An iterative ensemble Kalman smoother

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Ensemble variational methods

- New methods called ensemble variational methods that mix variational and ensemble approaches (see Lorenc, 2013 for an *almost* perfect definition): Hybrid methods, 4D-Var-Ben, 4D-En-Var, Ensemble of data assimilation (EDA) and IEnKF/IEnKS.

- The IEnKF/IEnKS differ from the other ones in that they are more natural (simple?), regardless of the numerical cost.

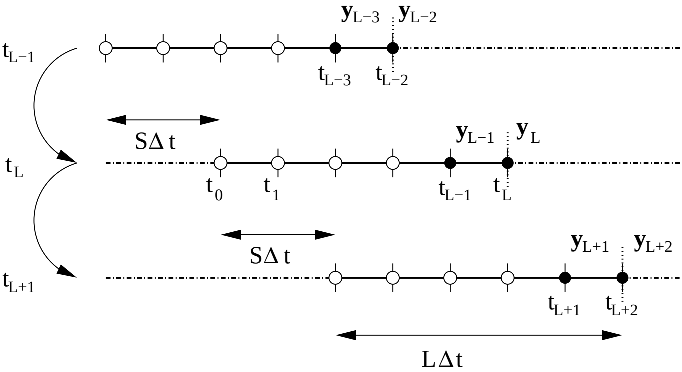
Lorenc A. 2013. Recommended nomenclature for EnVar data assimilation methods.
In Research Activities in Atmospheric and Oceanic Modelling , WGNE.

The IEnKS: at the crossroad between the EnKF and 4D-Var

- The IEnKS follows the scheme of the EnKF:
  - Analysis in ensemble space → Posterior ensemble generation → Ensemble forecast
- Except that
  - The analysis in ensemble space is variational [e.g. Zupanski, 2005] over a finite time windows. It may require several iterations in strongly nonlinear conditions [Gu & Oliver, 2007; Sakov et al., 2012; Bocquet and Sakov, 2012-2013].
  - The gradient of the 4D cost function is computed with the ensemble [Gu & Oliver, 2007;Liu et al., 2008]: no need for the tangent linear/adjoint.
- It generalises the iterative extended Kalman filter/smoother [Wishner et al., 1969; Jazwinski, 1970;Bell, 1994] to ensemble methods.
- It is a unified/straightforward scheme (no hybridization so to speak).

The IEnKS: the cycling

- L: length of the data assimilation window,
- S: shift of the data assimilation window in between two updates.



The IEnKS: a variational standpoint

- Analysis IEnKS cost function in state space $p(\mathbf{x}_0|\mathbf{y}_L) \propto \exp\left(-\mathscr{J}(\mathbf{x}_0)\right)$:

$$\mathscr{J}(\mathbf{x}_0) = \sum_{k=1}^{L} \frac{1}{2}\left(\mathbf{y}_k - H_k \circ \mathscr{M}_{k\leftarrow 0}(\mathbf{x}_0)\right)^{\mathrm{T}} \beta_k \mathbf{R}_k^{-1} \left(\mathbf{y}_k - H_k \circ \mathscr{M}_{k\leftarrow 0}(\mathbf{x}_0)\right) + \frac{1}{2}\left(\mathbf{x}_0 - \overline{\mathbf{x}}_0\right)\mathbf{P}_0^{-1}\left(\mathbf{x}_0 - \overline{\mathbf{x}}_0\right). \tag{1}$$

$\{\beta_0, \beta_1, \ldots, \beta_L\}$ weight the observations impact within the window.

- Reduced scheme in ensemble space, $\mathbf{x}_0 = \overline{\mathbf{x}}_0 + \mathbf{A}_0\mathbf{w}$, where $\mathbf{A}_0$ is the ensemble anomaly matrix:

$$\widetilde{\mathscr{J}}(\mathbf{w}) = \mathscr{J}\left(\overline{\mathbf{x}}_0 + \mathbf{A}_0\mathbf{w}\right). \tag{2}$$

- IEnKS cost function in ensemble space [Hunt et al., 2007; Bocquet and Sakov, 2012]:

$$\widetilde{\mathscr{J}}(\mathbf{w}) = \frac{1}{2}\sum_{k=1}^{L}\left(\mathbf{y}_k - H_k \circ \mathscr{M}_{k\leftarrow 0}\left(\overline{\mathbf{x}}_0 + \mathbf{A}_0\mathbf{w}\right)\right)^{\mathrm{T}} \beta_k \mathbf{R}_k^{-1}\left(\mathbf{y}_k - H_k \circ \mathscr{M}_{k\leftarrow 0}\left(\overline{\mathbf{x}}_0 + \mathbf{A}_0\mathbf{w}\right)\right) + \frac{1}{2}(N-1)\mathbf{w}^{\mathrm{T}}\mathbf{w}. \tag{3}$$

The IEnKS: minimisation scheme

- As a variational reduced method, one can use Gauss-Newton [Sakov et al., 2012], Levenberg-Marquardt [Bocquet and Sakov, 2012; Chen and Oliver, 2013], quasi-Newton, etc., minimisation schemes.
- Gauss-Newton scheme (the Hessian is approximate):

$$
\begin{aligned}
\mathbf{w}^{(p+1)} &= \mathbf{w}^{(p)} - \widetilde{\mathscr{H}}_{(p)}^{-1} \nabla \widetilde{\mathscr{J}}_{(p)}(\mathbf{w}^{(p)}) , \\
\mathbf{x}_0^{(p)} &= \mathbf{x}_0^{(0)} + \mathbf{A}_0 \mathbf{w}^{(p)} , \\
\nabla \widetilde{\mathscr{J}}_{(p)} &= - \sum_{k=1}^{L} \mathbf{Y}_{k,(p)}^{\mathrm{T}} \beta_k \mathbf{R}_k^{-1} \left(\mathbf{y}_k - H_k \circ \mathscr{M}_{k\leftarrow 0}(\mathbf{x}_0^{(p)}) \right) + (N-1)\mathbf{w}^{(p)} , \\
\widetilde{\mathscr{H}}_{(p)} &= (N-1)\mathbf{I}_N + \sum_{k=1}^{L} \mathbf{Y}_{k,(p)}^{\mathrm{T}} \beta_k \mathbf{R}_L^{-1} \mathbf{Y}_{(p)} , \\
\mathbf{Y}_{k,(p)} &= [H_k \circ \mathscr{M}_{k\leftarrow 0}]'_{|\mathbf{x}_0^{(p)}} \mathbf{A}_0 .
\end{aligned}
\tag{4}
$$

- One solution to compute the 4D sensitivities: the bundle scheme. It simply mimics the action of the tangent linear by finite difference:

$$
\mathbf{Y}_{k,(p)} \approx \frac{1}{\varepsilon} H_k \circ \mathscr{M}_{k\leftarrow 0} \left(\mathbf{x}^{(p)} \mathbf{1}^{\mathrm{T}} + \varepsilon \mathbf{A}_0 \right) \left(\mathbf{I}_N - \frac{\mathbf{1}\mathbf{1}^{\mathrm{T}}}{N} \right) . \tag{5}
$$

The IEnKS: ensemble update and the forecast step

- Generate an updated ensemble from the previous analysis:

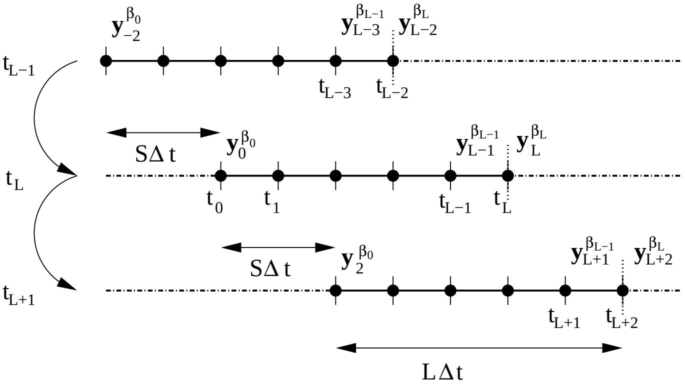
$$\mathbf{E}_0^\star = \mathbf{x}_0^\star \mathbf{1}^{\mathrm{T}} + \sqrt{N-1}\mathbf{A}_0 \widetilde{\mathscr{H}_\star}^{-1/2}\mathbf{U} \quad \text{where} \quad \mathbf{U}\mathbf{1} = \mathbf{1}\,. \tag{6}$$

- Just propagate the updated ensemble from t_0 to t_S:

$$\mathbf{E}_S = \mathscr{M}_{S\leftarrow 0}(\mathbf{E}_0)\,. \tag{7}$$

In the quasi-static case: $S = 1$.

IEnKS: single vs multiple data assimilation

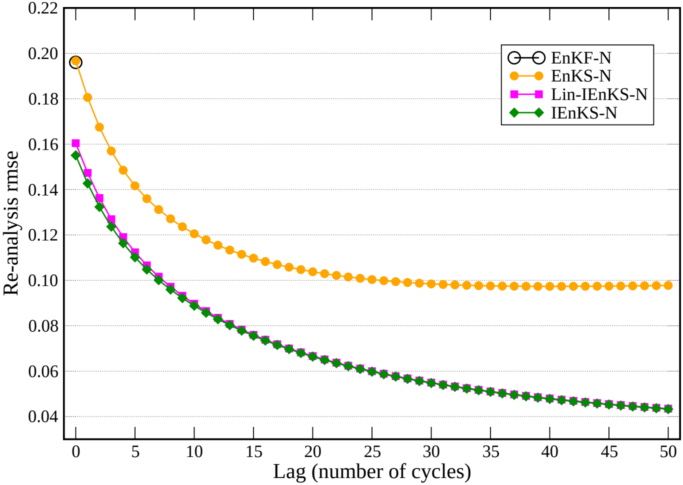


- SDA IEnKS: The observation vector are assimilated once and for all. Exact scheme.

- MDA IEnKS: The observation vector are assimilated several times and poundered with weights β_k within the window. Exact scheme in the linear/Gaussian limit. More stable for long windows than the SDA scheme.

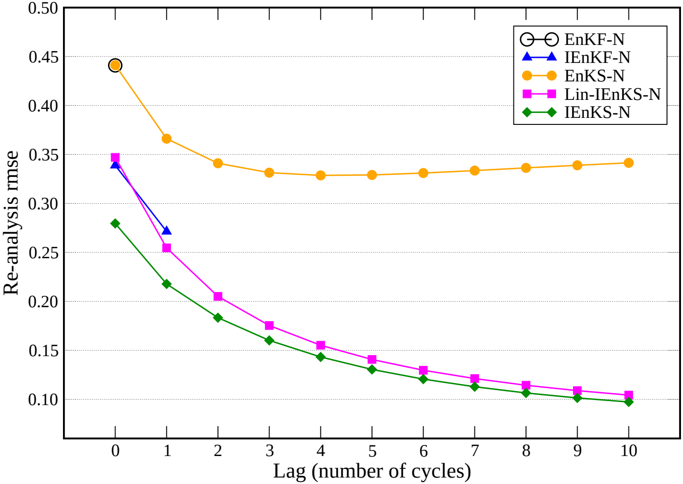
Application to the Lorenz '95 model

- Setup: Lorenz '95, $M = 40$, $N = 20$, $\Delta t = 0.05$, $\mathbf{R} = \mathbf{I}$.
- Lin-IEnKS $\equiv$ IEnKS with a single iteration (linearised IEnKS).
- Comparison of EnKF-N, MDA IEnKS-N, MDA Lin-IEnKS-N, EnKS-N, with $L = 50$.



Application to the Lorenz '95 model

- Setup: Lorenz '95, $M = 40$, $N = 20$, $\Delta t = 0.20$, $\mathbf{R} = \mathbf{I}$.
- Comparison of EnKF-N, IEnKF-N, MDA IEnKS-N, ETKS-N, with $L = 10$.
- Lin-IEnKS-N underperforms (because of the mild nonlinearity).

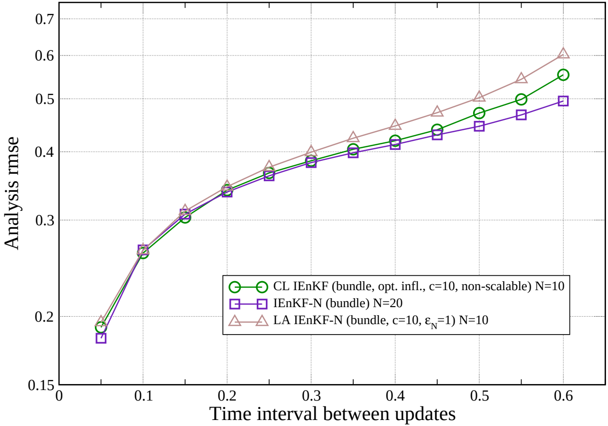


IEnKF/IEnKS: Localisation

- Localisation in an EnVar context is non-trivial because localisation and the evolution model do not commute:

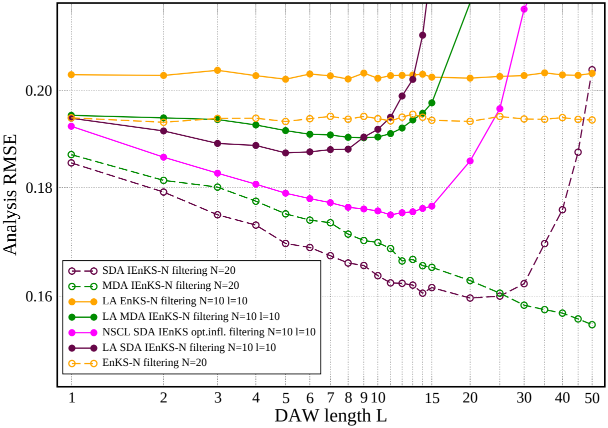
$$\mathbf{M}_{k\leftarrow 0}(\mathbf{C}\circ\mathbf{B}_0)\mathbf{M}_{k\leftarrow 0}^{\mathrm{T}} \neq \mathbf{C}\circ\left(\mathbf{M}_{k\leftarrow 0}\mathbf{B}_0\mathbf{M}_{k\leftarrow 0}^{\mathrm{T}}\right). \quad (8)$$

- Local analysis of IEnKF, and comparison with a non-scalable optimal approach.



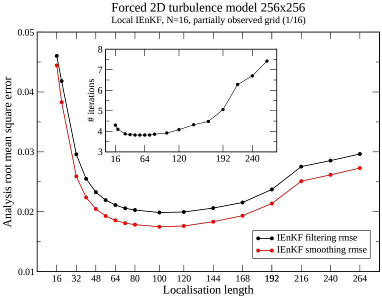
IEnKF/IEnKS: Localisation

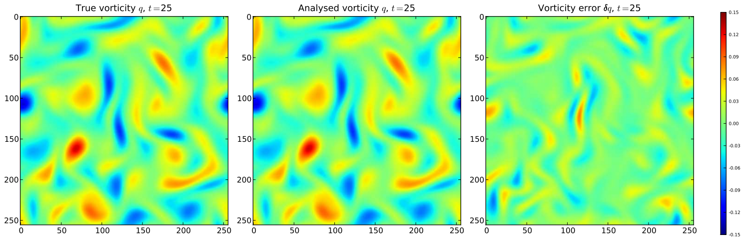
▶ Local analysis of IEnKS, and comparison with a non-scalable optimal approach (filtering performance).



IEnKF/IEnKS: Localisation

- Localisation of the IEnKF works fine on a forced 2D-turbulence model (256×256).



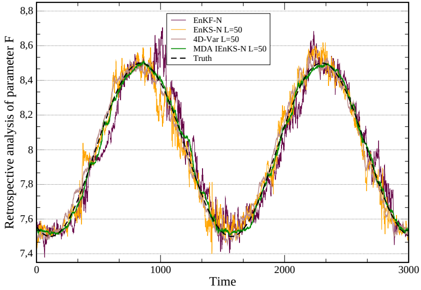


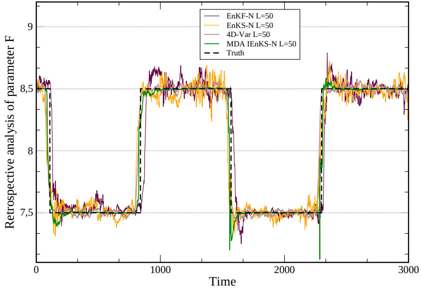
IEnKS: parameter estimation

- The augmented state formalism is convenient for the IEnKS, and offers an easy implementation of technically challenging data assimilation problems.

- Lorenz '95 with joint estimation of the forcing parameter F (41 variables): RMSEs.

Method / F profile	Sinusoidal	Step-wise
EnKF-N	0.063	0.079
EnKS-N L=50	0.040	0.063
4D-Var L=50	0.030	0.045
MDA IEnKS-N L=50	0.020	0.031





Conclusions

- The iterative ensemble Kalman smoother (IEnKS) is a way to elegantly combine the advantages of variational and ensemble Kalman filtering.
- The IEnKS is a generalisation of the iterative ensemble Kalman filter (IEnKF). It is an EnVar method. It is flow-dependent, tangent linear and adjoint free.
- Though based on Gaussian assumptions, it can offer (much) better retrospective analysis than standard Kalman smoothers in weak and mildly nonlinear conditions.
- Much more performing than other Kalman filter/smoothers in strongly non-linear conditions.
- Properly defined multiple assimilation of observations can stabilise the smoother over very large data assimilation window (20 days of Lorenz '95).
- More generally the IEnKF/IEnKS have the potential to outperform both the EnKF and the 4D-Var (IEnKS already does so with toy-models).
- Localisation remains a fundamental issue in this context (work in progress).
- Weak-constraint formalism not really explored yet (work in progress).

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