence of model error this solution involves cycling large state vectors and covariance matrices. One can readily construct approximate approaches involving same-sized quantities to present.

To overcome the limitations of a largely climatological prior covariance B a long window approach is still possible, though now costly.

Alternatively, several options exist for covariance cycling, including the use of appropriately constructed ensembles.