Finite-size ensemble Kalman filters (EnKF-N)
Iterative ensemble Kalman smoothers (IEnKS)

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Outline

1 The primal EnKF-N

2 The dual EnKF-N

3 The iterative ensemble Kalman filter & smoother

4 Conclusions
The primal EnKF-N

## Failure of the raw ensemble Kalman filter (EnKF)

- With the exception of Gaussian and linear systems, EnKF fails to provide a proper estimation on most systems.

- To properly work, it needs fixes: localisation and inflation.

- EnKF relies for its analysis on the first and second-order empirical moments:

\[
\bar{x} = \frac{1}{N} \sum_{n=1}^{N} x_k, \quad P = \frac{1}{N-1} \sum_{k=1}^{N} (x_k - \bar{x})(x_k - \bar{x})^T. \tag{1}
\]

Yet, \( \bar{x} \) and \( P \) may not be the true moments of the true filtering distribution (assuming there is one!). Hidden true moments of the true filtering distribution: \( x_b \) and \( B \).
Getting more from the ensemble

► Idea: even under Gaussian assumptions of the true distribution, the pdf $p(x|x_1,\ldots,x_N)$ extracts more information than $p(x|\bar{x},P)$.

► Using Gaussian assumptions, and being only interested in the filtering problem, one can get (hierarchical reasoning):

$$p(x|x_1,\ldots,x_N) = \frac{1}{p(x_1,\ldots,x_N)} \int dx_b dB \, p(x|x_b,B)p(x_1,\ldots,x_N|x_b,B)p(x_b,B). \tag{2}$$

► $p(x|x_b,B)$: the standard Gaussian prior but based on the true statistics.

► $p(x_1,\ldots,x_N|x_b,B) = \prod_{k=1}^{N} p(x_k|x_b,B)$

► $p(x_b,B)$: prior for the background statistics!
Choosing priors for the background statistics

To progress, we need to make assumptions on the background statistics $p(x_b, B)$: the statistics of the error statistics or hyperpriors.

A very simple choice is a weakly informative prior: the Jeffreys’ prior [Jeffreys 1961] with an additional assumption of independence for $x_b$ and $B$:

$$p(x_b, B) \equiv p_J(x_b, B) = p_J(x_b) p_J(B)$$

and

$$p_J(x_b) = 1, \quad p_J(B) = |B|^{-\frac{M+1}{2}}.$$ 

With Jeffreys prior, it is possible to perform the integral (with additional complications due to rank-deficiency usually not dealt with by mathematicians).
Principle of the EnKF-N

The prior of EnKF and the prior of EnKF-N:

\[
p(x|\bar{x},P) \propto \exp \left\{ -\frac{1}{2} (x - \bar{x})^T P^{-1} (x - \bar{x}) \right\}
\]

\[
p(x|x_1, x_2, \ldots, x_N) \propto \left| (x - \bar{x}) (x - \bar{x})^T + \varepsilon_N (N - 1) P \right|^{-\frac{N}{2}},
\]

with \( \varepsilon_N = 1 \) (mean-trusting variant), or \( \varepsilon_N = 1 + \frac{1}{N} \) (original variant).

Ensemble space decomposition (ETKF version of the filters): \( x = \bar{x} + A w \).

The variational principle of the analysis (in ensemble space):

\[
\mathcal{J}(w) = \frac{1}{2} (y - H(\bar{x} + A w))^T R^{-1} (y - H(\bar{x} + A w)) + \frac{N - 1}{2} w^T w
\]

\[
\mathcal{J}(w) = \frac{1}{2} (y - H(\bar{x} + A w))^T R^{-1} (y - H(\bar{x} + A w)) + \frac{N}{2} \ln \left( \varepsilon_N + w^T w \right).
\]
EnKF-N: algorithm

1. Requires: The forecast ensemble \( \{x_k\}_{k=1,...,N} \), the observations \( y \), and error covariance matrix \( R \).
2. Compute the mean \( \bar{x} \) and the anomalies \( A \) from \( \{x_k\}_{k=1,...,N} \).
3. Compute \( Y = HA, \ \delta = y - H\bar{x} \).
4. Find the minimum:
   \[
   w_a = \min_w \left\{ (\delta - Yw)^T R^{-1} (\delta - Yw) + N \ln \left( \epsilon_N + w^T w \right) \right\}
   \]
5. Compute \( x^a = \bar{x} + Aw_a \).
6. Compute \( \Omega_a = \left( Y^T R^{-1} Y + N \left( \frac{\epsilon_N + w_a^T w_a}{(\epsilon_N + w_a^T w_a)^2} \right) I_N - 2w_a w_a^T \right)^{-1} \).
7. Compute \( W^a = \left\{ (N - 1) \Omega_a \right\}^{1/2} U \).
8. Compute \( x^a_k = x^a + A W^a_k \)
The Lorenz '95 model

- The toy-model [Lorenz and Emmanuel 1998]:
  - It represents a mid-latitude zonal circle of the global atmosphere.
  - $M = 40$ variables $\{x_m\}_{m=1,...,M}$. For $m = 1, \ldots, M$:
    \[
    \frac{dx_m}{dt} = (x_{m+1} - x_{m-2})x_{m-1} - x_m + F,
    \]
    where $F = 8$, and the boundary is cyclic.
  - Chaotic dynamics, topological dimension of 13, a doubling time of about 0.42 time units, and a Kaplan-Yorke dimension of about 27.1.

- Setup of the experiment: Time-lag between update: $\Delta t = 0.05$ (about 6 hours for a global model), fully observed, $R = I$. 

Application to the Lorenz '95 model

- EnKF-N: analysis rmse versus ensemble size, for $\Delta t = 0.05$. 

![Graph showing EnKF-N: analysis rmse versus ensemble size, for $\Delta t = 0.05$.]
Application to the Lorenz '95 model

Local version: LETKF-N, with $N = 10$ (beware $\Delta t = 0.01$ requires a correction).
Forced 2D turbulence model

\[ \frac{\partial q}{\partial t} + J(q, \psi) = \lambda q + \nu \Delta^2 q + F, \quad q = \Delta \psi, \quad (5) \]

where \( J(q, \psi) = \partial_x q \partial_y \psi - \partial_y q \partial_x \psi \), \( q \) is the vorticity 2D field, \( \psi \) is the current function 2D field, \( F \) is the forcing, \( \lambda \) amplitude of the friction, \( \nu \) amplitude of the biharmonic diffusion, grid: \( 64 \times 64 \) small enough to be in the sufficient-rank regime.

Setup of the experiment: Time-lag between update: \( \Delta_t = 2 \), fully observed, \( R = 0.1 \mathbf{I} \).
Application to forced 2D turbulence

- Comparison of: EnKF with uniform inflation, EnKF-N, adaptive inflation EnKF (EnKF-ML), $N = 80$ (rank-sufficient regime). Starting away or close from the truth.

![Graph showing vorticity rmse analysis over cycles for different methods: Reference, EnKF $\lambda = 1.02$, EnKF-ML, EnKF-N, EnKF $\lambda = 1$, EnKF $\lambda = 1.02$, EnKF-ML, EnKF-N. The x-axis represents cycle numbers from 10 to 320, and the y-axis represents vorticity rmse analysis values. The graph illustrates the performance of each method over time, with EnKF-N showing a more stable and accurate analysis compared to the others.]
Also tested on . . .

- EnKF-N also tested on:
  - Lorenz ’63 model, [Lorenz, 1963]
  - Kuramato-Sivashinski model, [Kuramato, 1975; Sivashinski, 1977]
  - NEDyM economical model, [Hallegate, Ghil and co-authors, 2008-2012]
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The dual EnKF-N

**Lagrangian duality**

- The **primal** EnKF-N cost function:

\[
\mathcal{J}(w) = \frac{1}{2} (y - H(\bar{x} + Xw))^T R^{-1} (y - H(\bar{x} + Xw)) + \frac{N}{2} \ln \left( \varepsilon_N + w^T w \right). \tag{6}
\]

- **Idea:** Split the radial degree of freedom of \( w \), that is \( \sqrt{w^T w} \), from its angular degrees of freedom, that is \( w / \sqrt{w^T w} \).

- Lagrangian:

\[
\mathcal{L}(w, \rho, \zeta) = \frac{1}{2} (\delta - Yw)^T R^{-1} (\delta - Yw) + \frac{1}{2} \zeta \left( w^T w - \rho \right) + \frac{N}{2} \ln (\varepsilon_N + \rho), \tag{7}
\]

where \( \delta = y - H\bar{x} \).

- Saddle point equations:

\[
\begin{aligned}
\zeta^* &= \frac{N}{(\varepsilon_N + \rho^*)} \\
\zeta^* w^* &= -Y^T R^{-1} (\delta - Yw^*) 
\end{aligned} \quad \Rightarrow \quad \begin{aligned}
\rho^* &= \frac{N}{\zeta^*} - \varepsilon_N \\
w^* &= \left( \zeta^* + Y^T R^{-1} Y \right)^{-1} Y^T R^{-1} \delta
\end{aligned} \tag{8}
\]
Non-convex strong duality

- **Dual** cost function defined for $\zeta > 0$ by

\[
D(\zeta) = \inf_{w} \sup_{\rho \geq 0} L(w, \rho, \zeta)
\]

\[
= \frac{1}{2} \delta^T (R + Y \zeta^{-1} Y^T)^{-1} \delta + \frac{\varepsilon \sqrt{N}}{2} + \frac{N}{2} \ln \frac{N}{\zeta} - \frac{N}{2}.
\]  

(9)

- **Dual and primal problems:**

\[
\Delta = \inf_{\zeta > 0} D(\zeta) \quad \text{and} \quad \Pi = \inf_{w} J(w).
\]  

(10)

- **Strong duality result** (non quadratic, non-convex case!):

\[
\Delta = \Pi.
\]  

(11)
The dual EnKF-N scheme

1. Requires: The forecast ensemble \( \{x_k\}_{k=1,\ldots,N} \), the observations \( y \), and error covariance matrix \( R \).
2. Compute the mean \( \bar{x} \) and the anomalies \( A \) from \( \{x_k\}_{k=1,\ldots,N} \).
3. Compute \( Y = HA, \delta = y - H\bar{x} \).
4. Find the minimum:

\[
\zeta_a = \min_{\zeta \in [0,N/\epsilon_N]} \left\{ \delta^T \left( R + Y\zeta^{-1}Y^T \right)^{-1} \delta + \epsilon_N \zeta + N \ln \frac{N}{\zeta} - N \right\}
\]  

(12)

5. Compute \( w_a = \left( Y^T R^{-1} Y + \zeta_a \right)^{-1} Y^T R^{-1} \delta \).
6. Compute \( x_a = \bar{x} + A w_a \).
7. Compute \( \Omega_a = \left\{ Y^T R^{-1} Y + \zeta_a \left( \frac{2\epsilon_N}{N} \zeta_a - 1 \right) \right\}^{-1} \)
8. Compute \( W^a = \{(N-1)\Omega_a\}^{1/2} U \)
9. Compute \( x_k^a = x^a + AW_k^a \)
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- The iterative extended Kalman smoother [Bell, 1994] IEKS
Iterative ensemble Kalman filters

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Much too costly + needs the TLM and the adjoint $\rightarrow$ ensemble methods
Iterative ensemble Kalman filters

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Much too costly + needs the TLM and the adjoint $\rightarrow$ ensemble methods

- The iterative ensemble Kalman filter [Sakov et al., 2012; Bocquet and Sakov, 2012] IEnKF
- The iterative ensemble Kalman smoother [This talk...] IEnKS
Iterative ensemble Kalman filters

- The iterative extended Kalman filter [Wishner et al., 1969; Jazwinski, 1970] \textbf{IEKF}
- The iterative extended Kalman smoother [Bell, 1994] \textbf{IEKS}

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\textbf{Much too costly + needs the TLM and the adjoint $\rightarrow$ ensemble methods}
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**It’s TLM and adjoint free!**

**Don’t want to be bothered by inflation tuning?**
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Much too costly + needs the TLM and the adjoint $\rightarrow$ ensemble methods

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It’s TLM and adjoint free!

Don’t want to be bothered by inflation tuning?

- The finite-size iterative ensemble Kalman filter [Bocquet and Sakov, 2012] IEnKF-N
- The finite-size iterative ensemble Kalman smoother [This talk...] IEnKS-N
Iterative ensemble Kalman filters

- A fairly recent idea:
  [Gu & Oliver, 2007]: The idea.
  [Kalnay & Yang, 2010]: A step in the right direction.
  [Sakov, Oliver & Bertino, 2011]: The “pièce de résistance”
  [Bocquet & Sakov, 2012]: Correction of the bundle scheme + ensemble transform form.

- IEnKF cost function in ensemble space:

\[
\tilde{J}(w) = \frac{1}{2} (y_2 - H_2(M_1\rightarrow_2(x_1 + A_1w)))^T R_2^{-1} (y_2 - H_2(M_1\rightarrow_2(x_1 + A_1w))) \\
+ \frac{1}{2} (N - 1)w^T w. \tag{13}
\]

- Gauss-Newton scheme:

\[
w^{(p+1)} = w^{(p)} - \tilde{H}^{-1}(p) \nabla \tilde{J}(w^{(p)})
\]

\[
\nabla \tilde{J}(p) = -Y^T(p) R_2^{-1} \left( y_2 - H_2 M_1\rightarrow_2(x + A_1w^{(p)}) \right) + (N - 1)w^{(p)},
\]

\[
\tilde{H}(p) = (N - 1)I_N + Y^T(p) R_2^{-1} Y(p), \quad Y(p) = [H_2 M_2\leftarrow_1 A_1]'(p), \tag{14}
\]
Iterative ensemble Kalman filters

- Sensitivities $Y_p$ computed by ensemble propagation without TLM and adjoint.

- Finite-size versions of the filter are just defined by substituting the prior:

$$\frac{N-1}{2}w^Tw \rightarrow \frac{N}{2} \ln \left( \epsilon_N + w^Tw \right).$$  \hspace{1cm} (15)

- As a variational reduced method, one can use Gauss-Newton [Sakov et al., 2012], Levenberg-Marquardt [Bocquet and Sakov, 2012; Chen and Oliver, 2012], etc, minimisation schemes (not limited to quasi-Newton).

- Essentially a lag-one smoother. Does the job of a lag-one 4D-Var, with dynamical error covariance matrix and without the use of the TLM and adjoint! Very efficient in very nonlinear conditions if one can afford the multiple ensemble propagations.
Finite-size iterative ensemble Kalman filters

- Setup: Lorenz ’95, $M = 40$, $N = 40$, $\Delta t = 0.05 - 0.60$, $\mathbf{R} = \mathbf{I}$.
- Comparison of EnKF-N, EnKF (optimal inflation), IEnKF-N (bundle and transform), IEnKF (bundle and transform, optimal inflation)
Iterative ensemble Kalman smoothers

- In a mildly nonlinear context (built on linear and Gaussian hypotheses)
  Many earlier studies, see [Cosme et al., 2012] for a review, and [Cosme et al., 2010] for an application to oceanography.

- In a non-sequential but very non-linear context
  Many earlier studies, for instance [Evensen and van Leeuwen, 2000] [Chen & Oliver, 2012] in the context of reservoir modelling

- Sequential nonlinear context: [This talk]
  The IEnKS cost function is just the extension of the IEnKF cost function for a temporal window of $L$ cycles.
Finite-size iterative ensemble Kalman smoothers

 SETUP: Lorenz ’95, $M = 40$, $N = 20$, $\Delta t = 0.05$, $R = I$.


 ![Graph showing re-analysis rmse over lag (number of cycles).]
Finite-size iterative ensemble Kalman smoothers

- Setup: Lorenz '95, $M = 40$, $N = 20$, $\Delta t = 0.30$, $R = I$.
- Lin-IEnKS-N has (understandably) diverged.
Finite-size iterative ensemble Kalman smoothers

- Setup: 2D turbulence, $64 \times 64$, $N = 40$, $\Delta t = 2$, $R = 0.1I$.

![Graph showing vorticity re-analysis rmse over lag (number of cycles)]
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Conclusions

- A new prior for the ensemble forecast meant to be used in an EnKF analysis has been built. It takes into account sampling errors.
- It yields a new class of filters EnKF-N, that does not seem to require inflation supposed to account for sampling errors.
- Local variants (both LA and CL) available.
- Dual variant EnKF-N is an EnKF with built-in optimal inflation (accounting for sampling errors).
- Almost linear regime more problematic because of Jeffreys’ prior. Another hyperprior is needed.
- The iterative ensemble Kalman filter has been generalised to an iterative ensemble Kalman smoother (IEnKF). It is an En-Var method.
- It is tangent linear and adjoint free. It is, by construction, flow-dependent.
- Though based on Gaussian assumptions, it can offer better retrospective analysis than standard Kalman smoothers in midly nonlinear conditions.
- When affordable, it beats other Kalman filter/smoothers in strongly non-linear conditions.
Main references I


