Recent Advances in EnKF

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Data Assimilation



- Combine "optimally" short-term forecasts with observations.
- 3D-Var and Optimal Interpolation: used for many years, fixed background error covariance B
- Advanced methods: they evolve B ("errors of the day"):
 - 4D-Var: widely used in operations. Requires model adjoint. :-(
 - Ensemble Kalman Filter, no adjoint :-)
 - Hybrids: **B** from EnKF, variational solution

Conclusions from the THORPEX Workshop in Buenos Aires (2008)

- ✓ 4D-Var and EnKF are competitive in skill
- Hybrid approach best (Buehner et al, 2008, 2009)
- There are no fatal disadvantages for either system
- ✓ Computationally competitive
- ✓ About 40-100 ensemble members needed from storm to global scales for EnKF
- ✓ Both methods have developed approaches to deal with model errors and nonlinearities

As a result, Japan, NCEP, ECMWF, Canada, Brazil,... are exploring EnKF (or hybrid EnKF+variational) for operations.

Tools that improve LETKF/EnKF

We adapted ideas inspired by 4D-Var:

- ✓ **No-cost smoother** (Kalnay et al, Tellus 2007)
- "Quasi Outer loop", nonlinearities and long windows (Yang and Kalnay)
- ✓ Accelerating the spin-up with Running in Place (Kalnay and Yang, 2008)
- ✓ Forecast sensitivity to observations (Liu and Kalnay, QJ, 2008) (correction)
- Coarse analysis resolution without degradation (Yang et al., QJ, 2009)
- ✓ Low-dimensional **model bias correction** (Li et al., MWR, 2009)
- ✓ Simultaneous estimation of optimal inflation and observation errors (Li et al., QJ, 2009).

Examples of applications:

Estimates of surface carbon fluxes as parameters (Kang et al, 2011)

Local Ensemble Transform Kalman Filter (Ott et al, 2004, Hunt et al, 2004, 2007) (a square root filter)

(Start with initial ensemble)



- Model independent (black box)
- Obs. assimilated simultaneously at each grid point
- 100% parallel: fast
- No adjoint needed
- 4D LETKF extension
- Computes weights explicitly

Localization based on observations

Perform data assimilation in a local volume, choosing observations

The state estimate is updated at the central grid red dot



Localization based on observations

Perform data assimilation in a local volume, choosing observations

The state estimate is updated at the central grid red dot

All observations (purple diamonds) within the local region are assimilated



The LETKF algorithm can be described in a single slide!

Local Ensemble Transform Kalman Filter (LETKF)

Globally: Forecast step: $\mathbf{x}_{n,k}^{b} = M_{n} \left(\mathbf{x}_{n-1,k}^{a} \right)$ Analysis step: construct $\mathbf{X}^{b} = \left[\mathbf{x}_{1}^{b} - \overline{\mathbf{x}}^{b} \right] \dots \left[\mathbf{x}_{K}^{b} - \overline{\mathbf{x}}^{b} \right];$ $\mathbf{y}_{i}^{b} = H(\mathbf{x}_{i}^{b}); \mathbf{Y}_{n}^{b} = \left[\mathbf{y}_{1}^{b} - \overline{\mathbf{y}}^{b} \right] \dots \left[\mathbf{y}_{K}^{b} - \overline{\mathbf{y}}^{b} \right]$

Locally: Choose for each grid point the observations to be used, and compute the local analysis error covariance and perturbations in ensemble space:

$$\tilde{\mathbf{P}}^{a} = \left[\left(K - 1 \right) \mathbf{I} + \mathbf{Y}^{bT} \mathbf{R}^{-1} \mathbf{Y}^{b} \right]^{-1}; \mathbf{W}^{a} = \left[(K - 1) \tilde{\mathbf{P}}^{a} \right]^{1/2}$$
Analysis mean in ensemble space:
$$\overline{\mathbf{W}}^{a} = \tilde{\mathbf{P}}^{a} \mathbf{Y}^{bT} \mathbf{R}^{-1} (\mathbf{y}^{o} - \overline{\mathbf{y}}^{b})$$

and add to \mathbf{W}^{a} to get the analysis ensemble in ensemble space.

The new ensemble analyses in model space are the columns of $\mathbf{X}_{n}^{a} = \mathbf{X}_{n}^{b}\mathbf{W}^{a} + \overline{\mathbf{x}}^{b}$. Gathering the grid point analyses forms the new global analyses. Note that the the output of the LETKF are analysis weights $\overline{\mathbf{w}}^{a}$ and perturbation analysis matrices of weights \mathbf{W}^{a} . These weights multiply the ensemble forecasts.

No-cost LETKF smoother (x): apply at t_{n-1} the same weights found optimal at t_n. It works for 3D- or 4D-LETKF



The no-cost smoother makes possible:

- ✓ Quasi Outer loop (comparable to 4D-Var)
- ✓ "Running in place" (faster spin-up)
- ✓ Use of future data in reanalysis
- ✓ Ability to use longer windows and nonlinear perturbations

No-cost LETKF smoother tested on a QG model: it works...



This very simple smoother allows us to go back and forth in time within an assimilation window: it allows assimilation of **future** data in reanalysis¹⁰

Nonlinearities and "outer loop"

- The main disadvantage of EnKF is that it cannot handle nonlinear (non-Gaussian) perturbations and therefore needs short assimilation windows.
- It doesn't have the outer loop so important in 3D-Var and 4D-Var (DaSilva, pers. comm. 2006)

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Lorenz -3 variable model
(Kalnay et al. 2007a Tellus),
RMS analysis error:
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4D-Var LETKF ⁵⁰ ⁵⁰ ⁵¹ ⁵¹ ⁵¹ ⁵² ⁵²⁵ Window=8 steps 0.31 **0.30** (linear window) Window=25 steps **0.53** 0.66 (nonlinear window)

With long windows + Pires et al. => 4D-Var clearly wins! ¹¹

"Outer loop" in 4D-Var

Incremental 4D-Var

No-cost LETKF smoother (x): apply at t_{n-1} the same weights found optimal at t_n. It works for 3D- or 4D-LETKF

Quasi Outer Loop (QOL): correct the analysis mean at t_{n-1} Running in Place (RIP): correct all the analyses at t_{n-1}

...and then do the data assimilation to t_n again

Nonlinearities: "Quasi Outer Loop" (QOL)

Quasi Outer Loop: use the final weights to correct only the <u>mean</u> initial analysis, keeping the initial perturbations. Repeat the analysis once or twice. It re-centers the ensemble on a more accurate nonlinear solution.

0.30

0.66

Lorenz -3 variable model RMS analysis error 4D-Var LETKF LETKF

Window=8 steps0.31Window=25 steps0.53

0.48

Nonlinearities, "QOL" and "Running in Place"

Quasi Outer Loop: similar to 4D-Var: use the final weights to correct only the <u>mean</u> initial analysis, keeping the initial perturbations. Repeat the analysis once or twice. It centers the ensemble on a more accurate nonlinear solution.

Lorenz -3 variable model RMS analysis error

	4D-Var	LETKF	LETKF	LETKF
			+QOL	+RIP
Window=8 steps	0.31	0.30	0.27	0.27
Window=25 steps	0.53	0.66	0.48	0.39

"Running in place" smoothes both the analysis and the analysis error covariance and iterates a few times...

Running in Place: Results with a QG model

Spin-up depends on initial perturbations, but RIP works well even with random perturbations. It becomes as fast as 4D-Var (blue). RIP takes only 2-6 iterations.

24 hr forecast of simulated Typhoon Sinlaku (trajectory and intensity were both improved with RIP)

An application of LETKF-RIP to ocean data assimilation

*Data Assimilation of the Global Ocean using 4D-LETKF and MOM2 Steve Penny's defense April 15, 2011

With:

- Eugenia Kalnay •
- Jim Carton
- Brian Hunt

- Kayo Ide
- Takemasa Miyoshi
- Gennady Chepurin 18

*Key advantages of Ensemble Kalman Filter

- It is computed by a sequential method based on the state and uncertainty at the previous step.
- It explicitly propagates uncertainty. 3D-Var does not propagate uncertainty (uses constant B matrix as approximate uncertainty at all timesteps)
- It does not require a tangent linear model or adjoint (as is required by 4D-Var, very costly in man-hours)

*Primary Disadvantages of EnKF

- Computational cost and storage of the ensemble
- Solution is limited to the space spanned by the ensemble (Though this is improved upon by introducing methods such as Running in Place¹ and Hybrid Filters²)
- Under-predicts forecast uncertainty (Though this is improved by use of adaptive inflation³)

1.) Kalnay, Yang 2008
 2.) Hamill and Snyder 2000, Wang et al₂₀007
 3.) Miyoshi 2010

RMSD (°C) (All vertical levels)

*12-month moving average Salinity RMSD (psu)

RMSD (psu) (All vertical levels)

Forecast sensitivity to observations "Adjoint sensitivity without adjoint" (Liu and K, 2008)

 $\mathbf{e}_{t|0} = \overline{\mathbf{x}}_{t|0}^f - \overline{\mathbf{x}}_t^a$

(Adapted from Langland and Baker, 2004)

The only difference between $\mathbf{e}_{t|0}$ and $\mathbf{e}_{t|-6}$ is the assimilation of observations at 00hr:

$$(\overline{\mathbf{x}}_{0}^{a} - \overline{\mathbf{x}}_{0|-6}^{b}) = \mathbf{K}(\mathbf{y} - H(\mathbf{x}_{0|-6}^{b}))$$

Observation impact on the reduction of forecast error:

$$\Delta \mathbf{e}^{2} = (\mathbf{e}_{t|0}^{T} \mathbf{e}_{t|0} - \mathbf{e}_{t|-6}^{T} \mathbf{e}_{t|-6}) = (\mathbf{e}_{t|0}^{T} - \mathbf{e}_{t|-6}^{T})(\mathbf{e}_{t|0} + \mathbf{e}_{t|-6})$$

Forecast sensitivity to observations

$$\Delta \mathbf{e}^{2} = (\mathbf{e}_{t|0}^{T} \mathbf{e}_{t|0} - \mathbf{e}_{t|-6}^{T} \mathbf{e}_{t|-6}) = (\mathbf{e}_{t|0}^{T} - \mathbf{e}_{t|-6}^{T})(\mathbf{e}_{t|0} + \mathbf{e}_{t|-6})$$
$$= (\overline{\mathbf{x}}_{t|0}^{f} - \overline{\mathbf{x}}_{t|-6}^{f})^{T} (\mathbf{e}_{t|0} + \mathbf{e}_{t|-6})$$
$$= \left[\mathbf{M}(\overline{\mathbf{x}}_{0}^{a} - \overline{\mathbf{x}}_{0|-6}^{b}) \right]^{T} (\mathbf{e}_{t|0} + \mathbf{e}_{t|-6}), \text{ so that}$$
$$\Delta \mathbf{e}^{2} = \left[\mathbf{M}\mathbf{K}(\mathbf{y} - H(\mathbf{x}_{0|-6}^{b})) \right]^{T} (\mathbf{e}_{t|0} + \mathbf{e}_{t|-6})$$

Langland and Baker (2004), Gelaro, solve this with the adjoint:

$$\Delta \mathbf{e}^2 = \left[(\mathbf{y} - H(\mathbf{x}_{0|-6}^b)) \right]^T \mathbf{K}^T \mathbf{M}^T (\mathbf{e}_{t|0} + \mathbf{e}_{t|-6})$$

This requires the adjoint of the model \mathbf{M}^T and of the data assimilation system \mathbf{K}^T (Langland and Baker, 2004)

Forecast sensitivity to observations

Langland and Baker (2004):

$$\Delta \mathbf{e}^{2} = \left[\mathbf{M} \mathbf{K} (\mathbf{y} - H(\mathbf{x}_{0|-6}^{b})) \right]^{T} (\mathbf{e}_{t|0} + \mathbf{e}_{t|-6})$$
$$= \left[(\mathbf{y} - H(\mathbf{x}_{0|-6}^{b})) \right]^{T} \mathbf{K}^{T} \mathbf{M}^{T} (\mathbf{e}_{t|0} + \mathbf{e}_{t|-6})$$

With EnKF we can use the original equation without "adjointing": Recall that $\mathbf{K} = \mathbf{P}^{a}\mathbf{H}^{T}\mathbf{R}^{-1} = 1/(K-1)\mathbf{X}^{a}\mathbf{X}^{aT}\mathbf{H}^{T}\mathbf{R}^{-1}$ so that $\mathbf{M}\mathbf{K} = \mathbf{M}\mathbf{X}^{a}(\mathbf{X}^{aT}\mathbf{H}^{T})\mathbf{R}^{-1}/(K-1) = \mathbf{X}_{t|0}^{f}\mathbf{Y}^{aT}\mathbf{R}^{-1}/(K-1)$

Thus,
$$\Delta \mathbf{e}^{2} = \left[\mathbf{M}\mathbf{K}(\mathbf{y} - H(\mathbf{x}_{0|-6}^{b})) \right]^{T} (\mathbf{e}_{t|0} + \mathbf{e}_{t|-6})$$
$$= \left[(\mathbf{y} - H(\mathbf{x}_{0|-6}^{b})) \right]^{T} \mathbf{R}^{-1} \mathbf{Y}_{0}^{a} \mathbf{X}_{t|0}^{fT} (\mathbf{e}_{t|0} + \mathbf{e}_{t|-6}) / (K-1) \right]^{T}$$

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This is a product using the available **nonlinear** forecast ensemble $\mathbf{X}_{t|0}^{fT}$ and $\mathbf{Y}_{0}^{a} = (\mathbf{H}\mathbf{X}^{a})$

Test ability to detect a poor quality ob impact on the forecast in the Lorenz 40 variable model

✓ The adjoint and the ensemble sensitivity give identical observation impact on the 24 hr forecast.

✓ The ensemble sensitivity is nonlinear and is able to detect bad obs for longer forecasts

Impact of each real observation (Miyoshi et al., 2011)

Observation impact for each type

Typhoon Sinlaku forecast (9/8 12 UTC – 9/12 12UTC, NW Pacific)

All types of observations reduce the typhoon forecast error. Upper soundings (ADPUPA) have the largest impact.

Impact of dropsondes on a Typhoon

Denying negative impact data improves forecast!

Coarse analysis with interpolated weights Yang et al (2008)

- In LETKF the analysis is a weighted average of the forecast ensemble
- We performed experiments with a QG model **interpolating** <u>weights</u> compared to **analysis** <u>increments</u>.
- Coarse grids of 11%, 4% and 2% interpolated analysis points.
- Weight fields vary on large scales: they interpolate very well

1/(3x3)=11% analysis grid

Weight interpolation versus Increment interpolation

ANALYSIS INCREMENTS FROM INCREMENTS INTERPOLATION (FROM FULL ANALYSIS)

With increment interpolation, the analysis degrades quickly... With weight interpolation, there is almost no degradation! LETKF maintains balance and conservation properties

Impact of coarse analysis on accuracy

With increment interpolation, the analysis degrades With weight interpolation, there is no degradation, the analysis is actually slightly better! Model error: comparison of methods to correct model bias and inflation

Hong Li, Chris Danforth, Takemasa Miyoshi, and Eugenia Kalnay, MWR (2009)

Inspired by the work of Dee and DaSilva, but with model errors estimated in model space, not in obs space

Model error: If we assume a perfect model in EnKF, we underestimate the analysis errors (Li, 2007)

— Why is EnKF vulnerable to model errors?

The ensemble spread is 'blind' to model errors

Bias removal scheme: Low Dimensional Method

2.3 Low-dim method (Danforth et al, 2007: Estimating and correcting global weather model error. *Mon. Wea. Rev, J. Atmos. Sci., 2007*)

estimate the global model error beyond the bias

SPEEDY 6 hr model errors against NNR (diurnal cycle)

1987 Jan 1~ Feb 15

Error anomalies

• For temperature at lower-levels, in addition to the time-independent bias, SPEEDY has strong diurnal cycle errors because it lacks diurnal radiation forcing

Leading EOFs for 925 mb TEMP

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We compared several methods to handle bias and random model errors

Simultaneous estimation of EnKF inflation and obs errors in the presence of model errors

Hong Li, Miyoshi and Kalnay (AMS, Jan 2007, QJ, 2009)

Inspired by Houtekamer et al. (2001) and Desroziers et al. (2005)

Any data assimilation scheme requires accurate statistics for the observation and background errors (usually tuned or from gut feeling).

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EnKF needs inflation of the background error covariance: tuning is expensive

 We introduce a method to simultaneously estimate ob errors and inflation.

Now extended to correlated ob errors by Miyoshi et al. (2009)

Diagnosis of observation error statistics

Houtekamer et al (2001) well known statistical relationship:

$$OMB*OMB < \mathbf{d}_{o-b}\mathbf{d}_{o-b}^T >= \mathbf{H}\mathbf{P}^b\mathbf{H}^T + \mathbf{R}$$

Desroziers et al, 2005, introduced two new statistical relationships:

$$\mathsf{OMA*OMB} \qquad < \mathbf{d}_{o-a} \mathbf{d}_{o-b}^T >= \mathbf{R}$$

$$\mathbf{AMB*OMB} \qquad \qquad < \mathbf{d}_{a-b} \mathbf{d}_{o-b}^{T} >= \mathbf{HP}^{b} \mathbf{H}^{T}$$

These relationships are correct if the **R** and **B** statistics are correct and errors are uncorrelated!

With inflation:
$$\mathbf{HP}^{b}\mathbf{H}^{T} \rightarrow \mathbf{H}\Delta\mathbf{P}^{b}\mathbf{H}^{T}$$
 with $\Delta > 1$

Diagnosis of observation error statistics

Transposing, we get "observations" of Δ and σ_a^2

$$\Delta^{o} = \frac{(\mathbf{d}_{o-b}^{T} \mathbf{d}_{o-b}) - Tr(\mathbf{R})}{Tr(\mathbf{H}\mathbf{P}^{b}\mathbf{H}^{T})}$$
OMB²

$$\Delta^{o} = \sum_{j=1}^{p} (y_{j}^{a} - y_{j}^{b})(y_{j}^{o} - y_{j}^{b}) / Tr(\mathbf{HP}^{b}\mathbf{H}^{T})$$
AMB*OMB

$$(\tilde{\sigma}_{o})^{2} = \mathbf{d}_{o-a}^{T} \mathbf{d}_{o-b} / p = \sum_{j=1}^{p} (y_{j}^{o} - y_{j}^{a})(y_{j}^{o} - y_{j}^{b}) / p$$
 OMA*OMB

Here we use a simple KF to estimate both Δ and σ_o^2 online.

SPEEDY model: online estimated observational errors, each variable started with error 2 (not 1)

The original wrongly specified R quickly converges to the correct value of R (in about 5-10 days)

Estimation of the inflation

Using an initially wrong R and Δ but estimating them adaptively Using a perfect R and estimating Δ adaptively

After **R** converges, the time dependent inflation factors are quite similar $_{46}$

Adaptive inflation (Miyoshi, 2011)

T=t0 T=t1

Covariance inflation

T=t0 T=t1

Previous inflation methods

Previous inflation methods

Generally better spread, but an unfavorable high-frequency pattern appears.

Previous inflation methods

Zhang et al. (2004) showed this worked well.

Adaptive inflation

Anderson (2007; 2009) applied the Bayesian estimation theory to estimate the inflation parameter α adaptively.

$$p(\boldsymbol{\alpha}_{i}^{a}) = p(y_{i} | \boldsymbol{\alpha}_{i}) p(y_{i-1} | \boldsymbol{\alpha}_{i}) \cdots p(y_{i-p+1} | \boldsymbol{\alpha}_{i}) p(\boldsymbol{\alpha}_{i}^{b}) / norm$$
Posterior
Obs
Prior

Li et al. (2009) applied the Gaussian assumption.

Localization of inflation estimates

- ☆: Current grid point
- : Grid points
- : Local observations
- : Remote observations

Apply the maximum likelihood estimate at each grid point independently.

Miyoshi (2011)

$$\alpha = \alpha(x, y, z, t)$$

Application to CO_2 data assimilation

Results of Mars GCM

JMA operational NWP system

Application: parameter estimation in EnKF. The state vector is augmented with the parameters a,r,b

Example with Lorenz model (simulation with noisy obs.)

<u>Left:</u> estimation of parameters with LETKF from the error covariance; <u>Right</u>: standard regression from observations

Application: Parameter Estimation in EnKF

- Example of carbon cycle data assimilation
 - Surface CO_2 fluxes (CF): a forcing for atmospheric CO_2
- State vector augmentation
 - State vector is augmented by CF which is updated by error covariance between the variables in the state vector
- Variable localization
 - In a multivariate analysis of EnKF, error covariance is zeroed out when there is no significant physical relationship between variables, in order to reduce a sampling error
- Inflation
 - It helps represent background uncertainty more accurately
- Vertical localization of satellite column data
 - Averaging kernel is nearly uniform in the vertical, although a forcing term (our ultimate estimate) is at the surface. Then...?

Variable localization

- Analysis of surface CO₂ fluxes assimilating atmospheric CO₂ observations
 - A case with a constant forcing

CF

С

U

V

Т

q Ps

CF

С

U

V

т

q

Ps

1-way multivariate analysis with variable localization →

Fully multivariate analysis ->

Kang et al. (2011, JGR)

1205

aóu

Inflation methods also have an impact

standard: fixed multiplicative

Analysis @ 00Z01APR1997

Analysis @ 00Z01JUL1997

60 Adaptive inflation by Miyoshi (2011, Mon. Wea. Rev.)

Vertical localization of CO₂ column data

- OCO (Orbiting Carbon Observatory) & GOSAT (Greenhouse gases Observing Satellite)
 - Satellites dedicated to mapping Earth's CO₂ levels

Averaging kernel is quite flat from the surface to the middle troposphere

In order to estimate surface CO_2 fluxes with those satellite data, we have **localized the column CO₂ data, updating only lower atmospheric CO₂** rather than a full column of CO_2 .

(the vertical localizing function is broad in the lower troposphere but zero in the upper layers)

Forcing of CO₂ is at the surface!!!

Vertical localization improves results

• Time series of CF for one year

Indication of pattern correlation [LAND]
 Time state
 CF Pattern Correlation [LAND]

Miyoshi's LETKF code

Takemasa Miyoshi has a new LETKF code based on the work he did at JMA. He has made it available to all at "Google code Miyoshi LETKF".

It is MPI (parallel) modular and very efficient. The same code has been coupled to Lorenz (1996), SPEEDY, the Regional Ocean Modular System (ROMS) at high resolution and the WRF model.

It contains all the advances discussed

Summary

- EnKF and 4D-Var are competitive, hybrid seems best
- Several countries are now testing EnKF (quite a change!)
- Many ideas to further improve LETKF work very well:
 - No-cost smoothing and "running in place"
 - A simple outer loop to deal with nonlinearities
 - Forecast sensitivity without adjoint model, valid for longer forecasts
 - Analysis sensitivity and exact cross-validation
 - Coarse resolution analysis without degradation
 - Correction of model bias combined with additive inflation gives the best results
 - Can estimate simultaneously optimal inflation and ob. errors.
 - The impact of adaptive inflation is very large.
 - LETKF code with examples available at Miyoshi's Google Code

The estimation of surface fluxes of carbon as evolving parameters seems to work well if several improvements are implemented

Thoughts on hybrid

Dale Barker suggested that a fast path for NCEP to the use of hybrid would be to make first a GSI-EnKF hybrid, and then replace GSI with 4D-Var. Seems a very sensible idea.

As shown by Buehner et al., hybrid Var and EnKF may be the most accurate approach ("sweet spot").

