

Advances in data assimilation techniques and their relevance to satellite data assimilation

ECMWF Seminar on Use of Satellite Observations in NWP

Andrew Lorenc, , 8-12 September 2014.

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- 1. Developments in DA methods
 - Hybrid-4DVar
 - 4D-Ensemble-Var
 - EnKF (e.g. LETKF)
- 2. Some potentially difficult problems relevant to satellite DA
 - How do the various methods fare?
- 3. Some personal opinions



Developments in DA methods

- 1. The ability to predict the evolution and growth of forecast errors was at the heart of the THORPEX.
- 2. Evolving capabilities & requirements of NWP:
 - Computing
 - Nonlinearity
 - Ensembles

Hybrid-4DVar – using EOTD information from ensemble

4DEnVar – using ensemble trajectories instead of model & adjoint

EnKF – general & **LETKF** – a popular flavour (related to 4DEnVar)



4-Dimensional DA Methods

Each is a 4D best-fit to observations in a 6 hour window, assuming Gaussian background and observation errors. I use underline to denote 4D variables and operators:

 \mathbf{x}^{b} background trajectory 4D error covariance of \mathbf{x}^{b} \mathbf{P} $\delta \mathbf{x}$ 4D analysis increment $\mathbf{y} = \underline{H} \left(\underline{\mathbf{x}}^b + \delta \underline{\mathbf{x}} \right)$ model estimate of obs $J(\delta \mathbf{x}) = \frac{1}{2} \delta \mathbf{x}^T \mathbf{P}^{-1} \delta \mathbf{x} + \frac{1}{2} (\mathbf{y} - \mathbf{y}^o)^T \mathbf{R}^{-1} (\mathbf{y} - \mathbf{y}^o)$ penalty function <u>**P**</u> is **big**! We cannot even estimate it fully, let alone compute $\frac{1}{2}\delta \mathbf{x}^T \mathbf{P}^{-1} \delta \mathbf{x}$. The solution is to model \mathbf{P} using a sequence of operations we can compute, then use these to transform $\delta \mathbf{x}$ so that $\frac{1}{2} \delta \mathbf{x}^T \mathbf{P}^{-1} \delta \mathbf{x}$ simplifies.

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 $\mathbf{B} = \mathbf{U}\mathbf{U}^T$ Model 3D covariance using transforms 3D analysis increment $\delta \mathbf{x}_0 = \mathbf{U} \mathbf{v}^c$ $\delta \mathbf{x} = \mathbf{M} \delta \mathbf{x}_0$ made 4D using linear forecast model ${f M}$ $\mathbf{P} = \mathbf{M} \mathbf{B} \mathbf{M}^T$ Implicit 4D prior covariance Transformed penalty function $J(\mathbf{v}^c) = \frac{1}{2}\mathbf{v}^{cT}\mathbf{v}^c + \frac{1}{2}(\mathbf{y} - \mathbf{y}^o)^T \mathbf{R}^{-1}(\mathbf{y} - \mathbf{y}^o)$

4 DVar: using climatological covariance B





Weaknesses of 4DVar.

- \mathbf{B} no flow-dependent Errors Of The Day
 - 1. Use recent ensembles to train a new B
 - 2. Use current ensemble to supplement B
- Parallelisation sequential runs of $\underline{\mathbf{M}} \& \underline{\mathbf{M}}^T$
 - 1. Parallelise in time too
 - 2. Use an ensemble instead (4DEnVar)
- No direct analysis ensemble
 - 1. Use a perturbed observation ensemble of 4DVars
 - 2. Use a separate EnKF system



Ensemble covariance filtering

B is big! We need a large ensemble PLUS clever filtering to reduce sampling noise, based on 2 ideas:

- Assume local homogeneity apply smoothing: horizontal, rotational, and time
- Assume some correlations are near zero, & localise: horizontal, vertical, spectral, between transformed variables

Two approaches to hybrid covariances, using these ideas:

- 1. Train a covariance model using recent ensembles
- 2. Augment **B** by using localised ensemble perturbations







From Lorenc (2003)



From Lorenc (2003)



Convective-scale ensemble s.d. of humidity at 945hPa

AEARO 84



AEARO 06



AEARO 06 - filtered



Large ensemble (84 members)

Small ensemble (6 members)

Horizontally filtered small ensemble

Using the AROME ensemble (Ménétrier et al. 2014).



p: sigma at level 39 10402m, max=89.6044







p: sigma at level 39 10402m, max=71.6403







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Ensemble covariance filtering: Met Office

The two approaches to hybrid covariances:

Train a covariance model using recent ensembles
 Augment B by using localised ensemble perturbations
 start from different ends; 1 starts from a climatological
 covariance model, then adds ensemble derived coefficients,
 starts from a raw ensemble then filters the covariances.
 Eventually they might meet in the middle.

As we shall see later, there is less scope for these methods in the EnKF, other than simple spatial localisation.



En-4DVar: using an ensemble of 3D states which samples background errors Ensemble perturbation matrix $\mathbf{X} = \left| \mathbf{x}'_1 \cdots \mathbf{x}'_N \right|$ where $\mathbf{x}'_k = \frac{1}{\sqrt{N-1}} \left(\mathbf{x}_k - \bar{\mathbf{x}} \right)$ $\mathbf{P} = \mathbf{C} \circ \mathbf{X} \mathbf{X}^T$ Model 3D \mathbf{P} as localised ensemble covariance, $\mathbf{C} = \mathbf{U}^{\alpha} \mathbf{U}^{\alpha T}$ then model \mathbf{C} using transforms $\boldsymbol{\alpha}_k = \mathbf{U}^{\alpha} \mathbf{v}_k^{\alpha}$ 3D localised linear combination of ensemble perturbations $\delta \mathbf{x}_0 = \Sigma_{k-1}^N \boldsymbol{\alpha}_k \circ \mathbf{x}'_k$ then linear forecast model \mathbf{M} $\delta \mathbf{x} = \mathbf{M} \delta \mathbf{x}_0$ $\underline{\mathbf{P}} = \underline{\mathbf{M}} \left(\mathbf{C} \circ \mathbf{X} \mathbf{X}^T \right) \underline{\mathbf{M}}^T$ Localized 4D covariance $\mathbf{v}^T = \begin{bmatrix} \mathbf{v}_1^{\alpha T} \cdots \mathbf{v}_N^{\alpha T} \end{bmatrix}$ concatenated control vectors $J(\mathbf{v}) = \frac{1}{2}\mathbf{v}^T\mathbf{v} + \frac{1}{2}(\mathbf{y} - \mathbf{y}^o)^T\mathbf{R}^{-1}(\mathbf{y} - \mathbf{y}^o)$ Transformed penalty function © Crown copyright Met Office Andrew Lorenc 15



hybrid-4DVar

4D analysis increment
$$\delta \mathbf{x} = \mathbf{M} \left(\beta_c \mathbf{U} \mathbf{v}^c + \beta_e \boldsymbol{\Sigma}_{k=1}^N \mathbf{U}^\alpha \mathbf{v}_k^\alpha \circ \mathbf{x}_k' \right)$$

Localized 4D covariance
$$\mathbf{P} = \mathbf{M} \left(\beta_c^2 \mathbf{B} + \beta_e^2 \mathbf{C} \circ \mathbf{X} \mathbf{X}^T \right) \mathbf{M}^T$$

concatenated control vectors

$$\mathbf{v}^T = \begin{bmatrix} \mathbf{v}^{cT}, \mathbf{v}_1^{\alpha T} \cdots \mathbf{v}_N^{\alpha T} \end{bmatrix}$$

1% improvement in rms errors when implemented at Met Office (Clayton *et al.* 2013)



u increments fitting a single u ob at 500hPa, at different times.



4D-Var

Hybrid 4D-Var

Unfilled contours show T field. Clayton *et al.* 2013



Parallelisation





4DVar has several potential problems looming in the next decade - their timing for each centres will depend on their computers and models:

1. Need new design to use millions of parallel threads, especially in sequential runs of linear (PF) and Adjoint models.

2. Forecast models are being redesigned to address this – a maintenance issue for the PF and Adjoint models.

A simple solution is to use the ensemble trajectories, pre-calculated in parallel, instead of the models inside 4DVar.

If Fourier filters and Poisson solvers are not available then the LETKF is an easier approach.

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4DEnVar: using an ensemble of 4D trajectories which samples background errors

Ensemble trajectory matrix $\mathbf{X} = \left| \mathbf{x}'_1 \cdots \mathbf{x}'_N \right|$ where $\mathbf{x}'_k = \frac{1}{\sqrt{N-1}} \left(\mathbf{x}_k - \bar{\mathbf{x}} \right)$ $\mathbf{P} = \mathbf{C} \circ \mathbf{X} \mathbf{X}^T$ Model 4D \mathbf{P} directly, as localised ensemble covariance. $\underline{\mathbf{C}} = \mathbf{U}^{\alpha} \mathbf{U}^{\alpha T}$ then model $\underline{\mathbf{C}}$ using transforms $\underline{\boldsymbol{\alpha}}_k = \underline{\mathbf{U}}^{\alpha} \mathbf{v}_k^{\alpha}$ 4D localised linear combination of ensemble trajectories $\delta \mathbf{x} = \Sigma_{k-1}^N \, \boldsymbol{\alpha}_k \circ \mathbf{x}'_k$ $\mathbf{v}^T = \begin{bmatrix} \mathbf{v}_1^{\alpha T} \cdots \mathbf{v}_N^{\alpha T} \end{bmatrix}$ concatenated control vectors $J(\mathbf{v}) = \frac{1}{2}\mathbf{v}^T\mathbf{v} + \frac{1}{2}(\mathbf{y} - \mathbf{y}^o)^T\mathbf{R}^{-1}(\mathbf{y} - \mathbf{y}^o)$ Transformed penalty function

4DEnVar: using an ensemble of 4D trajectories which samples background errors *Extra Details*

model ${f C}$ using transforms

It is common to use a 3D C and persistence in time: I

4D localised linear combination of ensemble trajectories

can be built from 3D localised perturbations and constant $\boldsymbol{\alpha}_k$.

Matrix notation:

 $\mathbf{A} = \begin{bmatrix} \boldsymbol{\alpha}_1' \ \cdots \ \boldsymbol{\alpha}_N' \end{bmatrix}$ $\mathbf{1}_N \text{ is a column vector of N 1s}$ $\underline{\mathbf{C}} = \underline{\mathbf{U}}^{\alpha} \underline{\mathbf{U}}^{\alpha T}$

 $\mathbf{C} = \mathbf{U}^{\alpha}\mathbf{U}^{\alpha T}$ $\mathbf{\underline{C}} = \mathbf{I}\mathbf{C}\mathbf{I}^{T}$

$$\delta \underline{\mathbf{x}} = \Sigma_{k=1}^{N} \, \underline{\alpha}_{k} \circ \underline{\mathbf{x}}_{k}'$$

$$\boldsymbol{\alpha}_{k} = \mathbf{U}^{\alpha} \mathbf{v}_{k}^{\alpha}$$
$$\delta \mathbf{x}(t) = \Sigma_{k=1}^{N} \boldsymbol{\alpha}_{k} \circ \mathbf{x}_{k}'(t)$$

 $\delta \mathbf{x}\left(t\right) = \left(\mathbf{A} \circ \mathbf{X}\left(t\right)\right) \mathbf{1}_{N}$





En-4DVar analysis increment $\delta \mathbf{x} = \mathbf{M} \Sigma_{k=1}^{N} \boldsymbol{\alpha}_{k} \circ \mathbf{x}_{k}'$

4DEnVar analysis increment $\delta \mathbf{x} = \Sigma_{k=1}^{N} \boldsymbol{\alpha}_{k} \circ \mathbf{x}'_{k}$

Test with a single wind ob, in a jet, at the start of the window



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100% ensemble 1200km localization scale





Met Office trial of 4DEnVar Lorenc et al. (2014)

Our first trial copied settings from the hybrid-4DVar:

- C with localisation scale 1200km,
- hybrid weights β_c^2 =0.8, β_e^2 =0.5

Results were disappointing:



The reason was the large weight given to the climatological covariance, which is treated like 3DVar in 4DEnVar



hybrid-4DEnVar

4D analysis increment
$$\delta \mathbf{x} = \beta_c \mathbf{I} \delta \mathbf{x}_0 + \beta_e \Sigma_{k=1}^N \boldsymbol{\alpha}_k \circ \mathbf{x}'_k$$

Localized 4D covariance $\mathbf{P} = \beta_c^2 \mathbf{IBI}^T + \beta_e^2 \mathbf{C} \circ \mathbf{X} \mathbf{X}^T$

hybrid-4DVar

4D analysis increment $\delta \mathbf{x} = \mathbf{M} \left(\beta_c \delta \mathbf{x}_0 + \beta_e \Sigma_{k=1}^N \boldsymbol{\alpha}_k \circ \mathbf{x}'_k \right)$

Localized 4D covariance $\mathbf{P} = \mathbf{M} \left(\beta_c^2 \mathbf{B} + \beta_e^2 \mathbf{C} \circ \mathbf{X} \mathbf{X}^T \right) \mathbf{M}^T$



50-50% hybrid 1200km localization scale





EnKF – common properties

Produce an analysis ensemble – need to distinguish

Use the matrix of ensemble model-ob perturbations.

but it is calculated using nonlinear H:

 $\underline{\mathbf{y}}_{k}^{\prime} = \frac{1}{\sqrt{N-1}} \left(\underline{H} \left(\underline{\mathbf{x}}_{k}^{b} \right) - \overline{\underline{H} \left(\underline{\mathbf{x}}^{b} \right)} \right)$ $\underline{\mathbf{Y}}^{b} = \left[\underline{\mathbf{y}}_{1}^{\prime} \cdots \underline{\mathbf{y}}_{N}^{\prime} \right]$

Most use the localised ob-gridpoint covariance

Stochastic filters (Houtekamer *et al.*, 2014) use the same analysis equation for each member and perturb observations (as in ensembles of 4DVar).

SQRT filters (Tippett *et al.*, 2003) analyses the ensemble mean, then calculate perturbations such that $\underline{\mathbf{X}}^{a}\underline{\mathbf{X}}^{aT} = \underline{\mathbf{P}}^{a}$.

$$\mathbf{X}^b$$
 (previously \mathbf{X}) and \mathbf{X}^a

For linear H

 $\mathbf{Y}^b = \mathbf{H}\mathbf{X}^b$

 $\mathbf{C} \circ \mathbf{Y}^b \mathbf{X}^{bT}$



LETKF

The equations of Hunt *et al.* (2007); Harlim and Hunt (2007) apply the factor $1/\sqrt{N-1}$ to $\mathbf{w} \& \boldsymbol{\alpha}$ rather than \mathbf{X}^{b} .

ETKF for mean analysis $\delta \mathbf{x} = \mathbf{X}^b \mathbf{w}$ $\mathbf{w} = \tilde{\mathbf{P}}^a \left(\mathbf{Y}^b\right)^T \mathbf{R}^{-1} \left(\underline{\mathbf{y}}^o - H\left(\underline{\mathbf{x}}^b\right)\right)$ The ensemble-space matrix
inversion is solved directly $\tilde{\mathbf{P}}^a = \left[\mathbf{I} + \left(\mathbf{Y}^b\right)^T \mathbf{R}^{-1} \mathbf{Y}^b\right]^{-1}$ $\tilde{\mathbf{P}}^a = \left[\mathbf{I} + \left(\mathbf{Y}^b\right)^T \mathbf{R}^{-1} \mathbf{Y}^b\right]^{-1}$ $\tilde{\mathbf{SQRT-filter}}$ for the analysis
pertubations $\tilde{\mathbf{X}}^a = \left(\tilde{\mathbf{P}}^a\right)^{1/2} \mathbf{X}^b$

LETKF solves these equations separately for each grid-point, with local observations

Each point's ${\bf w}$ is a row of matrix

Equivalent to 4DEnVar

 $\mathbf{A} = \begin{bmatrix} \boldsymbol{\alpha}_1' \ \cdots \ \boldsymbol{\alpha}_N' \end{bmatrix}$

$$\delta \mathbf{x}\left(t\right) = \left(\mathbf{A} \circ \mathbf{X}\left(t\right)\right) \mathbf{1}_{N}$$

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- EnKF are usually implemented in more straightforwardly way than variational schemes: model-ob values are calculated from each member, and used to calculate covariances with all model variables.
- A design goal in to keep the analysis cost small compared to that of the ensemble forecasts.
- Spatial localisation is used, in observation space.
 The localisation should select <*N* useful observations.
- Ensemble sizes can be quite large, e.g. Houtekamer et al. (2014) showed benefit from increasing the ensemble size above 196. In an experiment with the SPEEDY model, Miyoshi *et al.* 2014 tested ensemble up to 10240!



Cost & benefit of improvements to the EC EnKF system (Houtekamer *et al.* 2014)



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Met Office DA

A small selection of potential difficulties -- their relevance depends on the application and NWP system.

- Dense but incomplete observations, tracers
- Synergistic observations
- Cloudy inversions
- Non-Gaussian observed variables
- Initialisation Spin-up Staying near the attractor



Dense but incomplete observations, tracers

- Remote sensing normally gives dense but incomplete obs
- Prognostic eqns link space & time gradients of variables
- Tracers give simplest example (but others as important)
- 4DVar can get winds from tracers (Mary Forsythe's talk)
- So can Extended KF, if obs network is good (Daley 1996)
- For the EnKF, strong spatial localisation hinders deriving longer-scales in wind field.
- For 4DEnVar, scale-dependent localisation may help (work in progress)

Met Office 100% ensemble 500km localization scale







Synergistic observations

- If observations' "footprints" (i.e. the model variables which predict them) overlap, then it helps to use them together
- Observation-space localisation $\underline{\mathbf{C}} \circ \underline{\mathbf{Y}}^b \underline{\mathbf{X}}^{bT} = \underline{\mathbf{C}} \circ \mathbf{H} \underline{\mathbf{X}}^b \underline{\mathbf{X}}^{bT}$ $\mathbf{C} \circ \mathbf{X}^b \mathbf{X}^{bT}$ damages this. Model-space localisation (as in 4DEnVar) does not.
- Campbell et al. (2010) showed that observation space localisation degraded a 1D ensemble DA of radiances.
- My example is >30 years old!



Analysis error for 500hPa height for different combinations of error-free observations.

- V500

Z500 -

1000hPa	1000-500hPa	500hPa wind	500hPa
height (m)	thickness (m)	component	height (m)
(surface P)	(layer-mean T)	(m/s)	5 ()
	weights		Error (m)
			21.0
0.143			20.8
	0.419		19.1
		0.441	18.9
	0.611	0.628	14.4
0.192		0.461	18.4
0.520	0.699		16.7
0.853	1.147	0.880	1.9



Lorenc, A.C. 1981: "A global three-dimensional multivariate statistical analysis scheme." *Mon. Wea. Rev.*, **109**, 701-721.

N.B. using perfect obs



- Top priority problem for Met Office users
- Lorenc (2007) study of cloudy inversions in sondes & model
 ⇒The prior PDF is highly non-Gaussian
 ⇒High variances, & small correlation across inversion
- Ensemble covariances can help the second problem, but NOT the first.

Error PDFs composited by cloudy inversion level: Left: mean of T & RH, \Rightarrow large bias Met Office Right: correlations with level 5, $\Rightarrow \sim 0$ across inversion

All740328 All740328 2Clb 2344 2Clb 2344 20 20 3Clb 4052 20 3Clb 4020 4Clb 6059 4Clb 6059 5Clb 7704 5Clb 7704 7Clb 6534 7Clb 6534 15 15 15 8Clb 6357 8Clb 6357 model level model level 10 10 10 10 5 5 5 5 -20-10 0 10 20 0 0 -2 -10 1 2 -1 $^{-1}$ T T 5 mean RH % RH RH 5 mean T

Lorenc (2007) © Crown copyright Met Office Andrew Lorenc 37

Left: MOGREPS-R T profiles for a cloudy inversion: control sonde. Right: T covariances. Met Office Profile for station (54.50, -6.33) VT: 00Z on 29/12/2008 T+06h Pressure (hPa) Temperature (K) **Neill Bowler**

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^{-3.87 -2.58 -1.29 0.43 1.72 3.01 4.3}



- Can be handled by 4DVar and 4DEnVar with outer-loop or nonlinear *H* in inner-loop.
- EnKF effectively linearises *H* using the background sample this is not as accurate (but it is more robust)
- Observations of model-derived variables such as ppn, cloud, radar-reflectivity have been tried in 4DVar and EnKF. The EnKF is simpler to do.



Idealised EnKF of a perfect wind-speed observation



Lorenc (2003) © Crown copyright Met Office Andrew Lorenc 40



Non-Gaussian cloud errors

Met Office (Renshaw and Francis 2011)



(Also VarQC, scatterometer de-aliasing, ...)

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Initialisation – Spin-up – Met Office Staying near the attractor

- In a linear world we would be blown away!
 We rely on nonlinear limits to growth of small perturbations,
- Resolution is increasing faster than observations, so the dependence on the model attractor is increasing. Diagnostic relationships are getting less useful.
- Technical fixes have been with us for years:

≻Incremental DA – leave the model alone if no obs!

Make increments smooth and balanced

Allow model to adjust when we add them: long enough window, 4DIAU, extra damping



Spin up of showery precipitation inside an inflow boundary

1.5km grid

UK1p5, Total Rain amount (mm) 18 hours, from 09UTC 20090617





variable grid

UKV, Total Rain amount (mm) 18 hours, from 09UTC 20090617





_(c)4km grid

UK4, Total Rain amount (mm) 18 hours, from 09UTC 20090617





Tang et al. 2013



Vision – ideal Global DA for NWP, using quasi-linear methods

- "Best estimate" DA of "known" scales (~12km), using 4D-Var because of:
 - Desire to treat all scales together;
 - Desire to make best use of satellite obs e.g. by bias correction, using high-resolution.
- Hybrid ensemble to carry forward error information from past few days.
- May still be scope for nested regional systems to give more rapid running and higher resolution.

N.B. This vision is good for perhaps a decade, while we are restricted to well known scales, so the KF theory of a "best estimate" + a covariance description of uncertainty is useful.

WWRP/THORPEX Workshop on 4D-Var and Ensemble Kalman Filter Inter-comparisons. © Crown copyright Met Office Andrew Lorenc 44 Buenos Aires - November 2008

Some Personal Conclusions Long-term

- The scientific advantages of 4DVar are decreasing and will eventually not outweigh the increasing technical difficulties. (4DEnVar could be a replacement for 4DVar.)
- Convective-scale ensembles essential
 forecast uncertainty.
 Model dev, getting obs, & computational cost will dominate.
 Perhaps this militates in favour of the simple EnKF,
 but I prefer nested 4DEnVar, to handle all scales.
- Global NWP may fall further behind in computing, nevertheless, unless we get many more observations, convective-scale global NWP models will be available long before we know how to do their DA.



Question re global NWP

- In 10~20 years we will be able to run global ensembles at resolutions such that the initial errors are non-Gaussian.
 If the ensemble mean is so smooth as to be significantly implausible as a real state, the errors are non-Gaussian.
- Kalman Filter based methods (i.e. 4D-Var & EnKF) are not appropriate.
- [Nonlinear initialisation / the model attractor / spin-up] will be very important because of assimilation of imagery data and the desire for short-period precipitation forecasts.
- Models and observations will still be imperfect.
- Particle filters will be unaffordable.
- What will you do? (I will be retired ③)

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