An iterative ensemble Kalman filter in presence of additive model error

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Outline

1. The iterative ensemble Kalman filter (IEnKF)

2. Theory of the IEnKF-Q
   - Formulation
   - Decoupling
   - Base algorithm

3. Numerics for the IEnKF-Q

4. Conclusions

5. References
Iterative ensemble Kalman filter and smoother

- Iterative ensemble Kalman smoother (IEnKS): exemplar of nonlinear four-dimensional EnVar methods.
  - Propagates the error statistics from one cycle to the next with the ensemble (errors of the day).
  - Performs a 4D-Var analysis at each cycle (within the ensemble subspace).
- Outperforms 4D-Var, the EnKF, and the EnKS, ... by construction.

Iterative ensemble Kalman filter: cycling

- Iterative ensemble Kalman filter (IEnKF) \(\equiv\) lag-1 IEnKS.

- Cycling:

Variational analysis in ens. space \(\rightarrow\) Posterior ens. generation \(\rightarrow\) Ens. forecast
Iterative ensemble Kalman filter: a variational standpoint

- Analysis IEnKF cost function in state space $p(x_1|y_2) \propto \exp(-J(x_1))$:

$$J(x_1) = \frac{1}{2} \|y_2 - \mathcal{H}_2 \circ \mathcal{M}_2(x_1)\|_{R_2^{-1}}^2 + \frac{1}{2} \|x_1 - \bar{x}_1\|_{P_1^{-1}}^2.$$ 

- Reduced scheme in ensemble subspace, $x_1 = \bar{x}_1 + A_1 w_1$, where $A_1$ is the normalized ensemble perturbation matrix:

$$\tilde{J}(w_1) = J(\bar{x}_1 + A_1 w_1).$$

- IEnKF cost function in ensemble subspace:

$$\tilde{J}(w_1) = \frac{1}{2} \|y_2 - \mathcal{H}_2 \circ \mathcal{M}_2 (\bar{x}_1 + A_1 w_1)\|_{R_2^{-1}}^2 + \frac{1}{2} \|w_1\|^2.$$ 


Iterative ensemble Kalman filter: minimization scheme

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, minimization schemes (not limited to quasi-Newton). Example: Gauss-Newton scheme

\[
\begin{align*}
    w_1^{i+1} &= w_1^i - \tilde{H}_i^{-1} \nabla \tilde{J}_i(w_1^i), \\
    x_1^i &= \bar{x}_1 + A_1 w_1^i, \\
    \nabla \tilde{J}_i &= w_1^i - Y_i^T R_2^{-1} (y_2 - H_2 \circ M_2(x_1^i)) , \\
    \tilde{H}_i &= I_N + Y_i^T R_2^{-1} Y_i, \\
    Y_i &= [H_2 \circ M_2]'_{x_1^i} A_1.
\end{align*}
\]

Perturbation update: same as the ETKF

\[
E_1^* = x_1^* 1^T + \sqrt{N-1} A_1 \tilde{H}_*^{-1/2} U \quad \text{where} \quad U 1 = 1. \tag{1}
\]

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

\[
E_2 = M_{2:1}(E_1). \tag{2}
\]
Iterative ensemble Kalman filter: computing the sensitivities

- Sensitivities $Y_{(p)}$ computed by ensemble propagation without TLM and adjoint ([Gu and Oliver, 2007; Liu et al., 2008; Buehner et al., 2010])

- First alternative [Sakov et al., 2012]: the transform scheme. The ensemble is preconditioned before its propagation using the ensemble transform

$$T^i = \left( I_N + Y^iT R^{-1} Y^i \right)^{-1/2},$$

obtained at the previous iteration. The inverse transformation is applied after propagation.

- Second alternative [Bocquet and Sakov, 2012]: the bundle scheme. It simply mimics the action of the tangent linear by finite difference:

$$Y^i \approx \frac{1}{\varepsilon} \mathcal{H}_2 \circ \mathcal{M}_2 \left( x^iT + \varepsilon A_1 \right) \left( I_N - \frac{11^T}{N} \right).$$
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IEnKF-Q: formulation

▶ Analysis cost function:

\[ J(x_1, x_2) = \|x_1 - x_1^a\|^2_{(P_1^a)^{-1}} + \|y_2 - H(x_2)\|^2_{R^{-1}} + \|x_2 - M(x_1)\|^2_{Q^{-1}}. \]

▶ Ensemble subspace representation:

\[ x_1 = x_1^a + A_1^a u, \quad A_1^a (A_1^a)^T = P_1^a, \quad A_1^a 1 = 0, \]

\[ x_2 = M(x_1) + A_2^q v, \quad A_2^q (A_2^q)^T = Q, \quad A_2^q 1 = 0. \]

▶ Cost function in ensemble subspace:

\[ J(u, v) = u^T u + v^T v + \|y_2 - H(x_2)\|^2_{R^{-1}}. \]
IEnKF-Q: formulation

▶ Compactification:

\[ w \equiv \begin{bmatrix} u \\ v \end{bmatrix} \implies J(w) = w^T w + \| y_2 - \mathcal{H}(x_2) \|_R^2 - 1. \]

\[ \rightarrow \text{enables to apply the perfect model/strong constraint IEnKF machinery!} \]

▶ Condition of zero gradient:

\[ w - (HA)^T R^{-1} [y_2 - \mathcal{H}(x_2)] = 0, \]

where

\[ A \equiv [MA_1^a, A_2^q], \quad H \equiv \nabla \mathcal{H}(x_2), \quad M \equiv \nabla \mathcal{M}(x_1). \]

▶ The cost function can be minimized using a Gauss-Newton method

\[ w^{i+1} = w^i - D^i \nabla J(w^i), \]

where the inverse Hessian is approximated as

\[ D^i \approx \left[ I + (H'A_i)^T R^{-1} H'A_i \right]^{-1}. \]
IEnKF-Q: formulation

- Posterior errors:
  \[ \delta x_1 = A^a_1 \delta u, \quad \delta x_2 = MA^a_1 \delta u + A^q_2 \delta v, \]

- Updated perturbations over \([t_1, t_2]\):
  \[ A^a_2 (A^a_2)^T = E[\delta x^*_2 (\delta x^*_2)^T] = A^* E[w^*(w^*)^T](A^*)^T = A^* D^*(A^*)^T, \]
  which implies
  \[ A^a_2 = A^* (D^*)^{1/2} = A^* \left[ I + (H^* A^*)^T R^{-1} H^* A^* \right]^{-1/2}. \]

- Updated (smoothed) perturbations at \(t_1\):
  \[ A^s_1 (A^s_1)^T = E[\delta x^*_1 (\delta x^*_1)^T] = A^a_1 E[u^*(u^*)^T](A^a_1)^T, \]
  which implies
  \[ A^s_1 = A^a_1 (D_{1:m,1:m}^*)^{1/2}. \]
IEnKF-Q: decoupling

▶ In all generality:

\[ J(x_1, x_2) = -2 \ln p(x_1, x_2 | y_2) = -2 \ln p(x_2 | x_1, y_2) p(x_1 | y_2). \]

▶ If the observation operator \( \mathcal{H} \) is linear:

\[ -2 \ln p(x_1 | y_2) = \| x_1 - x_1^a \|^2_{(P_1^a)^{-1}} + \| y_2 - \mathcal{H} \circ M(x_1) \|^2_{(R + HQH^T)^{-1}} + c_1, \]

and

\[ -2 \ln p(x_2 | x_1, y_2) = \| x_2 - M(x_1) - QH^T (R + HQH^T)^{-1} [y_2 - \mathcal{H} \circ M(x_1)] \|^2_{Q^{-1} + H^TR^{-1}H} + c_2, \]

▶ Then the MAP of \( J(x_1, x_2) \) can be computed in two simpler steps:

▶ Minimize \(-2 \ln p(x_1 | y_2)\) over \( x_1 \) just like the IEnKF in the absence of model error but with \( R \rightarrow R + HQH^T \).

▶ The MAP of \(-2 \ln p(x_2 | x_1^*, y_2)\) is then directly given by:

\[ x_2^* = M(x_1^*) + QH^T (R + HQH^T)^{-1} [y_2 - \mathcal{H} \circ M(x_1^*)]. \]
This decoupling also implies the decoupling of \((u, v)\):

\[
\begin{align*}
    u^{i+1} - u^i &= D_u^i \left\{ (HM^i A_1^a)^T (R_u^i)^{-1} \left[ y_2 - \mathcal{H} \circ \mathcal{M}(x_1^a + A_1^a u^i) \right] - u^i \right\}, \\
    v^* &= D_v^* (HA^q_2)^T (R_v^*)^{-1} \left[ y_2 - \mathcal{H}(x_2^*) + HM^* A_1^a u^* \right].
\end{align*}
\]

However, this decoupling does not convey to the perturbations update!

The same decoupling is used in particle filtering [Doucet et al., 2000] to build the optimal importance proposal particle filter.
IEnKF-Q: algorithm (transform flavor)

1: function $[E_2] = \text{ienkf\_cycle}(E^a_1, A^q_2, y_2, R, \mathcal{M}, \mathcal{H})$
2: \hspace{1em} $x^a_1 = E^a_1 1/m$
3: \hspace{1em} $A^a_1 = (E^a_1 - x^a_1 1^T) / \sqrt{m - 1}$
4: \hspace{1em} $D = I, \quad w = 0$
5: \hspace{1em} repeat
6: \hspace{2em} $x_1 = x^a_1 + A^a_1 w_{1:m}$
7: \hspace{2em} $T = (D^{1:m,1:m})^{1/2}$
8: \hspace{2em} $E_1 = x_1 1^T + A^a_1 T \sqrt{m - 1}$
9: \hspace{2em} $E_2 = \mathcal{M}(E_1)$
10: \hspace{2em} $HA_2 = H(E_2)(I - 11^T / m) T^{-1} / \sqrt{m - 1}$
11: \hspace{2em} $HA^q_2 = H(E_2 11^T / m + A^q_2 \sqrt{m - 1})(I - 11^T / m_q) / \sqrt{m_q - 1}$
12: \hspace{2em} $HA = [HA_2, HA^q_2]$
13: \hspace{2em} $x_2 = E_2 1 / m + A^q_2 w_{m+1:m+m_q}$
14: \hspace{2em} $\nabla J = w - (HA)^T R^{-1} [y_2 - H(x_2)]$
15: \hspace{2em} $D = [I + (HA)^T R^{-1} HA]^{-1}$
16: \hspace{2em} $\Delta w = -D \nabla J$
17: \hspace{2em} $w = w + \Delta w$
18: \hspace{2em} until $|\Delta w| < \varepsilon$
19: \hspace{2em} $A_2 = E_2 (I - 11^T / m) T^{-1}$
20: \hspace{2em} $A = [A_2 / \sqrt{m - 1}, A^q_2] D^{1/2}$
21: \hspace{2em} $A_2 = SR(A, m) \sqrt{m - 1}$
22: \hspace{2em} $E_2 = x_2 1^T + (1 + \delta) A_2$
23: end function
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IEnKF-Q: numerical experiments

Experiments performed on the Lorenz-96 model. Fully observed: $H = I$, $R = I$. We choose $m_q = 41$, so that $Q$ is full rank.

Random mean-preserving rotations of the ensemble perturbations are sometimes applied to the IEnKF-Q, typically in the very weak model error regime.

Comparisons with EnKF+accounting for $Q$ and IEnKF+accounting for $Q$: 

- [Rand] stochastic approach: $A_f^2 = MA_1^a + Q^{1/2} \Xi$
- [Det] deterministic approach: $A_f^2 = A \left[ I + A^\dagger Q (A^\dagger)^T \right]^{1/2}$, with $A = MA_1^a$.


Test 1: nonlinearity (diagonal $Q$)

$Q = 0.01TI, \ m = 20.$
Test 1: nonlinearity (non-diagonal $Q$)

$[Q]_{ij} = 0.05 T (\exp[-d^2(i,j)/30]) + 0.1 \delta_{ij}, \ m = 30$
Test 2: model noise magnitude (weakly nonlinear)

\[ Q = qT I, \quad T = 1, \quad m = 20. \]
Test 2: model noise magnitude (strongly nonlinear)

\[ Q = qT \mathbf{I}, \quad T = 10, \quad m = 20. \]
Test 3: ensemble size (weakly nonlinear)

\[ Q = 0.01 T I, \ T = 1. \]
Test 3: ensemble size (strongly nonlinear)

$Q = 0.01 T I, \ T = 10.$
Test 4: local variant (weakly nonlinear)

\[ Q = 0.01 \mathbf{1}, \ T = 1. \]

Test 4: local variant (strongly nonlinear)

$Q = 0.01 T I , \ T = 10.$

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We have extended the iterative ensemble Kalman filter (IEnKF) to iterative ensemble Kalman filter in presence of additive model error (IEnKF-Q).

P. Sakov, J.-M. Haussaire, and M. Bocquet, An iterative ensemble Kalman filter in presence of additive model error, Q. J. R. Meteorol. Soc., 0 (2018), pp. 0–0. Accepted for publication

It consistently outperforms ad hoc schemes that incorporate model error into the IEnKF with the L96 model, and any other EnKF-based scheme.

Not shown: we have extended the asynchronous ensemble Kalman filter (AEnKF) to the asynchronous ensemble Kalman filter in presence of model error (AEnKF-Q).

P. Sakov and M. Bocquet, Asynchronous data assimilation with the EnKF in presence of additive model error, Tellus A, 70 (2018), p. 1414545

Not shown: Full blown nonlinear IEnKS-Q is working. But the challenge is on its computational cost.

Ongoing work with A. Fillion, S. Gratton and S. Gürol.
Final word

Thank you for your attention!
Merci pour votre attention!
References


