An iterative ensemble Kalman filter in presence of additive model error

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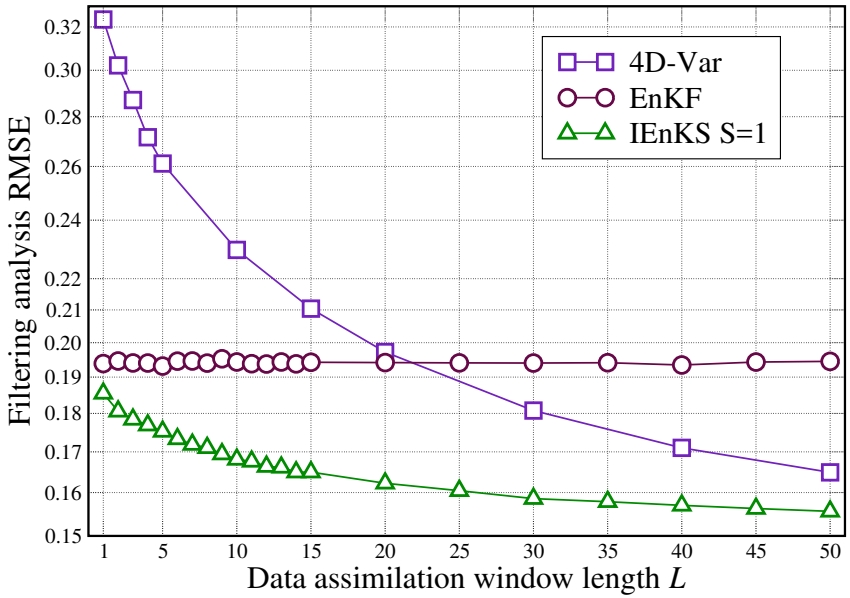
Outline

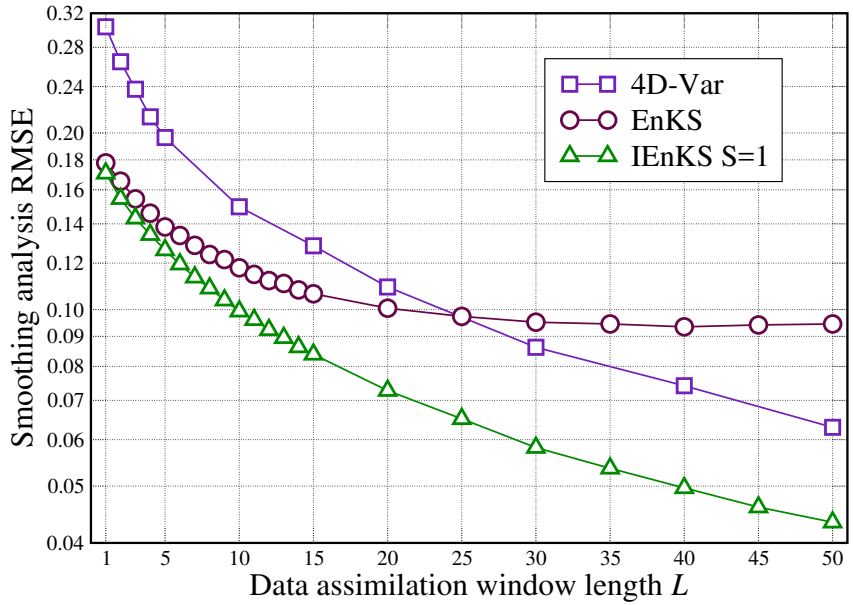
1. The iterative ensemble Kalman filter (IEnKF)
2. Theory of the IEnKF-Q
   - Formulation
   - Decoupling
   - Base algorithm
3. Numerics for the IEnKF-Q
4. Conclusions
5. References

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**.



Filtering

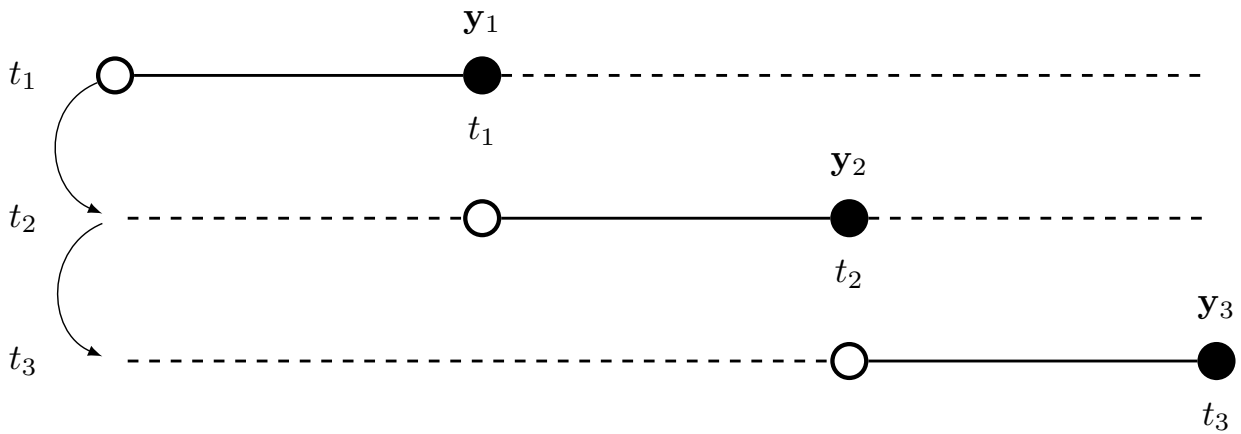


Smoothing

M. Bocquet and P. Sakov, *Joint state and parameter estimation with an iterative ensemble Kalman smoother*, Nonlin. Processes Geophys., 20 (2013), pp. 803–818

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 $p(\mathbf{x}_1|\mathbf{y}_2) \propto \exp\left(-J(\mathbf{x}_1)\right)$:

$$J(\mathbf{x}_1) = \frac{1}{2}\|\mathbf{y}_2 - \mathcal{H}_2 \circ \mathcal{M}_2(\mathbf{x}_1))\|^2_{\mathbf{R}_2^{-1}} + \frac{1}{2}\|\mathbf{x}_1 - \overline{\mathbf{x}}_1\|^2_{\mathbf{P}_1^{-1}}.$$

- Reduced scheme in ensemble subspace, $\mathbf{x}_1 = \overline{\mathbf{x}}_1 + \mathbf{A}_1\mathbf{w}_1$, where $\mathbf{A}_1$ is the normalized ensemble perturbation matrix:

$$\widetilde{J}(\mathbf{w}_1) = J(\overline{\mathbf{x}}_1 + \mathbf{A}_1\mathbf{w}_1).$$

- IEnKF cost function in ensemble subspace:

$$\widetilde{J}(\mathbf{w}_1) = \frac{1}{2}\|\mathbf{y}_2 - \mathcal{H}_2 \circ \mathcal{M}_2\left(\overline{\mathbf{x}}_1 + \mathbf{A}_1\mathbf{w}_1\right)\|^2_{\mathbf{R}_2^{-1}} + \frac{1}{2}\|\mathbf{w}_1\|^2.$$

P. Sakov, D. S. Oliver, and L. Bertino, *An iterative EnKF for strongly nonlinear systems*, Mon. Wea. Rev., 140 (2012), pp. 1988–2004

M. Bocquet and P. Sakov, *Combining inflation-free and iterative ensemble Kalman filters for strongly nonlinear systems*, Nonlin. Processes Geophys., 19 (2012), pp. 383–399

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

$$
\begin{aligned}
\mathbf{w}_1^{i+1} &= \mathbf{w}_1^i - \widetilde{\mathcal{H}}_i^{-1} \nabla \widetilde{\mathcal{J}}_i(\mathbf{w}_1^i), \\
\mathbf{x}_1^i &= \overline{\mathbf{x}}_1 + \mathbf{A}_1 \mathbf{w}_1^i, \\
\nabla \widetilde{\mathcal{J}}_i &= \mathbf{w}_1^i - \mathbf{Y}_i^{\mathrm{T}} \mathbf{R}_2^{-1} \left(\mathbf{y}_2 - \mathcal{H}_2 \circ \mathcal{M}_2(\mathbf{x}_1^i) \right), \\
\widetilde{\mathcal{H}}_i &= \mathbf{I}_N + \mathbf{Y}_i^{\mathrm{T}} \mathbf{R}_2^{-1} \mathbf{Y}_i, \\
\mathbf{Y}_i &= [\mathcal{H}_2 \circ \mathcal{M}_2]'_{|\mathbf{x}_1^i} \mathbf{A}_1 .
\end{aligned}
$$

- **Perturbation update:** same as the ETKF

$$
\mathbf{E}_1^\star = \mathbf{x}_1^\star \mathbf{1}^{\mathrm{T}} + \sqrt{N-1} \mathbf{A}_1 \widetilde{\mathcal{H}}_\star^{-1/2} \mathbf{U} \quad \text{where} \quad \mathbf{U}\mathbf{1} = \mathbf{1} . \tag{1}
$$

- **Forecast:** propagate the updated ensemble from t_0 to t_S:

$$
\mathbf{E}_2 = \mathcal{M}_{2:1}(\mathbf{E}_1) . \tag{2}
$$

Iterative ensemble Kalman filter: computing the sensitivities

- Sensitivities $\mathbf{Y}_{(p)}$ 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

$$\mathbf{T}^i = \left(\mathbf{I}_N + \mathbf{Y}^{i\mathrm{T}}\mathbf{R}^{-1}\mathbf{Y}^i\right)^{-1/2},$$

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:

$$\mathbf{Y}^i \approx \frac{1}{\varepsilon}\mathcal{H}_2 \circ \mathcal{M}_2\left(\mathbf{x}^i\mathbf{1}^{\mathrm{T}} + \varepsilon\mathbf{A}_1\right)\left(\mathbf{I}_N - \frac{\mathbf{1}\mathbf{1}^{\mathrm{T}}}{N}\right).$$

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IEnKF-Q: formulation

- Analysis cost function:

$$J(\mathbf{x}_1, \mathbf{x}_2) = \|\mathbf{x}_1 - \mathbf{x}_1^{\mathrm{a}}\|^2_{(\mathbf{P}_1^{\mathrm{a}})^{-1}} + \|\mathbf{y}_2 - \mathcal{H}(\mathbf{x}_2)\|^2_{\mathbf{R}^{-1}} + \|\mathbf{x}_2 - \mathcal{M}(\mathbf{x}_1)\|^2_{\mathbf{Q}^{-1}}.$$

- Ensemble subspace representation:

$$\begin{aligned} \mathbf{x}_1 &= \mathbf{x}_1^{\mathrm{a}} + \mathbf{A}_1^{\mathrm{a}}\mathbf{u}, & \mathbf{A}_1^{\mathrm{a}}(\mathbf{A}_1^{\mathrm{a}})^{\mathrm{T}} &= \mathbf{P}_1^{\mathrm{a}}, & \mathbf{A}_1^{\mathrm{a}}\mathbf{1} &= \mathbf{0}, \\ \mathbf{x}_2 &= \mathcal{M}(\mathbf{x}_1) + \mathbf{A}_2^{q}\mathbf{v}, & \mathbf{A}_2^{q}(\mathbf{A}_2^{q})^{\mathrm{T}} &= \mathbf{Q}, & \mathbf{A}_2^{q}\mathbf{1} &= \mathbf{0}. \end{aligned}$$

- Cost function in ensemble subspace:

$$J(\mathbf{u}, \mathbf{v}) = \mathbf{u}^{\mathrm{T}}\mathbf{u} + \mathbf{v}^{\mathrm{T}}\mathbf{v} + \|\mathbf{y}_2 - \mathcal{H}(\mathbf{x}_2)\|^2_{\mathbf{R}^{-1}}.$$

IEnKF-Q: formulation

- Compactification:

$$\mathbf{w} \equiv \begin{bmatrix} \mathbf{u} \\ \mathbf{v} \end{bmatrix} \quad \Longrightarrow \quad J(\mathbf{w}) = \mathbf{w}^{\mathrm{T}}\mathbf{w} + \|\mathbf{y}_2 - \mathcal{H}(\mathbf{x}_2)\|^2_{\mathbf{R}^{-1}} .$$

$\longrightarrow$ enables to apply the **perfect model/strong constraint IEnKF** machinery!

- Condition of zero gradient:

$$\mathbf{w} - (\mathbf{H}\mathbf{A})^{\mathrm{T}}\mathbf{R}^{-1}\left[\mathbf{y}_2 - \mathcal{H}(\mathbf{x}_2)\right] = \mathbf{0},$$

where

$$\mathbf{A} \equiv [\mathbf{M}\mathbf{A}_1^{\mathrm{a}}, \mathbf{A}_2^{q}], \quad \mathbf{H} \equiv \nabla\mathcal{H}(\mathbf{x}_2), \quad \mathbf{M} \equiv \nabla\mathcal{M}(\mathbf{x}_1).$$

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

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

where the inverse Hessian is approximated as

$$\mathbf{D}^{i} \approx \left[\mathbf{I} + (\mathbf{H}^{i}\mathbf{A}^{i})^{\mathrm{T}}\mathbf{R}^{-1}\mathbf{H}^{i}\mathbf{A}^{i}\right]^{-1}.$$

IEnKF-Q: formulation

- Posterior errors:

$$\delta \mathbf{x}_1 = \mathbf{A}_1^{\mathrm{a}}\, \delta \mathbf{u}, \qquad \delta \mathbf{x}_2 = \mathbf{M}\mathbf{A}_1^{\mathrm{a}}\, \delta \mathbf{u} + \mathbf{A}_2^{q}\, \delta \mathbf{v},$$

- Updated perturbations over $[t_1, t_2]$:

$$\mathbf{A}_2^{\mathrm{a}}(\mathbf{A}_2^{\mathrm{a}})^{\mathrm{T}} = \mathrm{E}[\delta \mathbf{x}_2^{\star}(\delta \mathbf{x}_2^{\star})^{\mathrm{T}}] = \mathbf{A}^{\star}\mathrm{E}[\mathbf{w}^{\star}(\mathbf{w}^{\star})^{\mathrm{T}}](\mathbf{A}^{\star})^{\mathrm{T}} = \mathbf{A}^{\star}\mathbf{D}^{\star}(\mathbf{A}^{\star})^{\mathrm{T}},$$

which implies

$$\mathbf{A}_2^{\mathrm{a}} = \mathbf{A}^{\star}(\mathbf{D}^{\star})^{1/2} = \mathbf{A}^{\star}\left[\mathbf{I} + (\mathbf{H}^{\star}\mathbf{A}^{\star})^{\mathrm{T}}\mathbf{R}^{-1}\mathbf{H}^{\star}\mathbf{A}^{\star}\right]^{-1/2}.$$

- Updated (smoothed) perturbations at t_1:

$$\mathbf{A}_1^{\mathrm{s}}(\mathbf{A}_1^{\mathrm{s}})^{\mathrm{T}} = \mathrm{E}[\delta \mathbf{x}_1^{\star}(\delta \mathbf{x}_1^{\star})^{\mathrm{T}}] = \mathbf{A}_1^{\mathrm{a}}\mathrm{E}[\mathbf{u}^{\star}(\mathbf{u}^{\star})^{\mathrm{T}}](\mathbf{A}_1^{\mathrm{a}})^{\mathrm{T}},$$

which implies

$$\mathbf{A}_1^{\mathrm{s}} = \mathbf{A}_1^{\mathrm{a}}\,(\mathbf{D}^{\star}_{1:m,1:m})^{1/2}.$$

IEnKF-Q: decoupling

- In all generality:

$$J(\mathbf{x}_1, \mathbf{x}_2) = -2 \ln p(\mathbf{x}_1, \mathbf{x}_2 | \mathbf{y}_2) = -2 \ln p(\mathbf{x}_2 | \mathbf{x}_1, \mathbf{y}_2) p(\mathbf{x}_1 | \mathbf{y}_2).$$

- If the observation operator $\mathcal{H}$ **is linear**:

$$-2 \ln p(\mathbf{x}_1 | \mathbf{y}_2) = \| \mathbf{x}_1 - \mathbf{x}_1^{\mathrm{a}} \|^2_{(\mathbf{P}_1^{\mathrm{a}})^{-1}} + \| \mathbf{y}_2 - \mathcal{H} \circ \mathcal{M}(\mathbf{x}_1) \|^2_{(\mathbf{R} + \mathbf{H}\mathbf{Q}\mathbf{H}^{\mathrm{T}})^{-1}} + c_1,$$

and

$$\begin{aligned} -2 \ln p(\mathbf{x}_2 | \mathbf{x}_1, \mathbf{y}_2) = & \| \mathbf{x}_2 - \mathcal{M}(\mathbf{x}_1) - \mathbf{Q}\mathbf{H}^{\mathrm{T}} (\mathbf{R} + \mathbf{H}\mathbf{Q}\mathbf{H}^{\mathrm{T}})^{-1} [\mathbf{y}_2 - \mathcal{H} \circ \mathcal{M}(\mathbf{x}_1)] \|^2_{\mathbf{Q}^{-1} + \mathbf{H}^{\mathrm{T}} \mathbf{R}^{-1} \mathbf{H}} \\ & + c_2, \end{aligned}$$

- Then the MAP of $J(\mathbf{x}_1, \mathbf{x}_2)$ can be computed in **two simpler steps**:
  - Minimize $-2 \ln p(\mathbf{x}_1 | \mathbf{y}_2)$ over $\mathbf{x}_1$ just like the IEnKF in the absence of model error but with $\mathbf{R} \to \mathbf{R} + \mathbf{H}\mathbf{Q}\mathbf{H}^{\mathrm{T}}$.
  - The MAP of $-2 \ln p(\mathbf{x}_2 | \mathbf{x}_1^\star, \mathbf{y}_2)$ is then directly given by:

$$\mathbf{x}_2^\star = \mathcal{M}(\mathbf{x}_1^\star) + \mathbf{Q}\mathbf{H}^{\mathrm{T}} \left(\mathbf{R} + \mathbf{H}\mathbf{Q}\mathbf{H}^{\mathrm{T}} \right)^{-1} [\mathbf{y}_2 - \mathcal{H} \circ \mathcal{M}(\mathbf{x}_1^\star)] .$$

IEnKF-Q: decoupling

- This decoupling also implies the decoupling of $(\mathbf{u}, \mathbf{v})$:

$$\mathbf{u}^{i+1} - \mathbf{u}^{i} = \mathbf{D}_u^i \left\{ (\mathbf{H}\mathbf{M}^i\mathbf{A}_1^{\mathrm{a}})^{\mathrm{T}} (\mathbf{R}_u^i)^{-1} \left[\mathbf{y}_2 - \mathcal{H} \circ \mathcal{M}(\mathbf{x}_1^{\mathrm{a}} + \mathbf{A}_1^{\mathrm{a}}\mathbf{u}^i) \right] - \mathbf{u}^i \right\}.$$

$$\mathbf{v}^\star = \mathbf{D}_v^\star (\mathbf{H}\mathbf{A}_2^q)^{\mathrm{T}} (\mathbf{R}_v^\star)^{-1} \left[\mathbf{y}_2 - \mathcal{H}(\mathbf{x}_2^\star) + \mathbf{H}\mathbf{M}^\star\mathbf{A}_1^{\mathrm{a}}\mathbf{u}^\star \right].$$

- 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)

function $[\mathbf{E}_2] = \mathbf{ienkf_cycle}(\mathbf{E}_1^{\mathrm{a}}, \mathbf{A}_2^q, \mathbf{y}_2, \mathbf{R}, \mathcal{M}, \mathcal{H})$

$\mathbf{x}_1^{\mathrm{a}} = \mathbf{E}_1^{\mathrm{a}} \mathbf{1}/m$

$\mathbf{A}_1^{\mathrm{a}} = (\mathbf{E}_1^{\mathrm{a}} - \mathbf{x}_1^{\mathrm{a}} \mathbf{1}^{\mathrm{T}})/\sqrt{m-1}$

$\mathbf{D} = \mathbf{I}, \quad \mathbf{w} = \mathbf{0}$

repeat

$\mathbf{x}_1 = \mathbf{x}_1^{\mathrm{a}} + \mathbf{A}_1^{\mathrm{a}} \mathbf{w}_{1:m}$

$\mathbf{T} = (\mathbf{D}_{1:m,1:m})^{1/2}$

$\mathbf{E}_1 = \mathbf{x}_1 \mathbf{1}^{\mathrm{T}} + \mathbf{A}_1^{\mathrm{a}} \mathbf{T} \sqrt{m-1}$

$\mathbf{E}_2 = \mathcal{M}(\mathbf{E}_1)$

$\mathbf{HA}_2 = \mathcal{H}(\mathbf{E}_2)(\mathbf{I} - \mathbf{1}\mathbf{1}^{\mathrm{T}}/m)\,\mathbf{T}^{-1}/\sqrt{m-1}$

$\mathbf{HA}_2^q = \mathcal{H}(\mathbf{E}_2 \mathbf{1}\mathbf{1}^{\mathrm{T}}/m + \mathbf{A}_2^q \sqrt{m_q - 1})(\mathbf{I} - \mathbf{1}\mathbf{1}^{\mathrm{T}}/m_q)/\sqrt{m_q - 1}$

$\mathbf{HA} = [\mathbf{HA}_2, \mathbf{HA}_2^q]$

$\mathbf{x}_2 = \mathbf{E}_2 \mathbf{1}/m + \mathbf{A}_2^q \mathbf{w}_{m+1:m+m_q}$

$\nabla J = \mathbf{w} - (\mathbf{HA})^{\mathrm{T}} \mathbf{R}^{-1} [\mathbf{y}_2 - \mathcal{H}(\mathbf{x}_2)]$

$\mathbf{D} = [\mathbf{I} + (\mathbf{HA})^{\mathrm{T}} \mathbf{R}^{-1} \mathbf{HA}]^{-1}$

$\Delta \mathbf{w} = -\mathbf{D}\,\nabla J$

$\mathbf{w} = \mathbf{w} + \Delta \mathbf{w}$

until $|\Delta \mathbf{w}| < \varepsilon$

$\mathbf{A}_2 = \mathbf{E}_2\,(\mathbf{I} - \mathbf{1}\mathbf{1}^{\mathrm{T}}/m)\,\mathbf{T}^{-1}$

$\mathbf{A} = [\mathbf{A}_2/\sqrt{m-1}, \mathbf{A}_2^q]\,\mathbf{D}^{1/2}$

$\mathbf{A}_2 = \mathrm{SR}(\mathbf{A}, m)\sqrt{m-1}$

$\mathbf{E}_2 = \mathbf{x}_2 \mathbf{1}^{\mathrm{T}} + (1+\delta)\mathbf{A}_2$

end function

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IEnKF-Q: numerical experiments

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

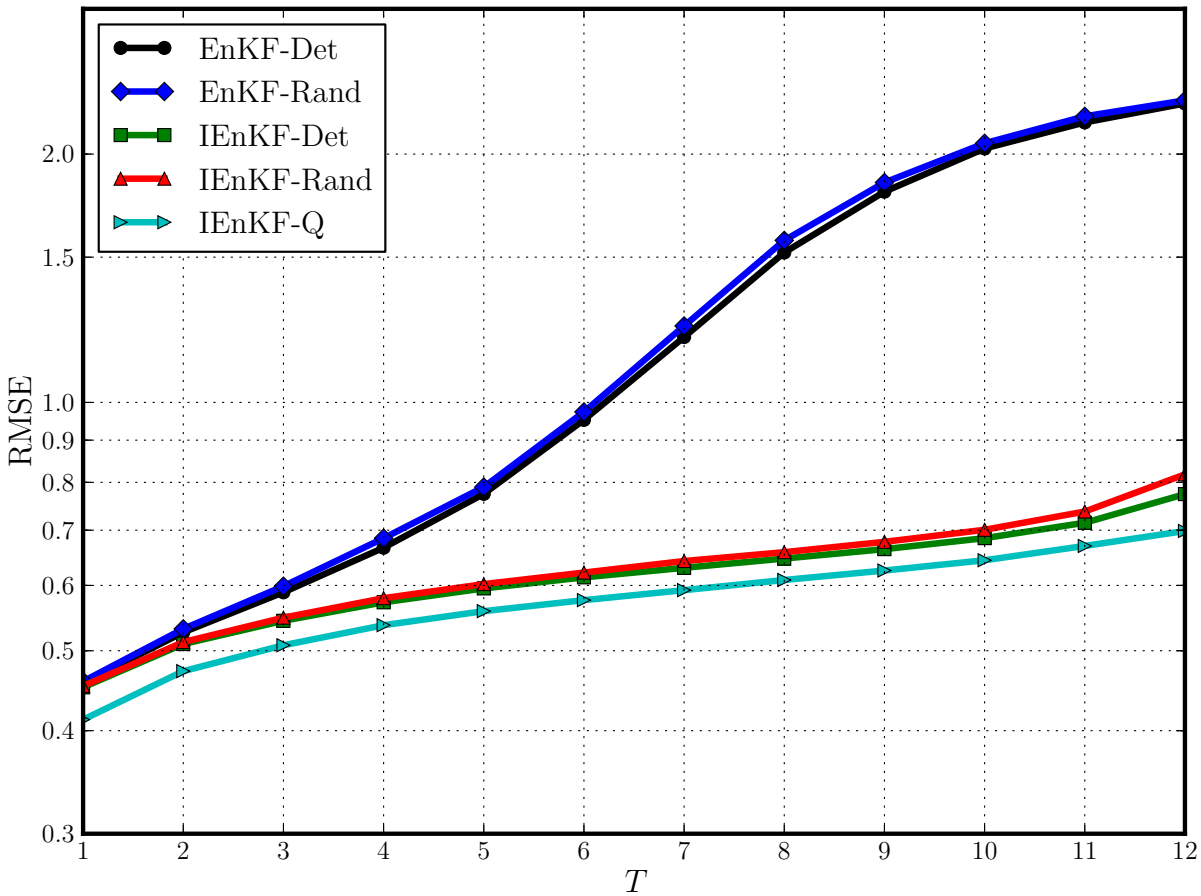
- **Random mean-preserving rotations** of the ensemble perturbations are sometimes applied to the IEnKF-Q, typically in the very weak model error regime.

- Comparisons with **EnKF+accounting for Q** and **IEnKF+accounting for Q**:
  - **[Rand]** stochastic approach: $\mathbf{A}_2^{\mathrm{f}} = \mathbf{M}\mathbf{A}_1^{\mathrm{a}} + \mathbf{Q}^{1/2}\Xi$,
  - **[Det]** deterministic approach: $\mathbf{A}_2^{\mathrm{f}} = \mathbf{A}\left[\mathbf{I} + \mathbf{A}^{\dagger}\mathbf{Q}(\mathbf{A}^{\dagger})^{\mathrm{T}}\right]^{1/2}$, with $\mathbf{A} = \mathbf{M}\mathbf{A}_1^{\mathrm{a}}$.

E. N. Lorenz and K. A. Emanuel, *Optimal sites for supplementary weather observations: simulation with a small model*, J. Atmos. Sci., 55 (1998), pp. 399–414

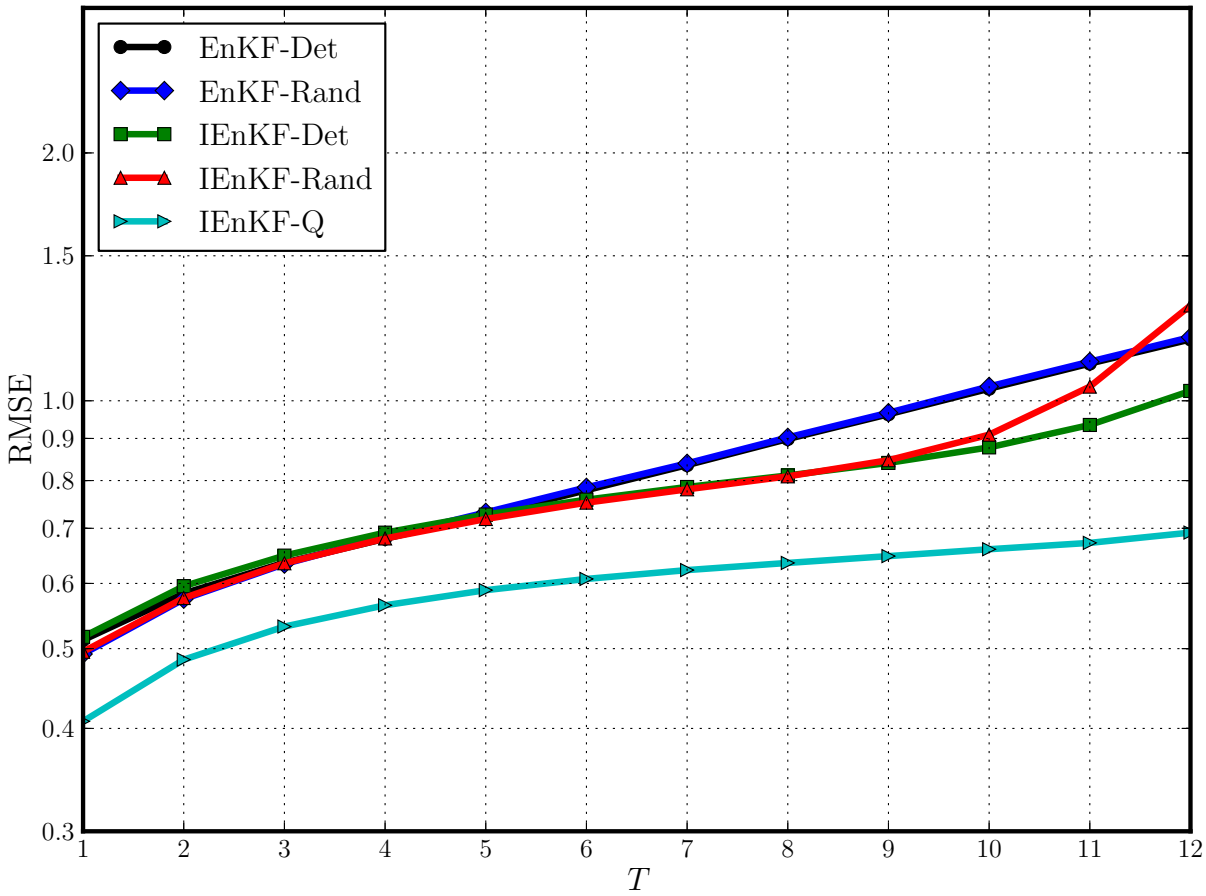
P. N. Raanes, A. Carrassi, and L. Bertino, *Extending the square root method to account for additive forecast noise in ensemble methods*, Mon. Wea. Rev., 143 (2015), pp. 3857–38730

Test 1: nonlinearity (diagonal $\mathbf{Q}$)



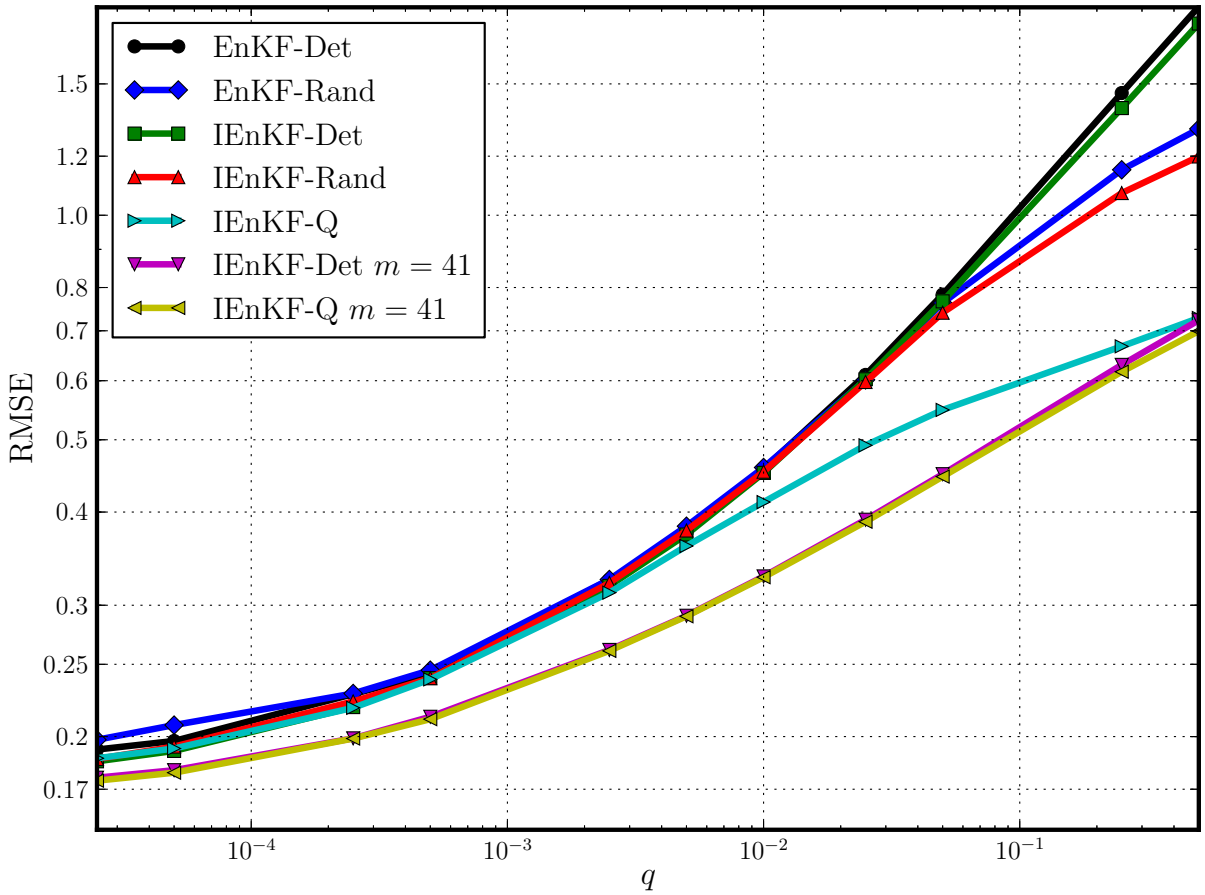
- $\mathbf{Q} = 0.01\,T\mathbf{I}$, $m = 20$.

Test 1: nonlinearity (non-diagonal $\mathbf{Q}$)



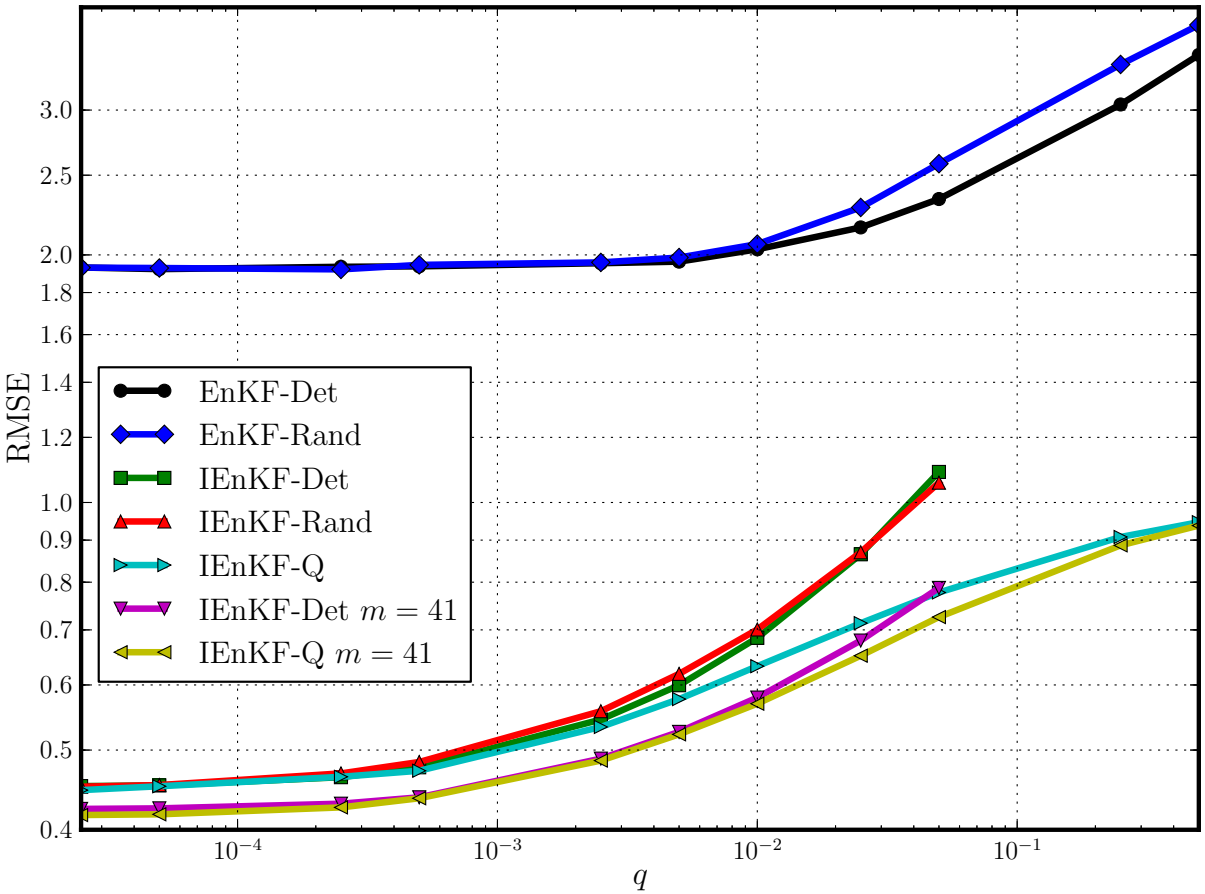
- $[\mathbf{Q}]_{ij} = 0.05\,T(\exp[-d^2(i,j)/30]) + 0.1\delta_{ij}$, $m = 30$

Test 2: model noise magnitude (weakly nonlinear)



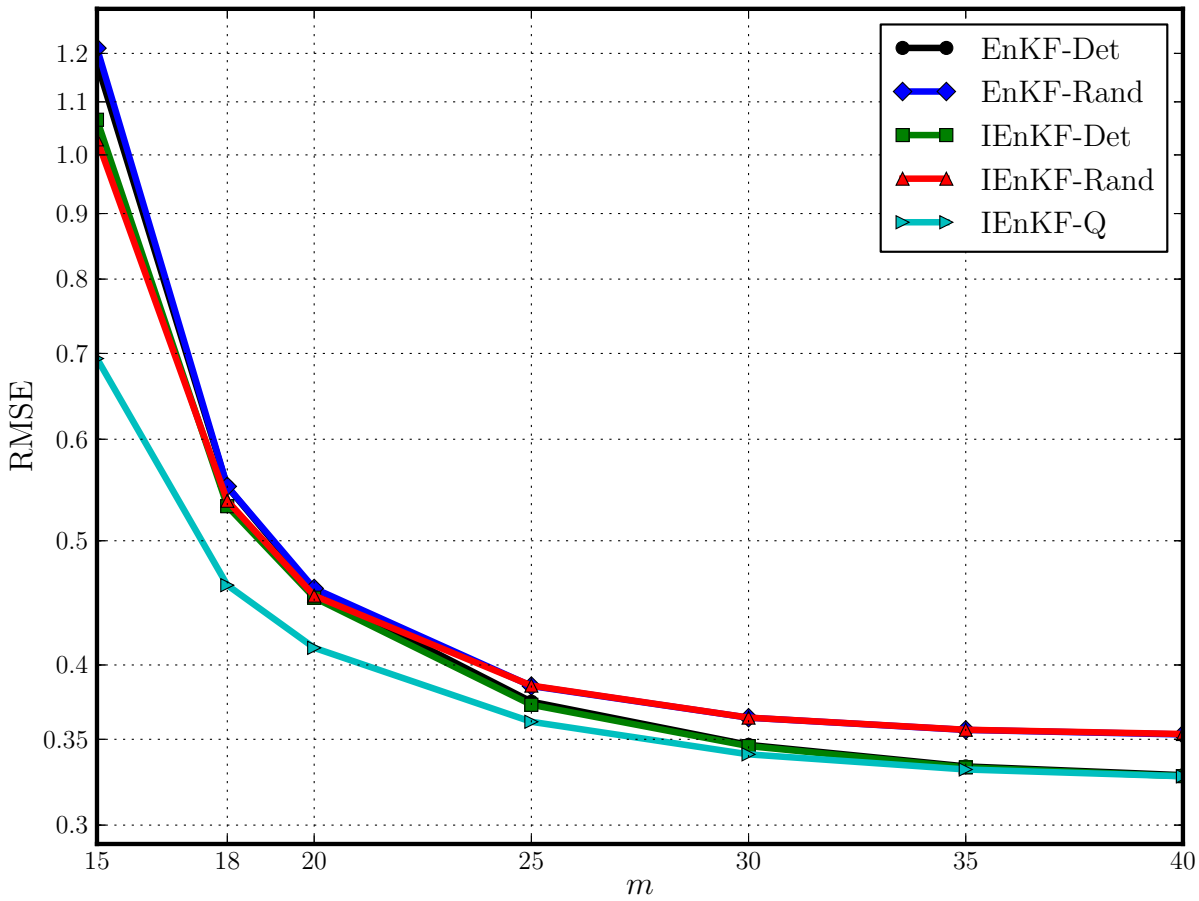
- $Q = qT\mathbf{I},\ T = 1,\ m = 20.$

Test 2: model noise magnitude (strongly nonlinear)



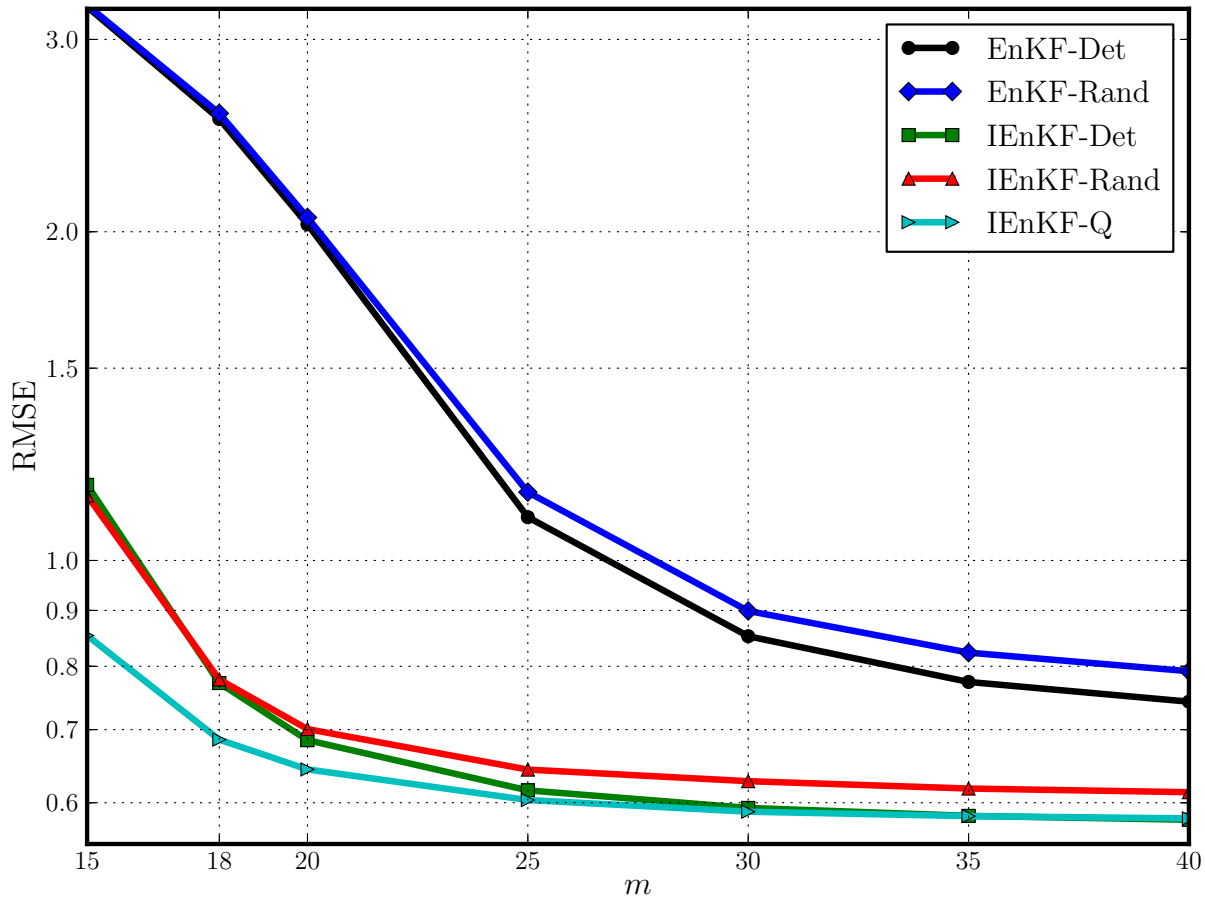
- $Q = qT\mathbf{I},\ T = 10,\ m = 20.$

Test 3: ensemble size (weakly nonlinear)



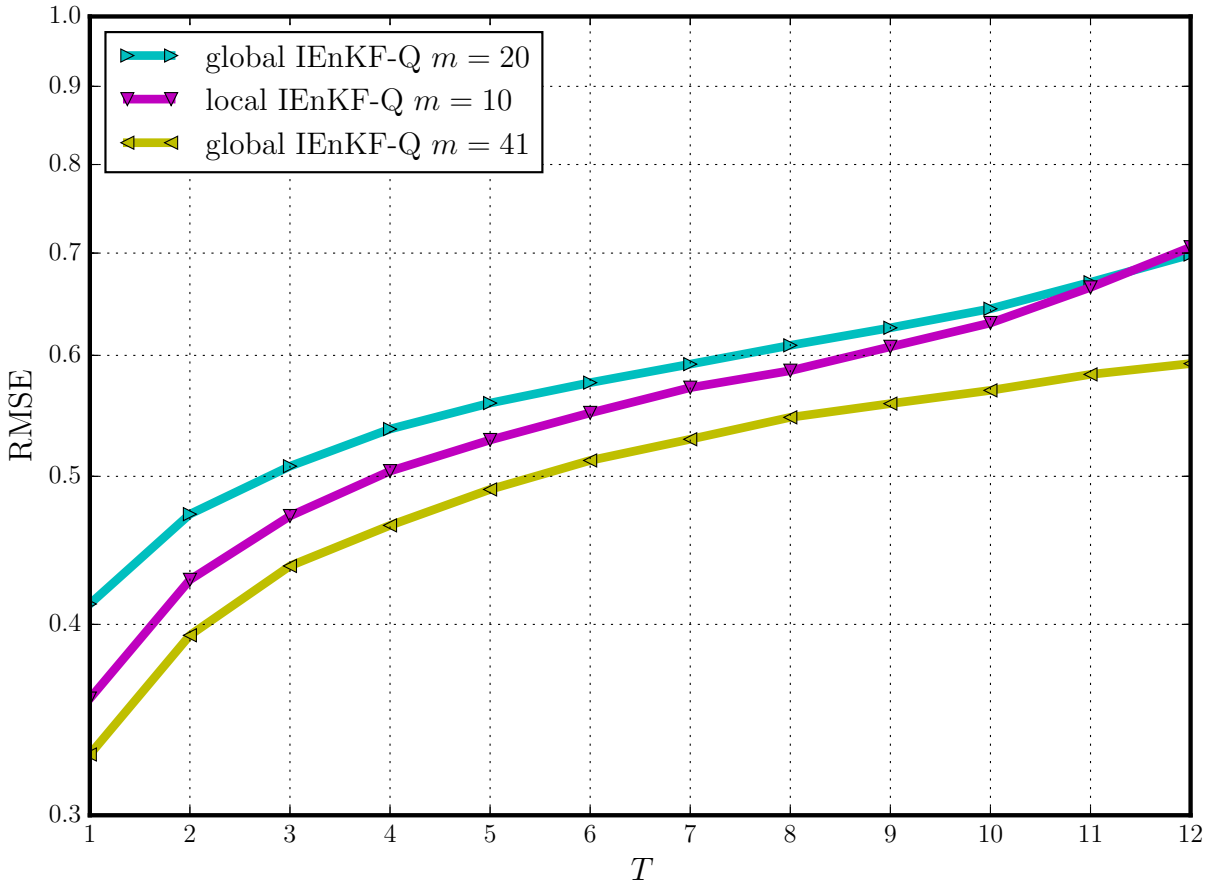
- $Q = 0.01\,T\mathbf{I},\ T = 1.$

Test 3: ensemble size (strongly nonlinear)



- $Q = 0.01\,T\mathbf{I},\ T = 10.$

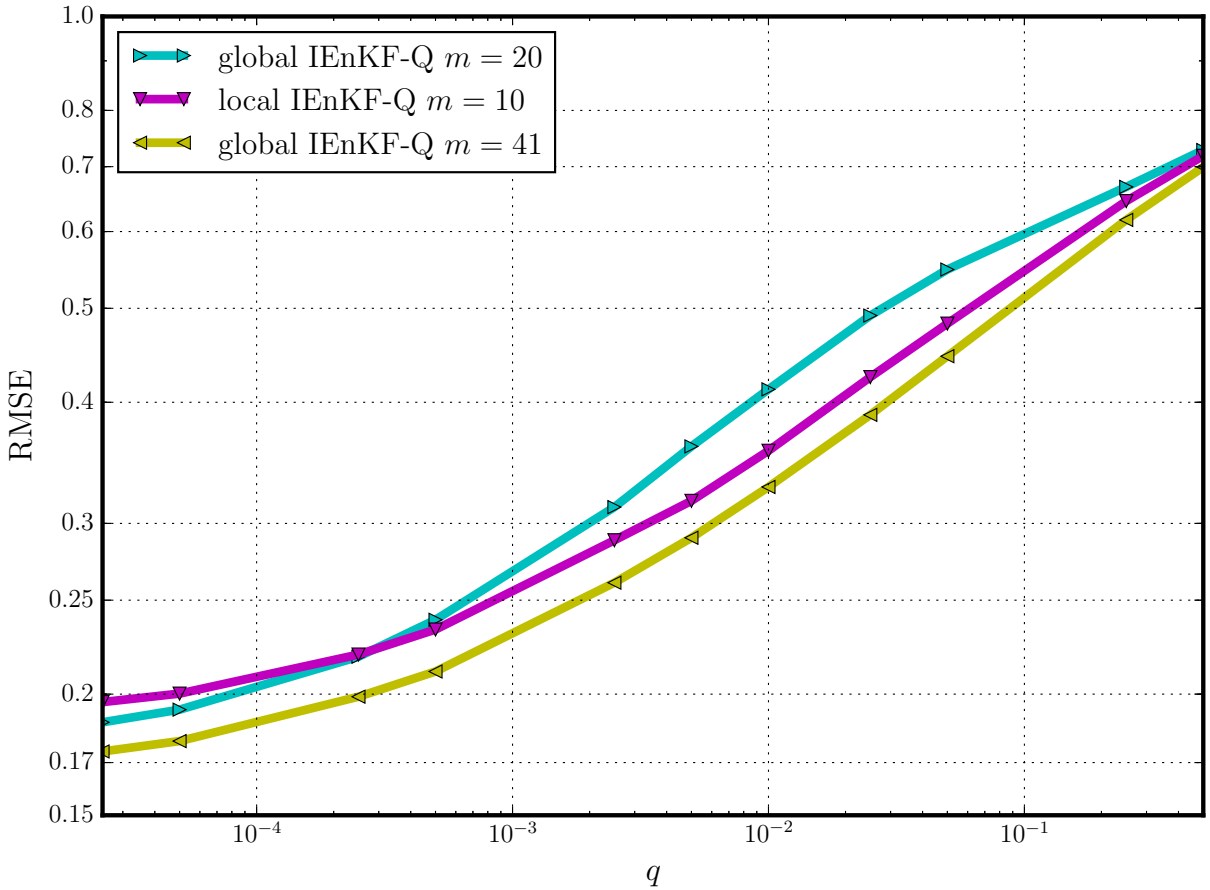
Test 4: local variant (weakly nonlinear)



- $Q = 0.01\,T\mathbf{I},\ T = 1.$

M. Bocquet, *Localization and the iterative ensemble Kalman smoother*, Q. J. R. Meteorol. Soc., 142 (2016), pp. 1075–1089

Test 4: local variant (strongly nonlinear)



- $Q = 0.01\,T\mathbf{I},\ T = 10.$

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Conclusions

- 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

[1] M. Bocquet, *Localization and the iterative ensemble Kalman smoother*, Q. J. R. Meteorol. Soc., 142 (2016), pp. 1075–1089.

[2] M. Bocquet and P. Sakov, *Combining inflation-free and iterative ensemble Kalman filters for strongly nonlinear systems*, Nonlin. Processes Geophys., 19 (2012), pp. 383–399.

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[5] P. N. Raanes, A. Carrassi, and L. Bertino, *Extending the square root method to account for additive forecast noise in ensemble methods*, Mon. Wea. Rev., 143 (2015), pp. 3857–38730.

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

[7] 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.
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