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/smootherr [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 $p(x_0|y_L) \propto \exp(-J(x_0))$:

$$J(x_0) = \sum_{k=1}^{L} \frac{1}{2} (y_k - H_k \circ M_{k \leftarrow 0}(x_0))^T \beta_k R_k^{-1} (y_k - H_k \circ M_{k \leftarrow 0}(x_0))$$

$$+ \frac{1}{2} (x_0 - \bar{x}_0) P_0^{-1} (x_0 - \bar{x}_0). \tag{1}$$

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

▶ Reduced scheme in ensemble space, $x_0 = \bar{x}_0 + A_0 w$, where $A_0$ is the ensemble anomaly matrix:

$$\tilde{J}(w) = J(\bar{x}_0 + A_0 w). \tag{2}$$

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

$$\tilde{J}(w) = \frac{1}{2} \sum_{k=1}^{L} (y_k - H_k \circ M_{k \leftarrow 0}(\bar{x}_0 + A_0 w))^T \beta_k R_k^{-1} (y_k - H_k \circ M_{k \leftarrow 0}(\bar{x}_0 + A_0 w))$$

$$+ \frac{1}{2} (N - 1) w^T w. \tag{3}$$
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):

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

\[ \mathbf{x}_0^{(p)} = \mathbf{x}_0^{(0)} + \mathbf{A}_0 \mathbf{w}(p), \]

\[ \nabla \tilde{\mathcal{J}}(p) = - \sum_{k=1}^{L} \mathbf{Y}_{k,(p)}^T \beta_k \mathbf{R}_k^{-1} \left( \mathbf{y}_k - H_k \circ \mathcal{M}_k \downarrow 0(\mathbf{x}_0^{(p)}) \right) + (N - 1) \mathbf{w}(p), \]

\[ \tilde{\mathcal{H}}(p) = (N - 1) \mathbf{I}_N + \sum_{k=1}^{L} \mathbf{Y}_{k,(p)}^T \beta_k \mathbf{R}_k^{-1} \mathbf{Y}(p), \]

\[ \mathbf{Y}_{k,(p)} = [H_k \circ \mathcal{M}_k \downarrow 0]'_{\mathbf{x}_0^{(p)}} \mathbf{A}_0. \quad (4) \]

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

\[ \mathbf{Y}_{k,(p)} \approx \frac{1}{\varepsilon} H_k \circ \mathcal{M}_k \downarrow 0 \left( \mathbf{x}^{(p)} \mathbf{1}_N + \varepsilon \mathbf{A}_0 \right) \left( \mathbf{I}_N - \frac{\mathbf{1}_N \mathbf{1}_N^T}{N} \right). \quad (5) \]
The IEnKS: ensemble update and the forecast step

Generate an updated ensemble from the previous analysis:

\[
E^*_0 = x^*_0 1^T + \sqrt{N-1} A_0 \tilde{H}_x^{-1/2} U \quad \text{where} \quad U1 = 1.
\]  

Just propagate the updated ensemble from \( t_0 \) to \( t_S \):

\[
E_S = M_{S \leftarrow 0}(E_0).
\]  

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 pondered with weights $\beta_k$ 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, $M = 40$, $N = 20$, $\Delta t = 0.05$, $R = I$.

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

![Graphs showing filtering and smoothing analysis RMSE vs. DAW length L for different methods.](image-url)
Application to the Lorenz-95 model

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

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Localisation

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

\[ M_{k\leftarrow 0} (C \circ B_0) M_{k\leftarrow 0}^T \neq C \circ \left( M_{k\leftarrow 0} B_0 M_{k\leftarrow 0}^T \right). \]  \hspace{1cm} (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 \( x \in \mathbb{R}^M \) to a vector

\[
\mathbf{z} = \begin{pmatrix} x \\ \theta \end{pmatrix} \in \mathbb{R}^{M+P},
\] (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 \( \theta_{k+1} = \theta_k + \epsilon_k \).
Augmented state formalism

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, $M = 40$, $N = 20$, $\Delta t = 0.05$, $R = I$.

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).

<table>
<thead>
<tr>
<th>Method / F profile</th>
<th>Sinusoidal</th>
<th>Step-wise</th>
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</thead>
<tbody>
<tr>
<td>EnKF-N</td>
<td>0.063</td>
<td>0.079</td>
</tr>
<tr>
<td>EnKS-N L=50</td>
<td>0.040</td>
<td>0.063</td>
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<tr>
<td>4D-Var L=50</td>
<td>0.030</td>
<td>0.045</td>
</tr>
<tr>
<td>MDA IEnKS-N L=50</td>
<td>0.020</td>
<td>0.031</td>
</tr>
</tbody>
</table>

Retrospective analysis of parameter $F$
Extending the Lorenz-95 model

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

\[
\begin{align*}
x_{m-1} & \quad c_{m-\frac{1}{2}} & \quad x_m & \quad c_{m+\frac{1}{2}} & \quad x_{m+1} \\
\Phi_{m-1} & \quad E_{m-\frac{1}{2}} & \quad \Phi_m & \quad E_{m+\frac{1}{2}} & \quad \Phi_{m+1}
\end{align*}
\]

- 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.

\[
\frac{dx_m}{dt} = (x_{m+1} - x_{m-2})x_{m-1} - x_m + F, \quad (10)
\]

\[
\frac{dc_{m+\frac{1}{2}}}{dt} = \Phi_m - \Phi_{m+1} - \lambda c_{m+\frac{1}{2}} + E_{m+\frac{1}{2}}, \quad (11)
\]

where \( \Phi_m \) = \( x_m c_{m-\frac{1}{2}} \) if \( x_m \geq 0 \),

\[
\Phi_m = x_m c_{m+\frac{1}{2}} \quad \text{if} \quad x_m < 0. \quad (13)
\]

- 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 \( \lambda \).
Extending the Lorenz-95 model

▶ Time evolution of the wind (top) and concentration (bottom) fields of the coupled Lorenz-95 - tracer model.
Mean filtering and smoothing analysis rmse of the wind variables (left) and concentration variables (right) of the online tracer model, as a function of the data assimilation window length for the IEnKS (finite-size variant), the EnKF/EnKS, and 4D-Var (with optimal inflation of the prior).
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.


