Joint state and parameter estimation with an iterative ensemble Kalman smoother

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- 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.

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

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

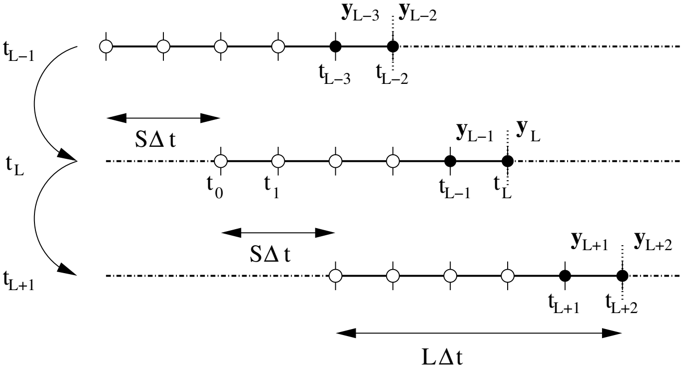
- The IEnKS has a great potential for parameter estimation, as it is variational but avoids the derivation of the adjoint.

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, 2012-2014].
  - 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 $p(\mathbf{x}_0|\mathbf{y}_L) \propto \exp\left(-\mathscr{J}(\mathbf{x}_0)\right)$:

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

$\{\beta_0, \beta_1, \ldots, \beta_L\}$ 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:

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

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

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

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:

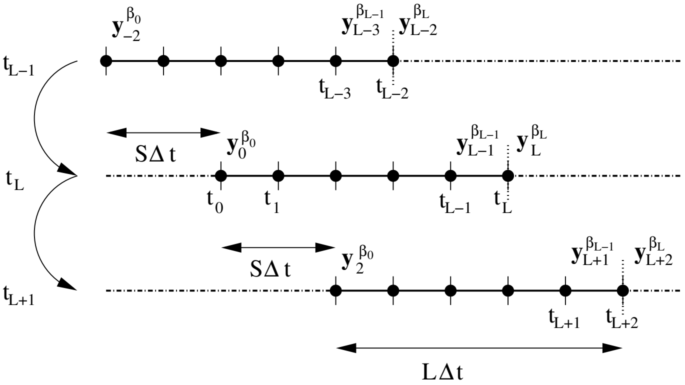
$$\mathbf{E}_0^\star = \mathbf{x}_0^\star \mathbf{1}^{\mathrm{T}} + \sqrt{N-1}\mathbf{A}_0 \widetilde{\mathscr{H}}_\star^{-1/2}\mathbf{U} \quad \text{where} \quad \mathbf{U}\mathbf{1} = \mathbf{1}\,. \tag{6}$$

- 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



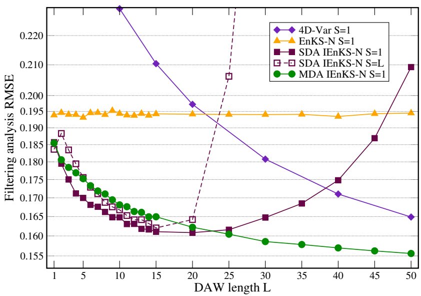
- SDA IEnKS: The observation vector are assimilated once and for all. Exact scheme.

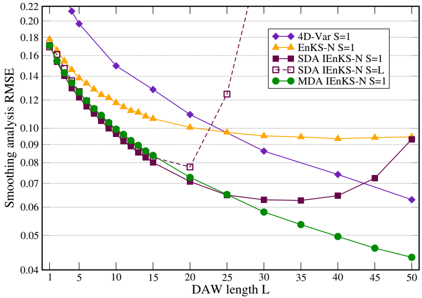
- MDA IEnKS: The observation vector are assimilated several times and poundered with weights β_k within the window. Exact scheme in the linear/Gaussian limit. More stable for long windows than the SDA scheme.

Application to the Lorenz-95 model

- Weakly nonlinear case: Lorenz-95, $M = 40$, $N = 20$, $\Delta t = 0.05$, $\mathbf{R} = \mathbf{I}$.

- Comparison of 4D-Var $S = 1$, EnKS $S = 1$, SDA IEnKS $S = 1$, SDA IEnKS $S = L$, and MDA IEnKS $S = 1$.

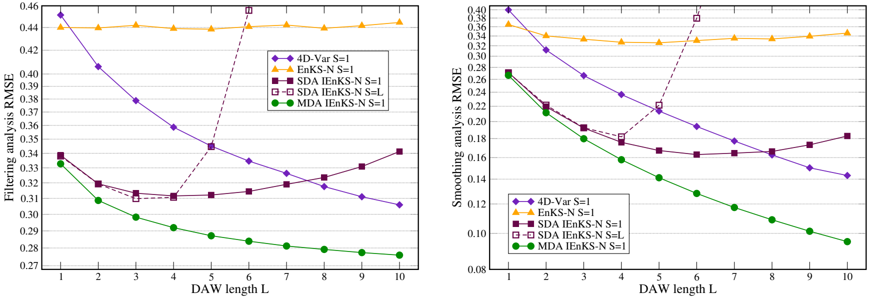




Application to the Lorenz-95 model

▶ Strongly nonlinear case: Lorenz-95, $M = 40$, $N = 20$, $\Delta t = 0.20$, $\mathbf{R} = \mathbf{I}$.

▶ Comparison of 4D-Var $S = 1$, EnKS $S = 1$, SDA IEnKS $S = 1$, SDA IEnKS $S = L$, and MDA IEnKS $S = 1$.

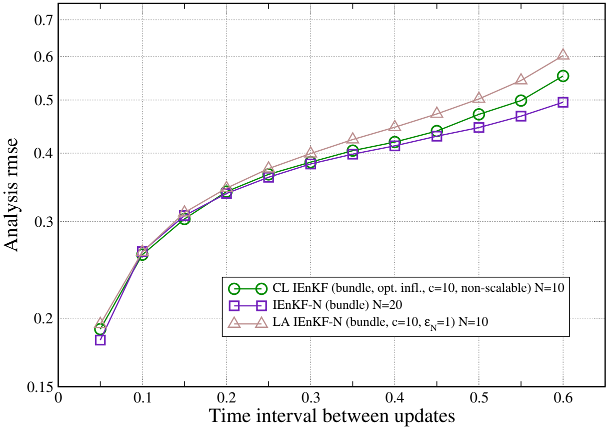


IEnKF/IEnKS: Localisation

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

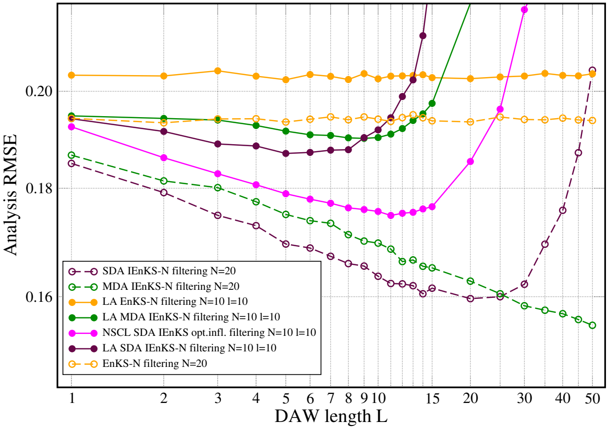
$$\mathbf{M}_{k\leftarrow 0}\left(\mathbf{C}\circ\mathbf{B}_0\right)\mathbf{M}_{k\leftarrow 0}^{\mathrm{T}} \neq \mathbf{C}\circ\left(\mathbf{M}_{k\leftarrow 0}\mathbf{B}_0\mathbf{M}_{k\leftarrow 0}^{\mathrm{T}}\right). \tag{8}$$

- 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: Augmented state formalism

- IEnKS treats parameters the way both 4D-Var and EnKF treat them.

- The state space is augmented from $\mathbf{x} \in \mathbb{R}^M$ to a vector

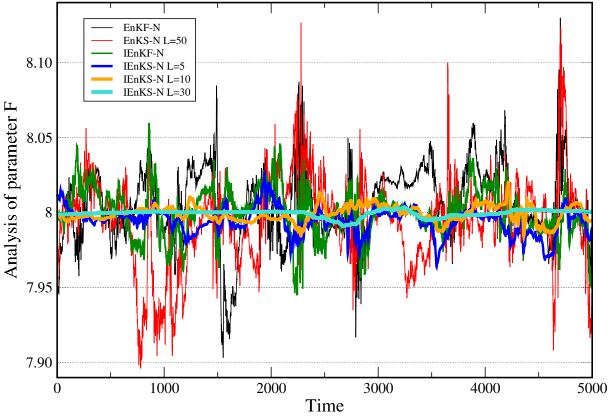
$$\mathbf{z} = \begin{pmatrix} \mathbf{x} \\ \theta \end{pmatrix} \in \mathbb{R}^{M+P}, \tag{9}$$

Technically, there is nothing more to the joint state and parameter IEnKS than in the state IEnKS.

- A forward model needs to be introduced for the parameters:
  - For instance, the persistence model ($\theta_{k+1} = \theta_k$),
  - or some jittering such as a Brownian motion ($\theta_{k+1} = \theta_k + \varepsilon_k$).

Estimation of the Lorenz-95 forcing parameter F

- F is static but unknown.

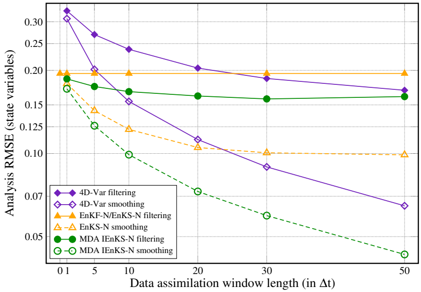


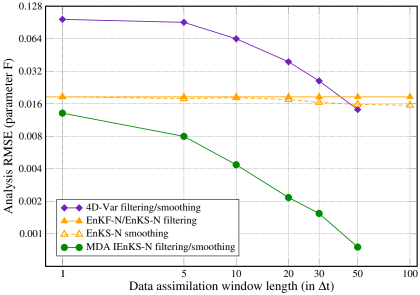
- Augmented state vector $\in \mathbb{R}^{41}$, $N = 20$. The forcing of the true model is $F = 8$.

Estimation of the Lorenz-95 forcing parameter F

- Setup: Lorenz-95, $M = 40$, $N = 20$, $\Delta t = 0.05$, $\mathbf{R} = \mathbf{I}$.

- Comparison of 4D-Var $S = 1$, EnKS $S = 1$, SDA IEnKS $S = 1$, SDA IEnKS $S = L$, and MDA IEnKS $S = 1$.

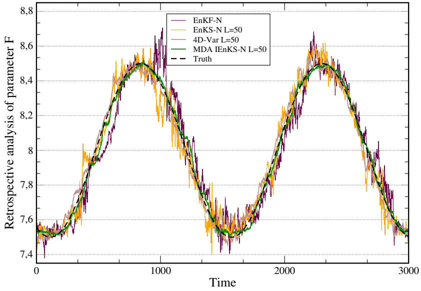


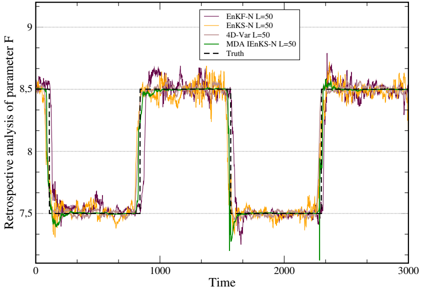


Estimation of the Lorenz-95 forcing parameter F

- The forcing parameter F is time-varying.
- Internalised model error (F is in the augmented state) + unaccounted external model error (the true F is time-varying $\neq$ persistence assumption).

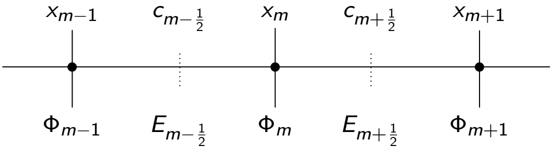
Method / F profile	Sinusoidal	Step-wise
EnKF-N	0.063	0.079
EnKS-N L=50	0.040	0.063
4D-Var L=50	0.030	0.045
MDA IEnKS-N L=50	0.020	0.031





Extending the Lorenz-95 model

▶ An online tracer model: Lorenz-95 (wind field) + tracer



▶ The tracer is advected by the *wind* field of the Lorenz-95 model. We have chosen to use the simple Godunov/upwind scheme which is positive and conservative.

$$\frac{\mathrm{d}x_m}{\mathrm{d}t} = (x_{m+1} - x_{m-2})x_{m-1} - x_m + F\,, \tag{10}$$

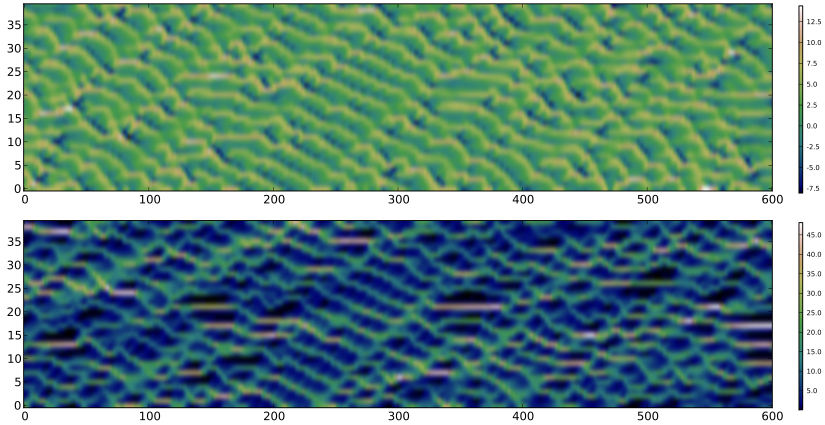
$$\frac{\mathrm{d}c_{m+\frac{1}{2}}}{\mathrm{d}t} = \Phi_m - \Phi_{m+1} - \lambda c_{m+\frac{1}{2}} + E_{m+\frac{1}{2}}\,, \tag{11}$$

$$\text{where} \quad \Phi_m = x_m c_{m-\frac{1}{2}} \quad \text{if} \quad x_m \geq 0\,, \tag{12}$$

$$= x_m c_{m+\frac{1}{2}} \quad \text{if} \quad x_m < 0\,. \tag{13}$$

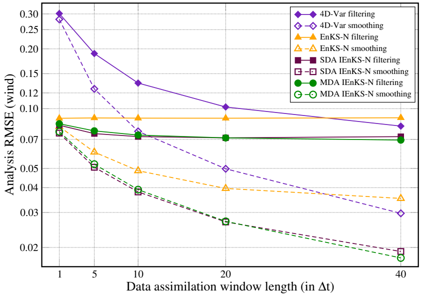
▶ Uniform emission of the tracer with the flux $E_{m+\frac{1}{2}}$. Deposited on the whole domain, using a simple scavenging scheme parametrised by a scavenging ratio λ.

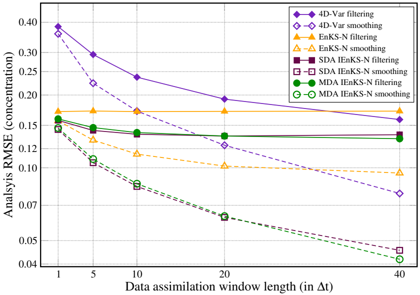
Extending the Lorenz-95 model



- Time evolution of the wind (top) and concentration (bottom) fields of the coupled Lorenz-95 - tracer model.

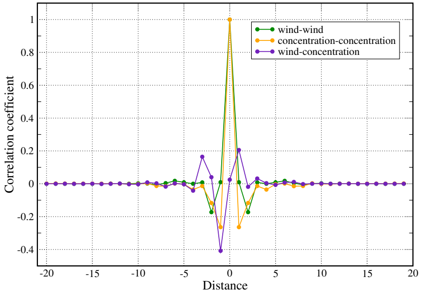
Extending the Lorenz-95 model

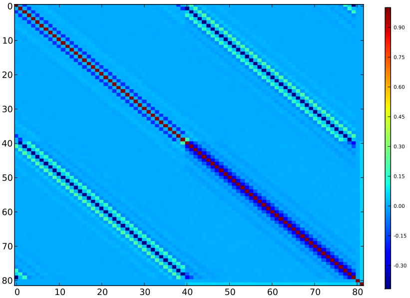




- Mean filtering and smoothing analysis rmses of the wind variables (left) and concentration variables (right) of the online tracer model, as a function of the DAW length for the IEnKS (finite-size variant), the EnKF/EnKS, and 4D-Var (with optimal inflation of the prior).

Extending the Lorenz-95 model





▶ Structure functions of the mean correlation of the errors of the initial condition from the IEnKS applied to the online tracer model.

▶ The full error covariance matrix obtained from the IEnKS can be used to help 4D-Var by building better background statistics. It does help 4D-Var in the estimation of parameters, but does little to the estimation of the state variables whose error covariance matrix is quite dynamical.

Conclusions

- The iterative ensemble Kalman smoother (IEnKS) is a method to seamlessly 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.
- The IEnKF/IEnKS have the potential to (significantly) outperform both the EnKF and the 4D-Var in all regimes. IEnKS already does so with toy-models.
- IEnKS is very well suited for parameter (or joint state/parameter) estimation, and does so in a very simple way via the augmented state formalism.
- More complex reactive air quality toy-model under development in order to test the IEnKS on challenging atmospheric chemistry problems.

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