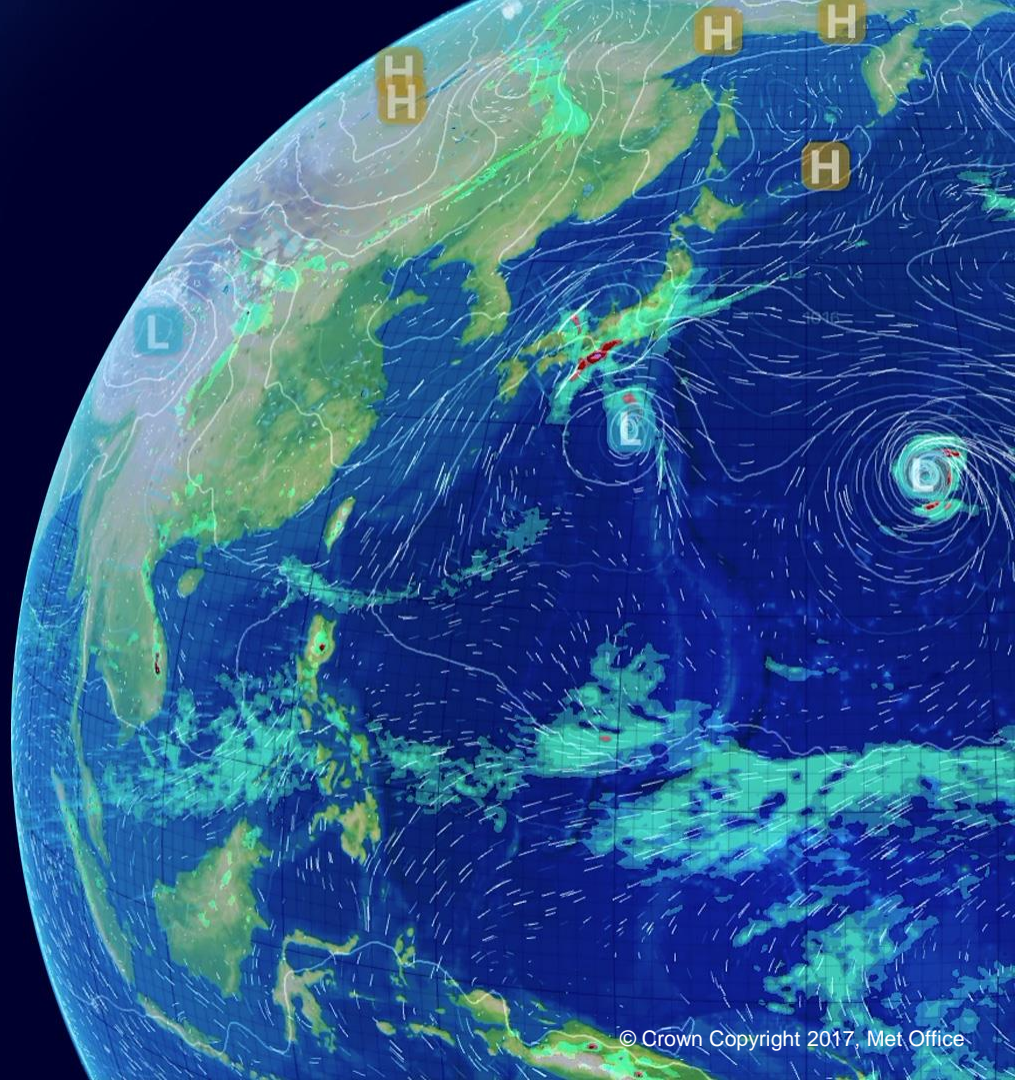


EnKF methods to initialize ensembles

Neill Bowler

ECMWF annual seminar



Contents

Basic derivation of EnKF

Localisation

Inflation

Inbreeding, non-linearity ...

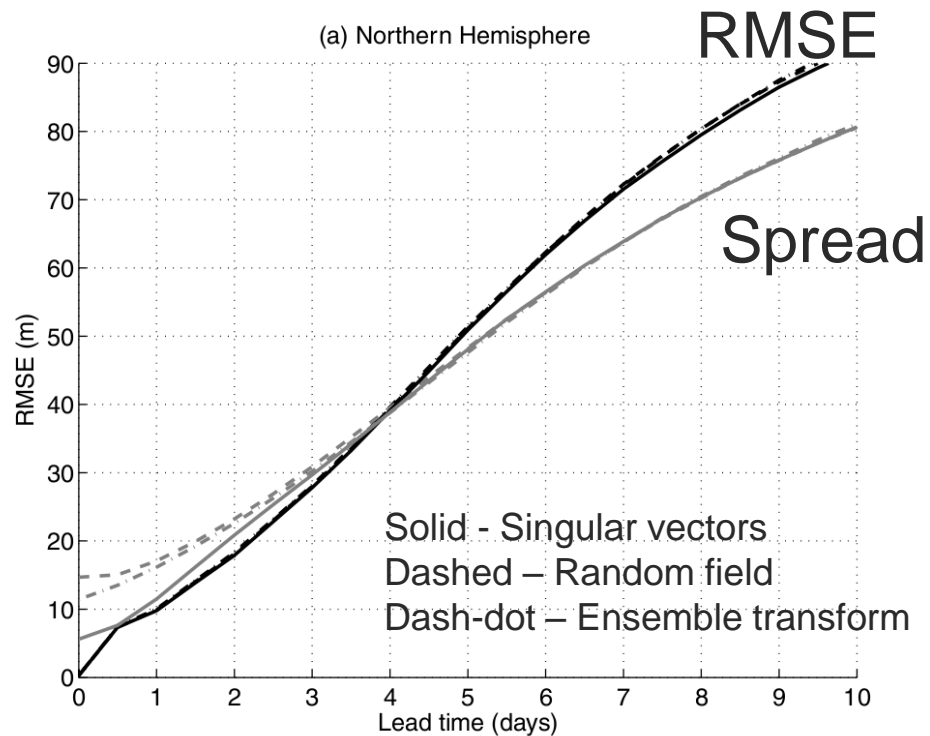
Conclusion

... before we begin

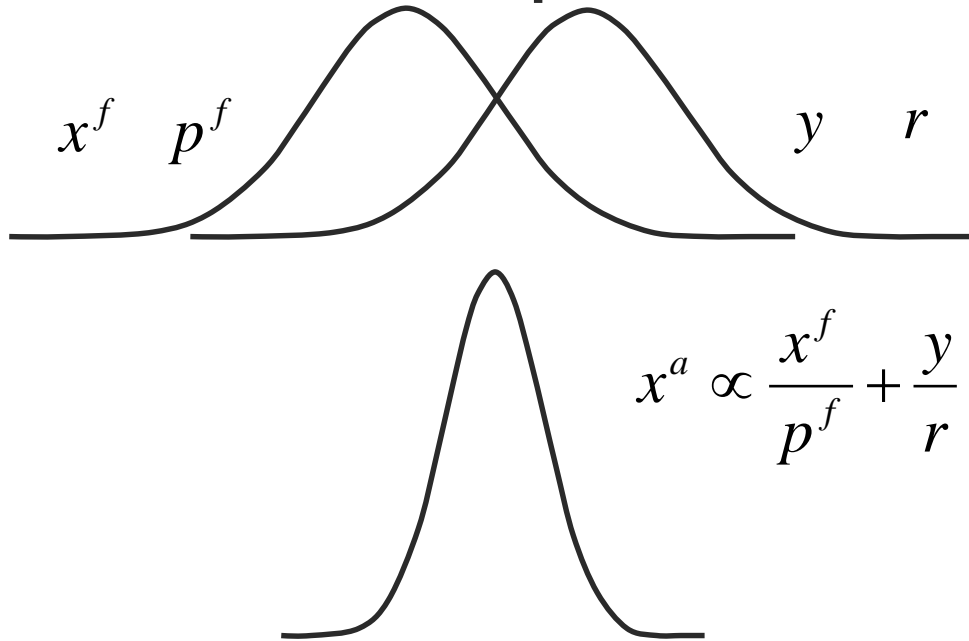
So what?

Magnusson et al (2009) showed that initialisation method matters little for medium-range ensemble forecasting

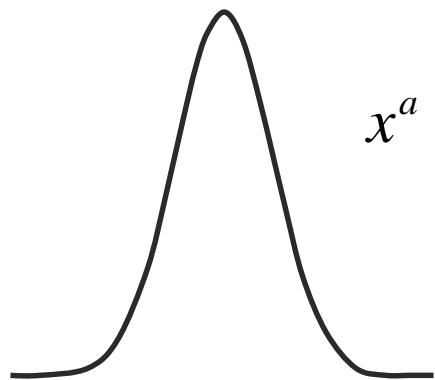
Increased focus on data assimilation as a way to measure performance



How to make an optimal estimate



How to make an optimal estimate



$$x^a \propto \frac{x^f}{p^f} + \frac{y}{r}$$

$$x^a = \frac{rp^f}{r + p^f} \left(\frac{x^f}{p^f} + \frac{y}{r} \right) = x^f + \frac{p^f}{r + p^f} (y - x^f)$$

$$p^a = \left(1 - \frac{p^f}{r + p^f} \right) p^f$$

Kalman filter equations

Update $\mathbf{K}_n = \mathbf{P}_n^f \mathbf{H}^T \left(\mathbf{H} \mathbf{P}_n^f \mathbf{H}^T + \mathbf{R}_n \right)^{-1}$

$$\mathbf{x}_n^a = \mathbf{x}_n^f + \mathbf{K}_n \left(\mathbf{y}_n - \mathbf{H} \mathbf{x}_n^f \right)$$

$$\mathbf{P}_n^a = \mathbf{P}_n^f - \mathbf{K}_n \mathbf{H} \mathbf{P}_n^f$$

Forecast $\mathbf{x}_n^f = \mathbf{M} \mathbf{x}_{n-1}^a$ $\mathbf{P}_n^f = \mathbf{M} \mathbf{P}_{n-1}^a \mathbf{M}^T + \mathbf{Q}_n$

NWP approximations

Update $\mathbf{K}_n = \mathbf{P}_n^f \mathbf{H}^T (\mathbf{H} \mathbf{P}_n^f \mathbf{H}^T + \mathbf{R}_n)^{-1}$

$$\mathbf{x}_n^a = \mathbf{x}_n^f + \mathbf{K}_n (\mathbf{y}_n - \mathbf{H} \mathbf{x}_n^f)$$

$$\mathbf{P}_n^a = \mathbf{P}_n^f - \mathbf{K}_n \mathbf{H} \mathbf{P}_n^f$$

Forecast $\mathbf{x}_n^f = \mathbf{M} \mathbf{x}_{n-1}^a$ $\mathbf{P}_n^f = \mathbf{M} \mathbf{P}_{n-1}^a \mathbf{M}^T + \mathbf{Q}_n$

The model-size problem

Operational model has 2.7×10^9 variables

\mathbf{P}^f has 7×10^{18} entries (thousands of peta-bytes)

Use an ensemble to sample from this

$$\mathbf{X}_n^f = \frac{1}{\sqrt{N-1}} \left(\mathbf{x}_n^{f,1} - \overline{\mathbf{x}_n^f} \quad \mathbf{x}_n^{f,2} - \overline{\mathbf{x}_n^f} \quad \dots \quad \mathbf{x}_n^{f,N} - \overline{\mathbf{x}_n^f} \right)$$

Ensemble Kalman filter equations

Update $\mathbf{K}_n = \mathbf{P}_n^f \mathbf{H}^T \left(\mathbf{H} \mathbf{P}_n^f \mathbf{H}^T + \mathbf{R}_n \right)^{-1}$

$$\mathbf{x}_n^{a,i} = \mathbf{x}_n^{f,i} + \mathbf{K}_n \left(\mathbf{y}_n + \gamma_n^i - H \left(\mathbf{x}_n^{f,i} \right) \right)$$

$$\gamma_n^i \sim N(0, \mathbf{R}_n)$$

Forecast $\mathbf{x}_n^{f,i} = M \left(\mathbf{x}_{n-1}^{a,i} \right) + \eta_n^i$ $\mathbf{P}_n^f = \mathbf{L} \circ \mathbf{X}_n^f \mathbf{X}_n^{f,T}$

Danger!

In making the switch to using ensembles and nonlinear models we have introduced many potential problems, mostly related to sampling error

- Localisation
- Inflation
- Perturbed observations
- Inbreeding

Perturbations or analyses?

Update state

$$\mathbf{x}_n^{a,i} = \mathbf{x}_n^{f,i} + \mathbf{K}_n \left(\mathbf{y}_n + \gamma_n^i - H \left(\mathbf{x}_n^{f,i} \right) \right)$$

Like an EDA

Update mean

$$\overline{\mathbf{x}}_n^a = \overline{\mathbf{x}}_n^f + \mathbf{K}_n \left(\mathbf{y}_n - H \left(\overline{\mathbf{x}}_n^f \right) \right)$$

Update perturbations

$$\hat{\mathbf{x}}_n^{a,i} = \hat{\mathbf{x}}_n^{f,i} + \mathbf{K}_n \left(\gamma_n^i - \mathbf{H} \hat{\mathbf{x}}_n^{f,i} \right)$$

Localisation

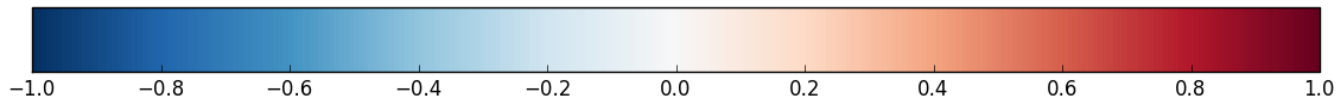
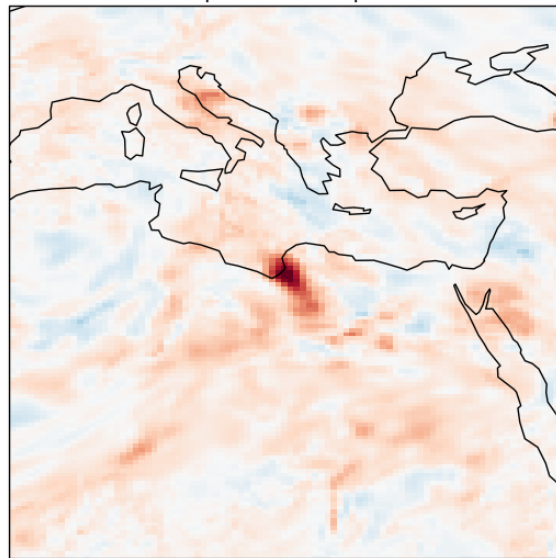
Localisation

An ensemble can provide a sample of a background-error covariance matrix

These samples are typically small

We need to remove the noise

Covariance for air potential temperature at level 20



Localisation

Covariance matrices have certain properties

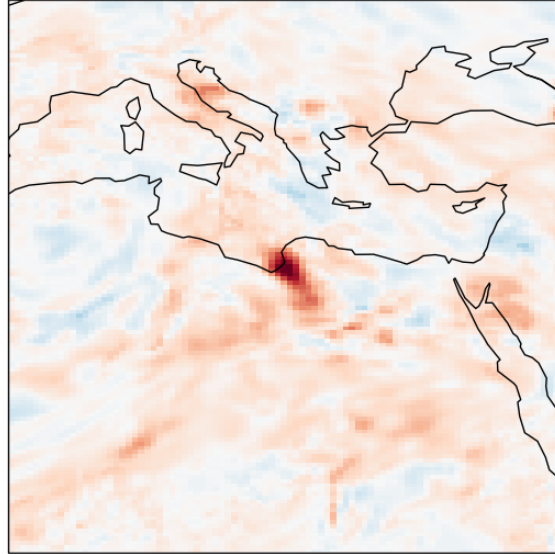
- Positive semi-definite
- Symmetric, etc

Hadamard (Schur, elementwise) product of two covariance matrices is a covariance matrix

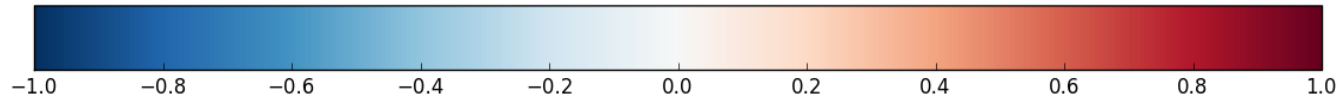
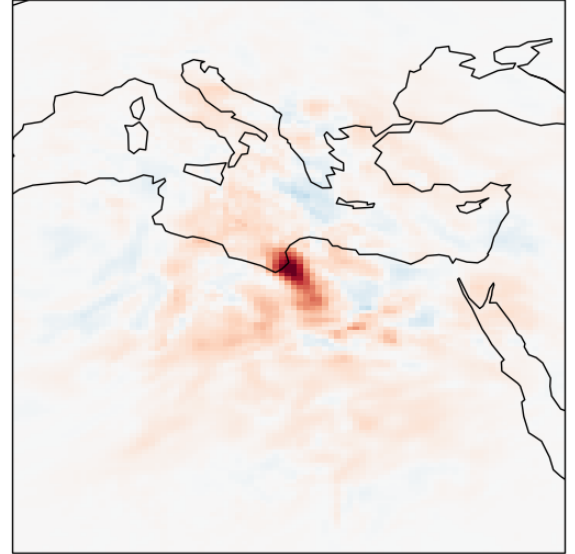
Assume that distant points are uncorrelated, and define a localising covariance matrix which enforces this

Localisation

Covariance for air potential temperature at level 20



Localised covariance for air potential temperature at level 20



Perturbed observations

Perturbed observations and square-root filters

$$\mathbf{x}_n^{a,i} = \mathbf{x}_n^{f,i} + \mathbf{K}_n \left(\mathbf{y}_n + \gamma_n^i - H \left(\mathbf{x}_n^{f,i} \right) \right)$$

$$\gamma_n^i \sim N(\mathbf{0}, \mathbf{R}_n)$$

Perturbed observations -> extra sampling error

Avoid this using square-root filters

$$\mathbf{P}_n^a = (\mathbf{I} - \mathbf{K}_n \mathbf{H}) \mathbf{P}_n^f$$

$$\mathbf{X}_n^a = (\mathbf{I} - \mathbf{K}_n \mathbf{H})^{1/2} \mathbf{X}_n^f$$

EnSRF

Ensemble square-root filter (Whitaker & Hamill 2002)

Treat observations one at a time

$$\hat{\mathbf{x}}_n^{a,i} = (\mathbf{I} - \alpha \mathbf{K}_n \mathbf{H}) \hat{\mathbf{x}}_n^{f,i}$$

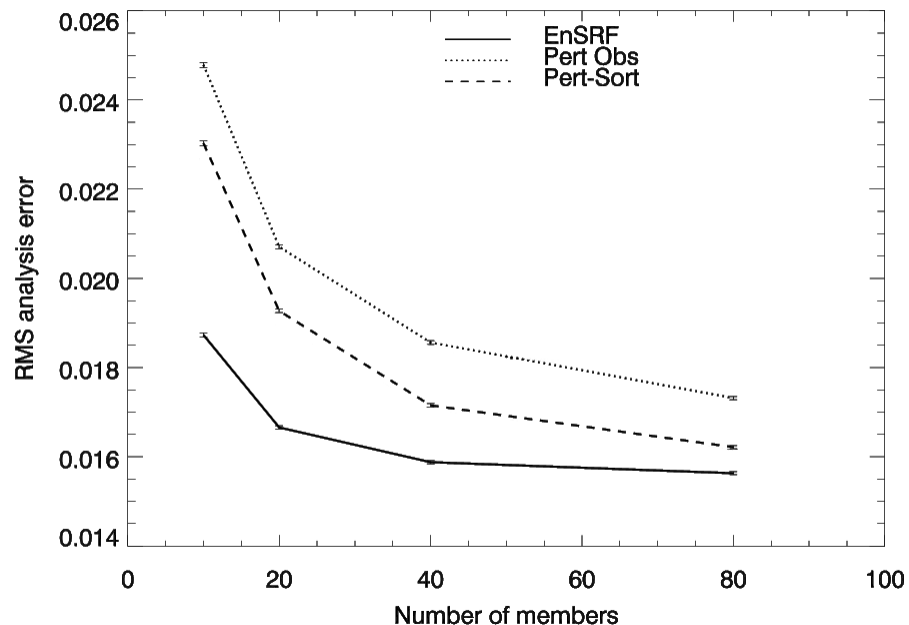
Gain reduction factor

$$\alpha = \left(1 + \sqrt{\frac{\mathbf{R}}{\mathbf{H} \mathbf{P}^f \mathbf{H}^T + \mathbf{R}}} \right)^{-1}$$

Perturbed observations and square-root filters

Comparison within Lorenz (1996) model (40 variables, mild nonlinearity)

Observations every grid-point (Bowler & Flowerdew, 2013)



Perturbed observations may be good

Square-root filters use simplified analysis-error covariance

$$\mathbf{P}_n^a = (\mathbf{I} - \mathbf{K}_n \mathbf{H}) \mathbf{P}_n^f$$

Perturbed-observations actually samples from

$$\mathbf{P}_n^a = (\mathbf{I} - \mathbf{K}_n \mathbf{H}) \mathbf{P}_n^f (\mathbf{I} - \mathbf{K}_n \mathbf{H})^T + \mathbf{K}_n \mathbf{R} \mathbf{K}_n^T$$

In a nonlinear system the perturbations can become substantially non-Gaussian. Perturbed observations help maintain Gaussianity (Lawson & Hansen, 2004)

Inflation

The need for inflation

Tight localisation -> Imbalance in perturbations, slow growth

Broad localisation -> Over-estimation of observation impact, small spread

There is no single correct answer

Typically inflation is needed to increase spread

Model error?

Multiplicative inflation

- Simplest method to counter lack of spread in the ensemble
- Multiply perturbations by inflation factor

$$\mathbf{x}^{a,i} \rightarrow \overline{\mathbf{x}^a} + \beta \left(\mathbf{x}^{a,i} - \overline{\mathbf{x}^a} \right)$$

- Tuning required

Adaptive inflation

Wang and Bishop (2003) proposed a simple adaptive scheme

$$\beta_n = \beta_{n-1} \sqrt{\frac{(\mathbf{d}_f^o)^T \mathbf{d}_f^o - \text{Tr}(\mathbf{R})}{\text{Tr}(\mathbf{H}\mathbf{P}^f \mathbf{H}^T)}}$$

This can be estimated for different regions (Bowler et al (2009), Flowerdew & Bowler (2013))

An alternative adaptive inflation scheme was developed by Anderson (2008)

Inflation oscillations

The observing network varies (more sondes 0, 12 UTC)

Wang & Bishop method based on what the inflation factor should have been

$$\beta_n = \beta_{n-1} \sqrt{\frac{(\mathbf{d}_f^o)^T \mathbf{d}_f^o - \text{Tr}(\mathbf{R})}{\text{Tr}(\mathbf{H}\mathbf{P}^f \mathbf{H}^T)}}$$

Larger inflation factor needed at 0, 12 UTC, but applied at 6, 18 UTC

Adaptive inflation

Ying & Zhang (2015) proposed a different method

$$\beta_n = \sqrt{\frac{(\mathbf{d}_a^f)^T \mathbf{d}_o^a}{\text{Tr}(\mathbf{H}\mathbf{P}_a\mathbf{H}^T)}}$$

$$\mathbf{d}_o^a = \mathbf{y} - H(\mathbf{x}_a)$$

$$\mathbf{d}_a^f = H(\mathbf{x}_a) - H(\mathbf{x}_f)$$

Ratio of measured analysis spread to actual analysis spread

Should avoid oscillation issues, since dealing with analysis spread at current time

Inflation in the Météo-France system

A global factor to counter under-spread in the ensemble system (Raynaud et al, 2012)

Uses ratio of cost-function minimum to optimal minimum

$$J_b^{theo}(\mathbf{x}_a) = Tr(\mathbf{HK})$$

$$\beta_n = \sqrt{\frac{\mathbf{V}_s}{\sigma_f^2} \frac{J_b(\mathbf{x}_a)}{J_b^{theo}(\mathbf{x}_a)}}$$

\mathbf{V}_s

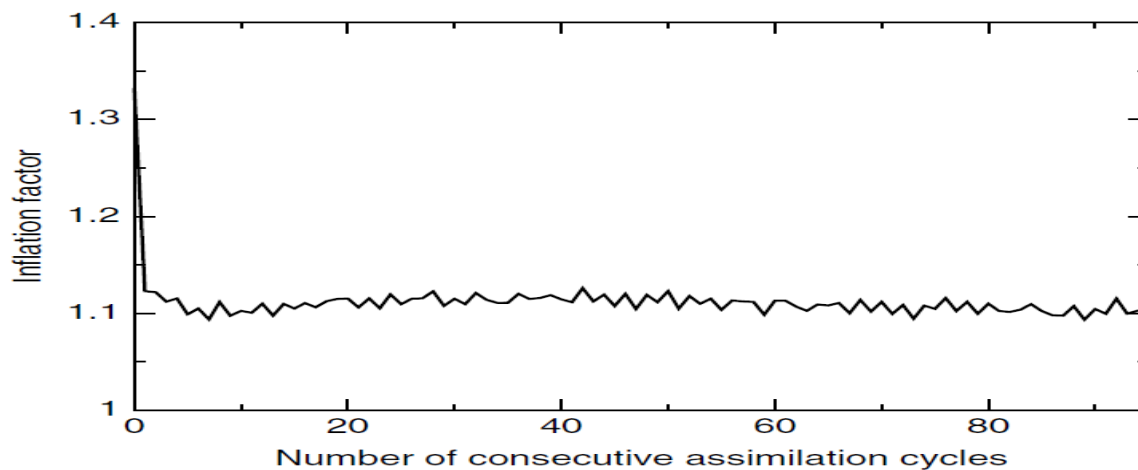
Specified variance from a climatological ensemble

Theoretical cost-function minimum, calculated from the EDA (Desroziers et al., 2009)

Inflation in the Météo-France system

Compensation for model error
neglect in En-DA

Relatively stable



Relaxation methods

Multiplicative inflation can lead to over-spread in poorly observed regions

Relax perturbations back towards the forecast perturbations / spread

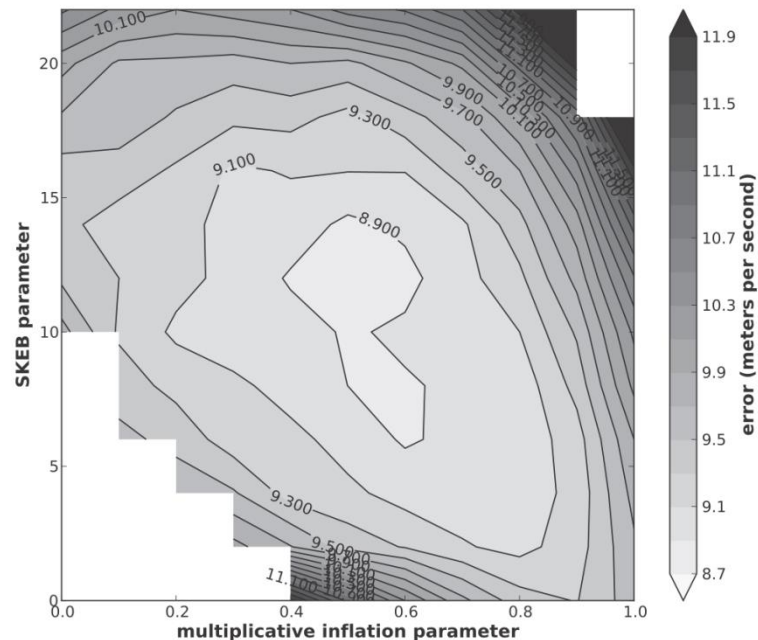
RTPP / RTPS

Popular

Inflation and model error

Whitaker and Hamill (2012) looked at combining model error representation with inflation methods

Showed that multiplicative inflation and representing model error are complementary – both are needed



Other issues

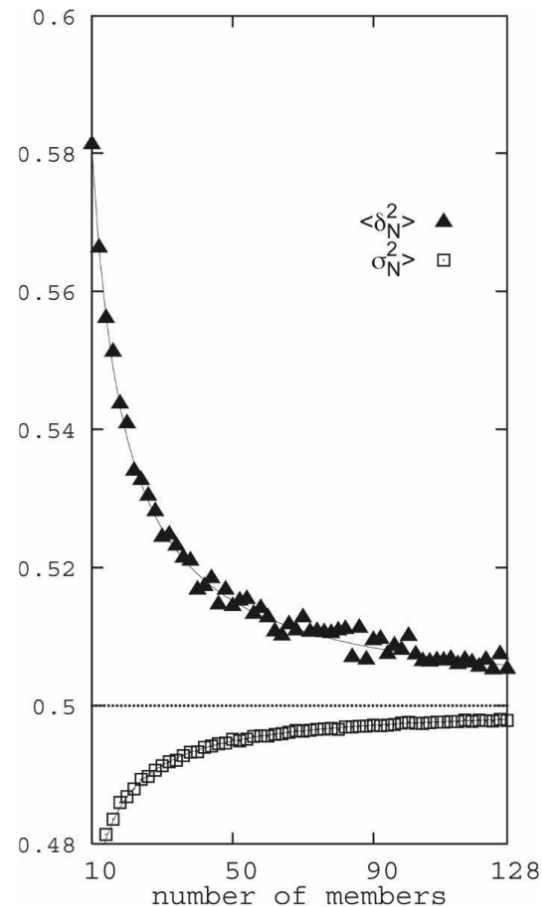
Inbreeding

The standard EnKF has a bias – with a finite ensemble the error is increased, but the spread decreased (Sacher & Bartello, 2009)

Inbreeding – using each ensemble perturbation in the covariance used to update that ensemble

Solution – split the ensemble into M sub-ensembles; use the $M-1$ other sub-ensembles when updating

Introduces positive bias into ensemble spread



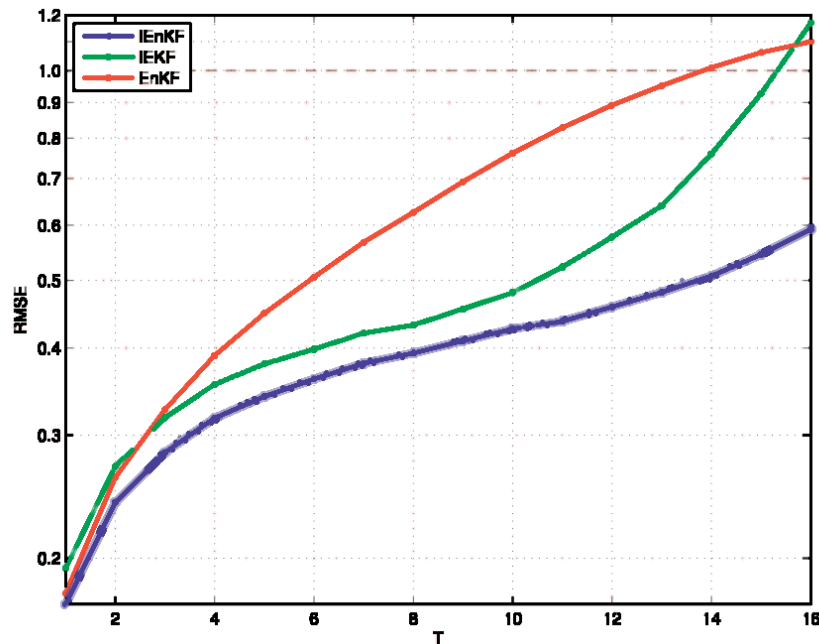
Iterative EnKF

EnKF struggles in non-linear systems

Variational DA can use outer-loops

EnKF can be iterated by re-running the ensemble member forecasts with updated information (Sakov et al, 2012)

Costly



Comparison with other methods

Increased focus on short-range

Compared with error-breeding or singular vectors

- Slower growth of perturbations
- Useful in data assimilation

Comparison with EDA

Essentially the same method

- Easier to set up
 - Better for coupled modelling
- Update algorithm cheaper, and very scalable
- Can't use hybrid covariances
- Outer loop (iterative EnKF) expensive
- Either batches of observations, or observation-space localisation
 - Extracts less benefit from satellite observations

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Other developments

Proposal for hybrid EnKF

Successive covariance localisation

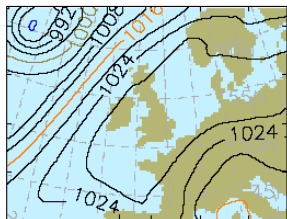
Relaxation to prior perturbations (RTPP)

Multiplicative inflation can lead to $\sigma_a^2 > \sigma_f^2$

Therefore apply a relaxation rather than inflation (Zhang et al, 2004)

$$\mathbf{x}^{a,i} \rightarrow \overline{\mathbf{x}^a} + (1 - \beta)(\mathbf{x}^{a,i} - \overline{\mathbf{x}^a}) + \beta(\mathbf{x}^{f,i} - \overline{\mathbf{x}^f})$$

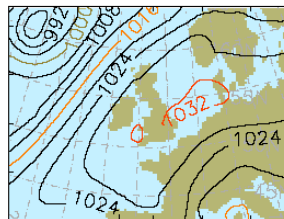
$(1 - \beta)$



Analysis perturbation

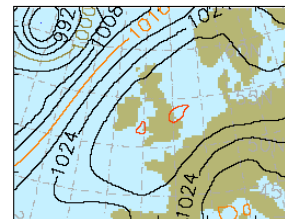
+

β



Forecast perturbation

=



Relaxed perturbation

Relaxation to prior spread (RTPS)

RTPP mixes analysis and forecast perturbations

Forecast perturbations are larger-scale, more balanced

Therefore relax the spread, not the perturbations (Whitaker & Hamill, 2012)

$$\mathbf{x}^{a,i} \rightarrow \overline{\mathbf{x}}^a + \beta \left(\mathbf{x}^{a,i} - \overline{\mathbf{x}}^a \right)$$

$$\beta = \frac{\varphi \sigma_f + (1 - \varphi) \sigma_a}{\sigma_a}$$