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

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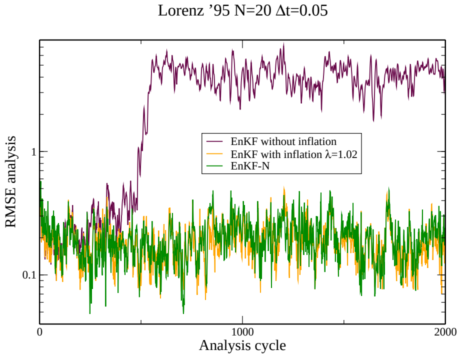
Outline

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:

$$\bar{\mathbf{x}} = \frac{1}{N}\sum_{n=1}^{N}\mathbf{x}_k\,, \qquad \mathbf{P} = \frac{1}{N-1}\sum_{k=1}^{N}\left(\mathbf{x}_k-\bar{\mathbf{x}}\right)\left(\mathbf{x}_k-\bar{\mathbf{x}}\right)^{\mathrm{T}}\,. \tag{1}$$

Yet, $\bar{\mathbf{x}}$ and $\mathbf{P}$ may not be the true moments of the true filtering distribution (assuming there is one!). Hidden true moments of the true filtering distribution: $\mathbf{x}_b$ and $\mathbf{B}$.

Getting more from the ensemble

- Idea: even under Gaussian assumptions of the true distribution, the pdf $p(\mathbf{x}|\mathbf{x}_1,\ldots,\mathbf{x}_N)$ extracts more information than $p(\mathbf{x}|\overline{\mathbf{x}},\mathbf{P})$.

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

$$p(\mathbf{x}|\mathbf{x}_1,\ldots,\mathbf{x}_N) = \frac{1}{p(\mathbf{x}_1,\ldots,\mathbf{x}_N)} \int \mathrm{d}\mathbf{x}_b \mathrm{d}\mathbf{B}\, p(\mathbf{x}|\mathbf{x}_b,\mathbf{B}) p(\mathbf{x}_1,\ldots,\mathbf{x}_N|\mathbf{x}_b,\mathbf{B}) p(\mathbf{x}_b,\mathbf{B})\,. \tag{2}$$

  - $p(\mathbf{x}|\mathbf{x}_b,\mathbf{B})$: the standard Gaussian prior but based on the true statistics.
  - $p(\mathbf{x}_1,\ldots,\mathbf{x}_N|\mathbf{x}_b,\mathbf{B}) = \prod_{k=1}^{N} p(\mathbf{x}_k|\mathbf{x}_b,\mathbf{B})$
  - $p(\mathbf{x}_b,\mathbf{B})$: prior for the background statistics!

Choosing priors for the background statistics

▶ To progress, we need to make assumptions on the background statistics $p(\mathbf{x}_b, \mathbf{B})$: 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 $\mathbf{x}_b$ and $\mathbf{B}$:

$$p(\mathbf{x}_b, \mathbf{B}) \equiv p_\mathrm{J}(\mathbf{x}_b, \mathbf{B}) = p_\mathrm{J}(\mathbf{x}_b) p_\mathrm{J}(\mathbf{B})$$

and

$$p_\mathrm{J}(\mathbf{x}_b) = 1 , \quad p_\mathrm{J}(\mathbf{B}) = |\mathbf{B}|^{-\frac{M+1}{2}} .$$

▶ 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:

$$p(\mathbf{x}|\overline{\mathbf{x}},\mathbf{P}) \propto \exp\left\{-\frac{1}{2}(\mathbf{x}-\overline{\mathbf{x}})^{\mathrm{T}}\mathbf{P}^{-1}(\mathbf{x}-\overline{\mathbf{x}})\right\}$$

$$p(\mathbf{x}|\mathbf{x}_1,\mathbf{x}_2,\ldots,\mathbf{x}_N) \propto \left|(\mathbf{x}-\overline{\mathbf{x}})(\mathbf{x}-\overline{\mathbf{x}})^{\mathrm{T}} + \varepsilon_N(N-1)\mathbf{P}\right|^{-\frac{N}{2}}, \qquad (3)$$

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

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

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

$$\mathscr{J}(\mathbf{w}) = \frac{1}{2}(\mathbf{y}-H(\overline{\mathbf{x}}+\mathbf{A}\mathbf{w}))^{\mathrm{T}}\mathbf{R}^{-1}(\mathbf{y}-H(\overline{\mathbf{x}}+\mathbf{A}\mathbf{w})) + \frac{N-1}{2}\mathbf{w}^{\mathrm{T}}\mathbf{w}$$

$$\mathscr{J}(\mathbf{w}) = \frac{1}{2}(\mathbf{y}-H(\overline{\mathbf{x}}+\mathbf{A}\mathbf{w}))^{\mathrm{T}}\mathbf{R}^{-1}(\mathbf{y}-H(\overline{\mathbf{x}}+\mathbf{A}\mathbf{w})) + \frac{N}{2}\ln\left(\varepsilon_N + \mathbf{w}^{\mathrm{T}}\mathbf{w}\right). \qquad (4)$$

EnKF-N: algorithm

1. Requires: The forecast ensemble $\{\mathbf{x}_k\}_{k=1,\ldots,N}$, the observations $\mathbf{y}$, and error covariance matrix $\mathbf{R}$
2. Compute the mean $\overline{\mathbf{x}}$ and the anomalies $\mathbf{A}$ from $\{\mathbf{x}_k\}_{k=1,\ldots,N}$.
3. Compute $\mathbf{Y} = \mathbf{HA}$, $\delta = \mathbf{y} - \mathbf{H}\overline{\mathbf{x}}$
4. Find the minimum:
$$\mathbf{w}_a = \min_{\mathbf{w}} \left\{ (\delta - \mathbf{Yw})^{\mathrm{T}} \mathbf{R}^{-1} (\delta - \mathbf{Yw}) + N \ln \left(\varepsilon_N + \mathbf{w}^{\mathrm{T}} \mathbf{w} \right) \right\}$$
5. Compute $\mathbf{x}^a = \overline{\mathbf{x}} + \mathbf{A}\mathbf{w}_a$.
6. Compute $\mathbf{\Omega}_a = \left(\mathbf{Y}^{\mathrm{T}} \mathbf{R}^{-1} \mathbf{Y} + N \frac{(\varepsilon_N + \mathbf{w}_a^{\mathrm{T}} \mathbf{w}_a) \mathbf{I}_N - 2 \mathbf{w}_a \mathbf{w}_a^{\mathrm{T}}}{(\varepsilon_N + \mathbf{w}_a^{\mathrm{T}} \mathbf{w}_a)^2} \right)^{-1}$
7. Compute $\mathbf{W}^a = \{(N-1)\mathbf{\Omega}_a\}^{1/2} \mathbf{U}$
8. Compute $\mathbf{x}_k^a = \mathbf{x}^a + \mathbf{A}\mathbf{W}_k^a$

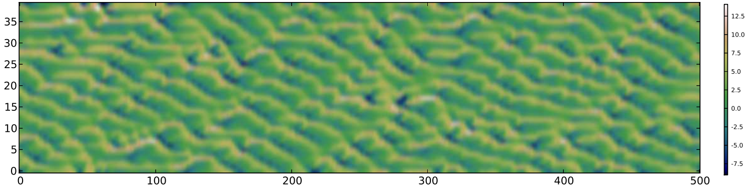
The Lorenz '95 model

- The toy-model [Lorenz and Emmanuel 1998]:
  - It represents a mid-latitude zonal circle of the global atmosphere.
  - $M = 40$ variables $\{x_m\}_{m=1,\ldots,M}$. For $m = 1, \ldots, M$:

$$\frac{\mathrm{d}x_m}{\mathrm{d}t} = (x_{m+1} - x_{m-2})x_{m-1} - x_m + F\,,$$

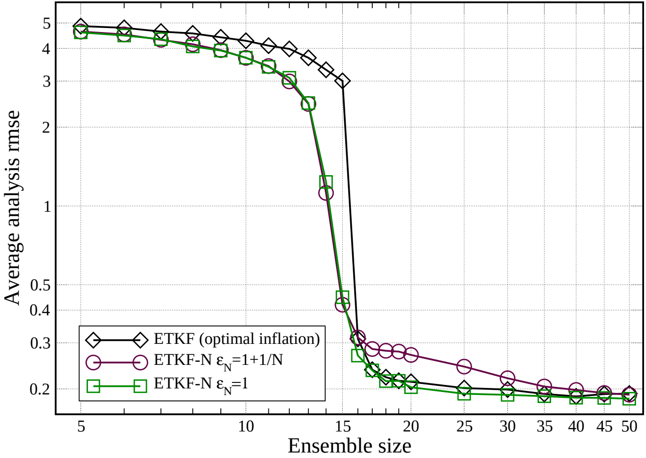
    where $F = 8$, and the boundary is cyclic.
  - Chaotic dynamics, topological dimension of 13, a doubling time of about 0.42 time units, and a Kaplan-Yorke dimension of about 27.1.

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



Application to the Lorenz '95 model

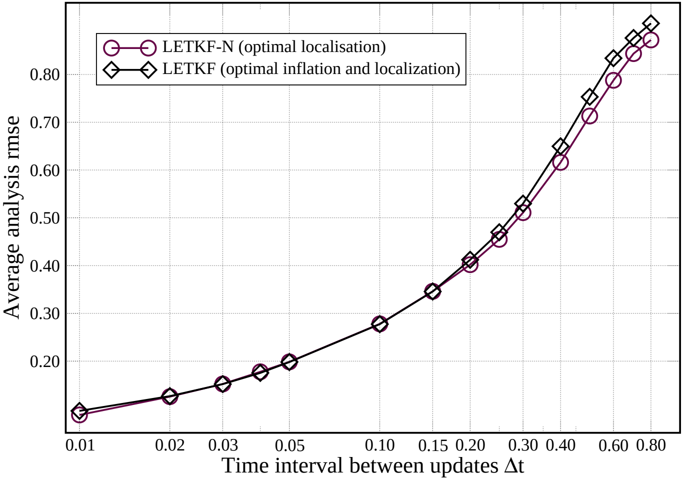
- EnKF-N: analysis rmse versus ensemble size, for $\Delta t = 0.05$.



rank-deficient regime rank-sufficient regime

Application to the Lorenz '95 model

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



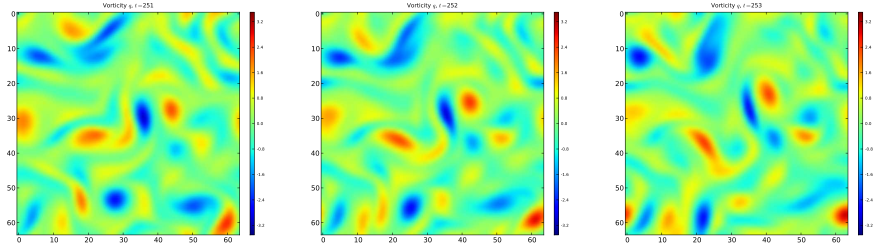
Forced 2D turbulence model

- Forced 2D turbulence model

$$\frac{\partial q}{\partial t} + J(q,\psi) = \lambda q + \nu \Delta^2 q + F\,, \qquad q = \Delta\psi\,, \tag{5}$$

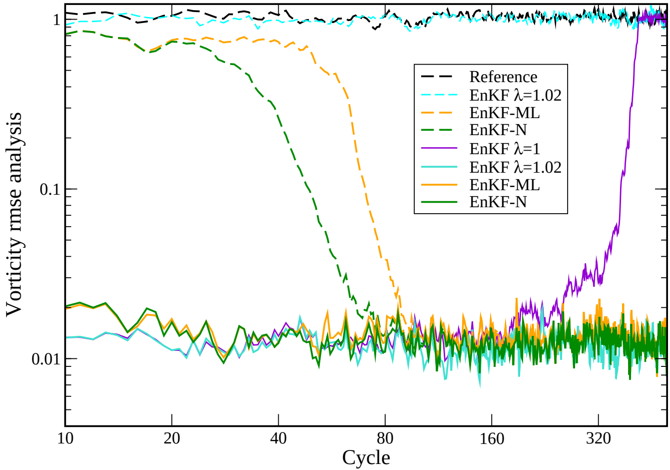
where $J(q,\psi) = \partial_x q \partial_y \psi - \partial_y q \partial_x \psi$, q is the vorticity 2D field, ψ is the current function 2D field, F is the forcing, λ amplitude of the friction, ν amplitude of the biharmonic diffusion, grid: 64×64 small enough to be in the sufficient-rank regime.

- Setup of the experiment: Time-lag between update: $\Delta_t = 2$, fully observed, $\mathbf{R} = 0.1\mathbf{I}$.



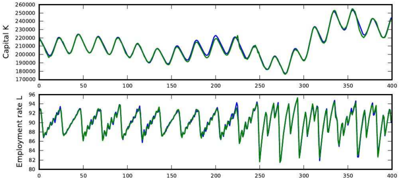
Application to forced 2D turbulence

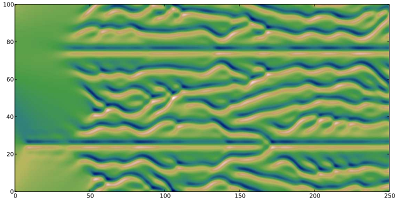
▶ Comparison of: EnKF with uniform inflation, EnKF-N, adaptive inflation EnKF (EnKF-ML), $N = 80$ (rank-sufficient regime). Starting away or close from the truth.



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]





Credit: `http://images.math.cnrs.fr`

Outline

Lagrangian duality

- The primal EnKF-N cost function:

$$\mathscr{J}(\mathbf{w}) = \frac{1}{2}\left(\mathbf{y} - H(\overline{\mathbf{x}} + \mathbf{X}\mathbf{w})\right)^{\mathrm{T}} \mathbf{R}^{-1} \left(\mathbf{y} - H(\overline{\mathbf{x}} + \mathbf{X}\mathbf{w})\right) + \frac{N}{2} \ln\left(\varepsilon_N + \mathbf{w}^{\mathrm{T}}\mathbf{w}\right). \tag{6}$$

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

- Lagrangian:

$$\mathscr{L}(\mathbf{w}, \rho, \zeta) = \frac{1}{2}\left(\delta - \mathbf{Y}\mathbf{w}\right)^{\mathrm{T}} \mathbf{R}^{-1} \left(\delta - \mathbf{Y}\mathbf{w}\right) + \frac{1}{2}\zeta\left(\mathbf{w}^{\mathrm{T}}\mathbf{w} - \rho\right) + \frac{N}{2} \ln\left(\varepsilon_N + \rho\right), \tag{7}$$

where $\delta = \mathbf{y} - \mathbf{H}\overline{\mathbf{x}}$.

- Saddle point equations:

$$\begin{cases} \zeta^\star = N/(\varepsilon_N + \rho^\star) \\ \zeta^\star \mathbf{w}^\star = -\mathbf{Y}^{\mathrm{T}}\mathbf{R}^{-1}(\delta - \mathbf{Y}\mathbf{w}^\star) \end{cases} \Rightarrow \begin{cases} \rho^\star = N/\zeta^\star - \varepsilon_N \\ \mathbf{w}^\star = \left(\zeta^\star + \mathbf{Y}^{\mathrm{T}}\mathbf{R}^{-1}\mathbf{Y}\right)^{-1} \mathbf{Y}^{\mathrm{T}}\mathbf{R}^{-1}\delta \end{cases} \tag{8}$$

Non-convex strong duality

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

$$\begin{aligned} \mathscr{D}(\zeta) &= \inf_{\mathbf{w}} \sup_{\rho \geq 0} \mathscr{L}(\mathbf{w}, \rho, \zeta) \\ &= \frac{1}{2}\delta^{\mathrm{T}} \left(\mathbf{R} + \mathbf{Y}\zeta^{-1}\mathbf{Y}^{\mathrm{T}}\right)^{-1} \delta + \frac{\varepsilon_N \zeta}{2} + \frac{N}{2} \ln \frac{N}{\zeta} - \frac{N}{2}. \end{aligned} \tag{9}$$

- Dual and primal problems:

$$\Delta = \inf_{\zeta > 0} \mathscr{D}(\zeta) \quad \text{and} \quad \Pi = \inf_{\mathbf{w}} \mathscr{J}(\mathbf{w}). \tag{10}$$

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

$$\Delta = \Pi. \tag{11}$$

The dual EnKF-N scheme

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

$$\zeta_a = \min_{\zeta \in]0, N/\varepsilon_N]} \left\{ \delta^{\mathrm{T}} \left(\mathbf{R} + \mathbf{Y}\zeta^{-1}\mathbf{Y}^{\mathrm{T}} \right)^{-1} \delta + \varepsilon_N \zeta + N \ln \frac{N}{\zeta} - N \right\} \tag{12}$$

5. Compute $\mathbf{w}_a = \left(\mathbf{Y}^{\mathrm{T}}\mathbf{R}^{-1}\mathbf{Y} + \zeta_a \right)^{-1} \mathbf{Y}^{\mathrm{T}}\mathbf{R}^{-1}\delta$.
6. Compute $\mathbf{x}_a = \overline{\mathbf{x}} + \mathbf{A}\mathbf{w}_a$.
7. Compute $\mathbf{\Omega}_a = \left\{ \mathbf{Y}^{\mathrm{T}}\mathbf{R}^{-1}\mathbf{Y} + \zeta_a \left(\frac{2\varepsilon_N}{N}\zeta_a - 1 \right) \right\}^{-1}$
8. Compute $\mathbf{W}^a = \{(N-1)\mathbf{\Omega}_a\}^{1/2}\mathbf{U}$
9. Compute $\mathbf{x}_k^a = \mathbf{x}^a + \mathbf{A}\mathbf{W}_k^a$

Outline

Iterative ensemble Kalman filters

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

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- 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:

$$\begin{aligned}\widetilde{\mathscr{J}}(\mathbf{w}) \quad = \quad & \frac{1}{2}\left(\mathbf{y}_2 - H_2(\mathscr{M}_{1\to 2}(\overline{\mathbf{x}}_1 + \mathbf{A}_1\mathbf{w}))\right)^{\mathrm{T}} \mathbf{R}_2^{-1} \left(\mathbf{y}_2 - H_2(\mathscr{M}_{1\to 2}(\overline{\mathbf{x}}_1 + \mathbf{A}_1\mathbf{w}))\right) \\ & + \frac{1}{2}(N-1)\mathbf{w}^{\mathrm{T}}\mathbf{w}\,. \end{aligned} \tag{13}$$

- Gauss-Newton scheme:

$$\begin{aligned} \mathbf{w}^{(p+1)} &= \mathbf{w}^{(p)} - \widetilde{\mathscr{H}}_{(p)}^{-1}\nabla\widetilde{\mathscr{J}}(\mathbf{w}^{(p)}) \\ \nabla\widetilde{\mathscr{J}}_{(p)} &= -\mathbf{Y}_{(p)}^{\mathrm{T}}\mathbf{R}_2^{-1}\left(\mathbf{y}_2 - H_2\mathscr{M}_{1\to 2}(\overline{\mathbf{x}} + \mathbf{A}_1\mathbf{w}^{(p)})\right) + (N-1)\mathbf{w}^{(p)}\,, \\ \widetilde{\mathscr{H}}_{(p)} &= (N-1)\mathbf{I}_N + \mathbf{Y}_{(p)}^{\mathrm{T}}\mathbf{R}_2^{-1}\mathbf{Y}_{(p)}\,, \qquad \mathbf{Y}_{(p)} = [H_2\mathscr{M}_{2\leftarrow 1}\mathbf{A}_1]'_{(p)}\,, \end{aligned} \tag{14}$$

Iterative ensemble Kalman filters

- Sentivities $\mathbf{Y}_{(p)}$ computed by ensemble propagation without TLM and adjoint.

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

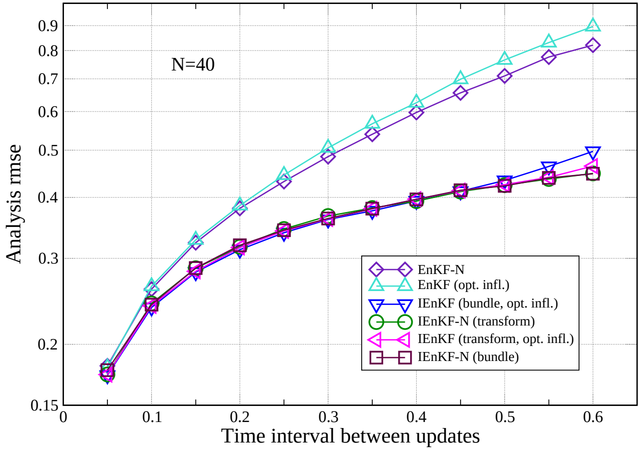
$$\frac{N-1}{2}\mathbf{w}^{\mathrm{T}}\mathbf{w} \longrightarrow \frac{N}{2}\ln\left(\varepsilon_N + \mathbf{w}^{\mathrm{T}}\mathbf{w}\right) . \tag{15}$$

- 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.

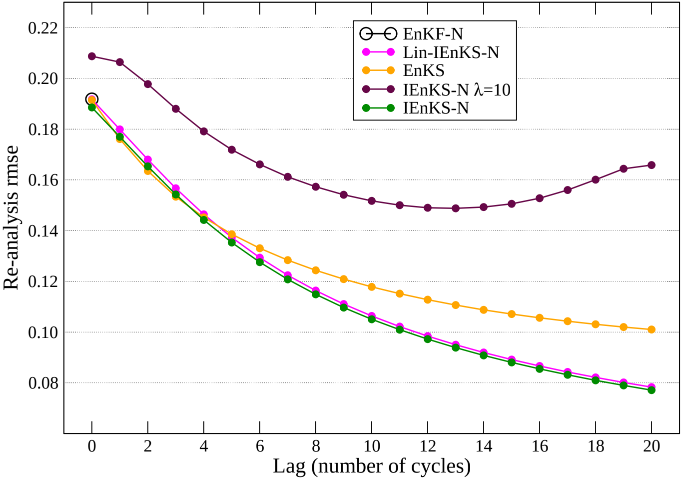
- In a non-sequential but very non-linear context
  Many earlier studies, for instance [Evensen and van Leeuwen, 2000]
  [Chen & Oliver, 2012] in the context of reservoir modelling

- 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

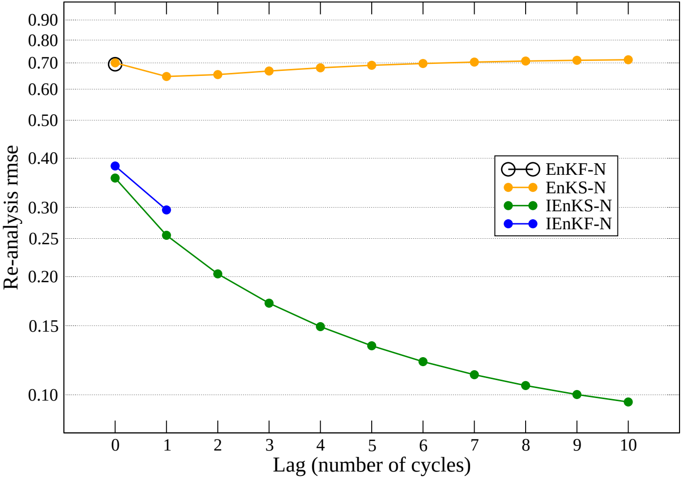
▶ Setup: Lorenz '95, $M = 40$, $N = 20$, $\Delta t = 0.05$, $\mathbf{R} = \mathbf{I}$.

▶ Comparison of EnKF-N, IEnKS-N, Lin-IEnKS-N, EnKS-N, IEnKS-N with a large inflation (reduced-rank 4D-Var?), with $L = 20$.



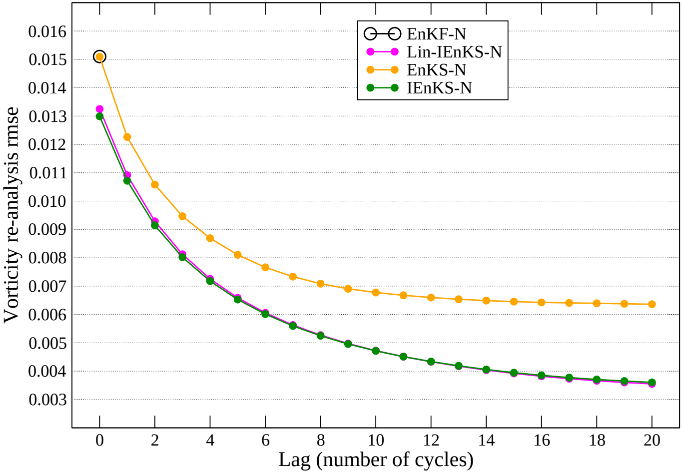
Finite-size iterative ensemble Kalman smoothers

- Setup: Lorenz '95, $M = 40$, $N = 20$, $\Delta t = 0.30$, $\mathbf{R} = \mathbf{I}$.
- Comparison of EnKF-N, IEnKF-N, IEnKS-N, ETKS-N, with $L = 10$.
- Lin-IEnKS-N has (understandably) diverged.



Finite-size iterative ensemble Kalman smoothers

- Setup: 2D turbulence, 64×64, $N = 40$, $\Delta t = 2$, $\mathbf{R} = 0.1\mathbf{I}$.
- Comparison of EnKF-N, IEnKF-N, IEnKS-N, ETKS-N, with $L = 20$.



Outline

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

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