A generalisation of the updating step in EnKF

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EnKF Workshop 2021

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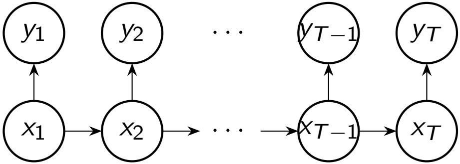
Talk outline

- ⋆ The state-space model
- ⋆ Ensemble Kalman filter (EnKF)
  - model and algorithm
  - simulation example
  - identify some issues
- ⋆ An improved model (and algorithm)
  - modified model
  - modified updating algorithm
  - simulation example (revisited)
- ⋆ Closing remarks
- ⋆ Note: We do not consider
  - variance inflation
  - localisation
  - computational efficiency

The state-space model

- State-space model



- Model components

$$
\begin{aligned}
x_1 &\sim p(x_1) \\
x_t|x_{t-1} &\sim p(x_t|x_{t-1}) \\
y_t|x_t &\sim \mathrm{N}(Hx_t, R)
\end{aligned}
$$

- Goal: Find/represent the filtering distribution

$$p(x_t|y_{1:t})$$

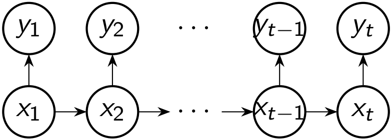
  - represent $p(x_t|y_{1:t})$ by an ensemble $\{x_t^1, \ldots, x_t^M\}$

Ensemble Kalman filter — recursive solution

- From $p(x_t|y_{1:t})$ to $p(x_{t+1}|y_{1:t+1})$ in to steps

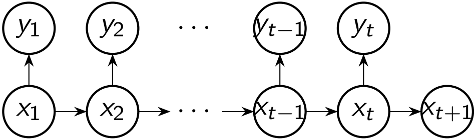
$p(x_t|y_{1:t})$

$\{x_t^1, \ldots, x_t^M\}$



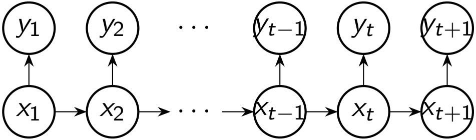
$p(x_{t+1}|y_{1:t})$

$\{\tilde{x}_{t+1}^1, \ldots, \tilde{x}_{t+1}^M\}$



$p(x_{t+1}|y_{1:t+1})$

$\{x_{t+1}^1, \ldots, x_{t+1}^M\}$



Ensemble Kalman filter — recursive solution

- ⋆ From $p(x_t|y_{1:t})$ to $p(x_{t+1}|y_{1:t+1})$ in to steps

$p(x_t|y_{1:t})$

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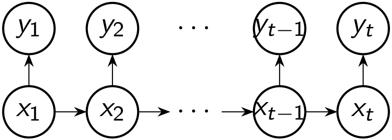

$p(x_{t+1}|y_{1:t})$

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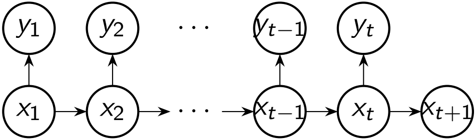

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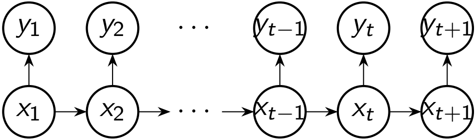
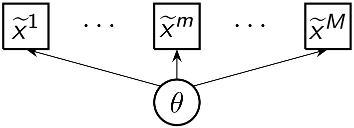
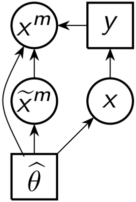


- ⋆ From now on: remove the time index notation

Ensemble Kalman filter — update step

- Assumed models when updating $\widetilde{x}^m$ to x^m (new data: y)





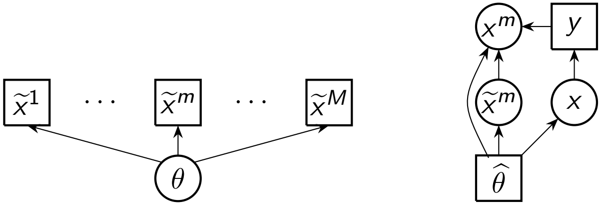
- First assumed model

$$\widetilde{x}^1, \ldots, \widetilde{x}^M | \theta \overset{\text{iid}}{\sim} \mathsf{N}(\mu, \Sigma)$$

  - $\theta = (\mu, \Sigma)$
  - $\widehat{\theta} = (\widehat{\mu}, \widehat{\Sigma})$: empirical quantities

Ensemble Kalman filter — update step

⋆ Assumed models when updating $\widetilde{x}^m$ to x^m (new data: y)



⋆ Second assumed model

$$\widetilde{x}^m, x|\widehat{\theta} \overset{\text{iid}}{\sim} \mathrm{N}(\widehat{\mu}, \widehat{\Sigma})$$

$$y|x \sim \mathrm{N}(Hx, R)$$

⋆ Require: $x^m|\widehat{\theta}, y \quad \overset{\text{d}}{=} \quad x|\widehat{\theta}, y$

Ensemble Kalman filter — update step

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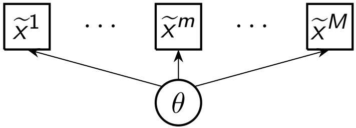
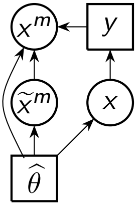




- Second assumed model

$$\widetilde{x}^m, x|\widehat{\theta} \overset{\text{iid}}{\sim} \mathrm{N}(\widehat{\mu}, \widehat{\Sigma})$$

$$y|x \sim \mathrm{N}(Hx, R)$$

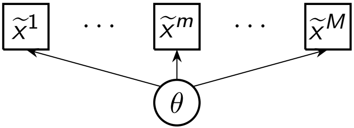
- Require: $x^m|\widehat{\theta}, y \;\overset{\text{d}}{=}\; x|\widehat{\theta}, y$
- Stochastic EnKF:

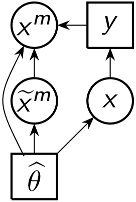
$$x^m = \widetilde{x}^m + K(y + \varepsilon - H\widetilde{x}^m)$$

where $K = \widehat{\Sigma}H^T(H\widehat{\Sigma}H^T + R)^{-1}$ and $\varepsilon \sim \mathrm{N}(0, R)$

Ensemble Kalman filter — update step

- ⋆ Assumed models when updating $\widetilde{x}^m$ to x^m (new data: y)





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$$\widetilde{x}^m, x | \widehat{\theta} \overset{\text{iid}}{\sim} \mathrm{N}(\widehat{\mu}, \widehat{\Sigma})$$

$$y | x \sim \mathrm{N}(Hx, R)$$

- ⋆ Require: $x^m | \widehat{\theta}, y \quad \overset{\text{d}}{=} \quad x | \widehat{\theta}, y$
- ⋆ Deterministic EnKF (square root filter)

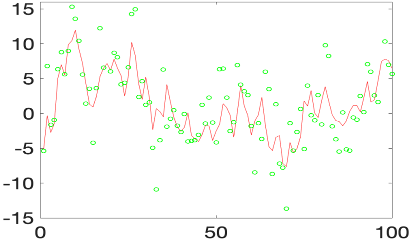
$$x^m = \widehat{\mu} + K(y - H\widehat{\mu}) + B(\widetilde{x}^m - \widetilde{\mu})$$

where $B\widehat{\Sigma}B^T = (\mathbb{I} - KH)\widetilde{\Sigma}$

Simulation example with stochastic EnKF

- ⋆ Use an example introduced in Myrseth and Omre (2010)
- ⋆ State vector x_t is a vector of size 100
- ⋆ $x_1 \sim \mathrm{N}(0, \Sigma)$, exponential correlation function
- ⋆ Forward function ($p(x_{t+1}|x_t)$) is deterministic
  - linear: smoothing for ten nodes
  - (non-linear example)
- ⋆ Likelihood, $y_n|x_n \sim \mathrm{N}(x_n, 20\mathbb{I})$

$t = 1$



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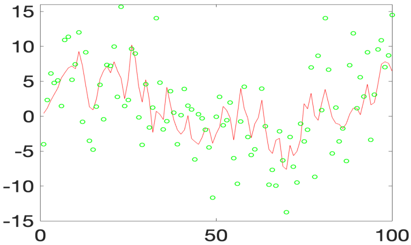
$t = 2$



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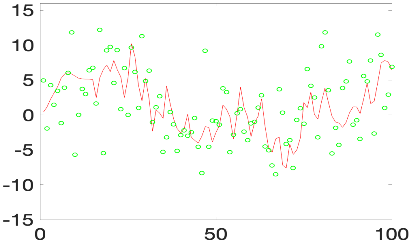
$t = 3$



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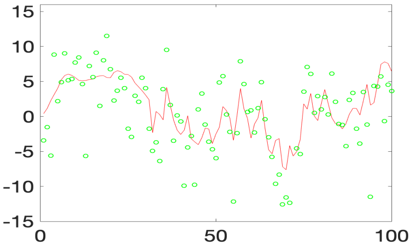
$t = 6$



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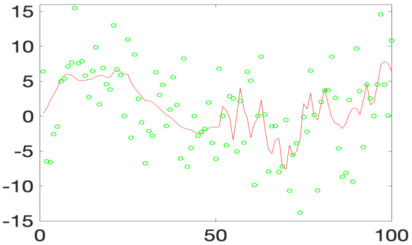
$t = 10$



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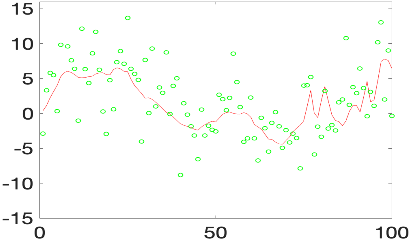
$t = 15$



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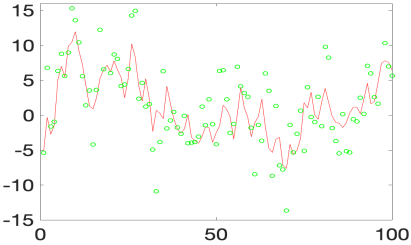
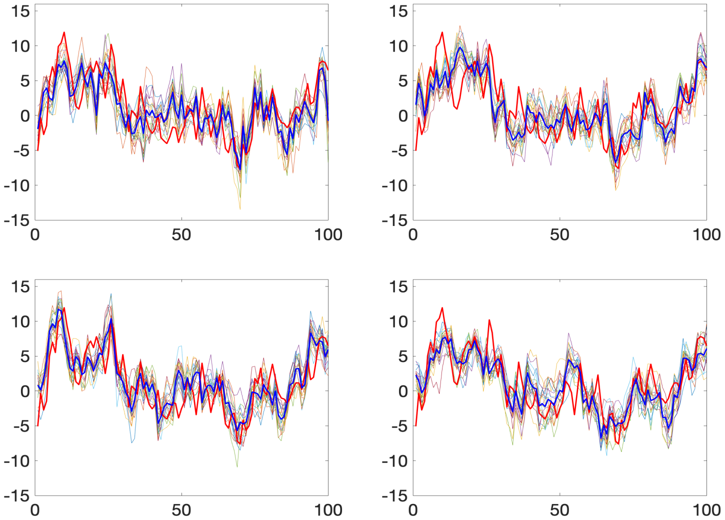
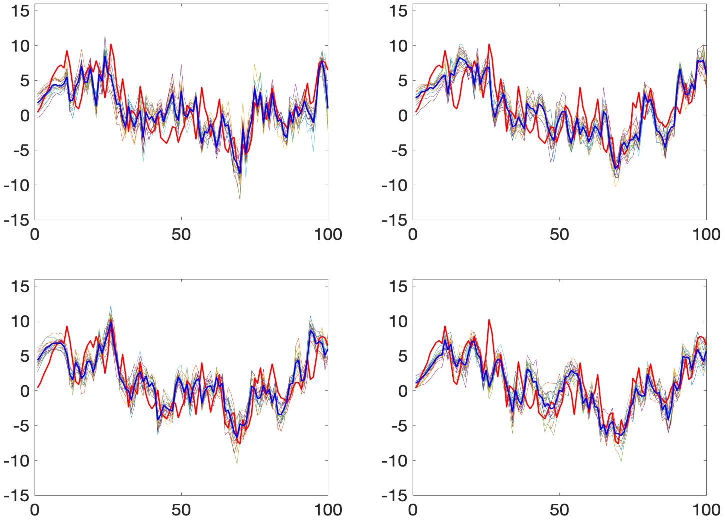
$t = 1$



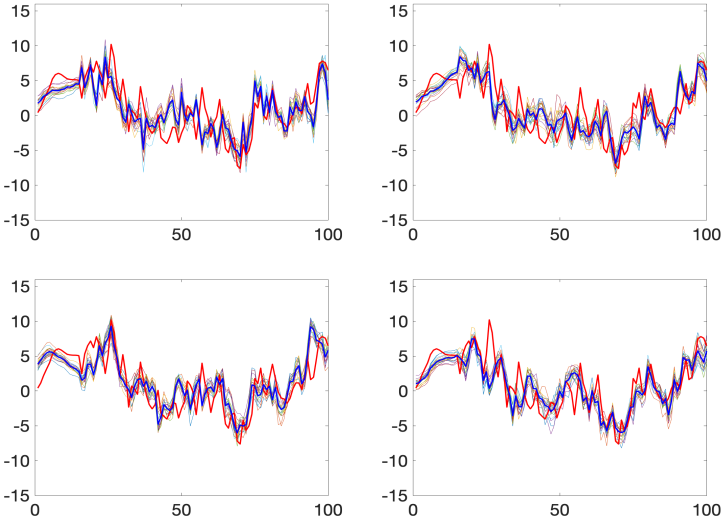
EnKF results with $M = 19$ ensemble members, time $t = 1$



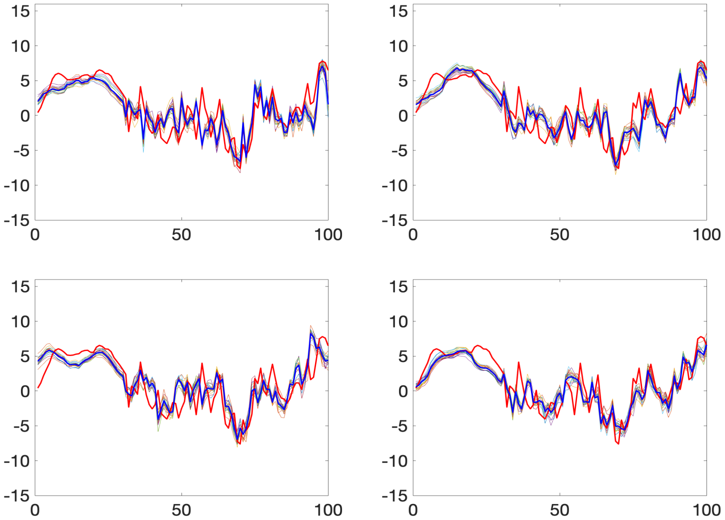
EnKF results with $M = 19$ ensemble members, time $t = 2$



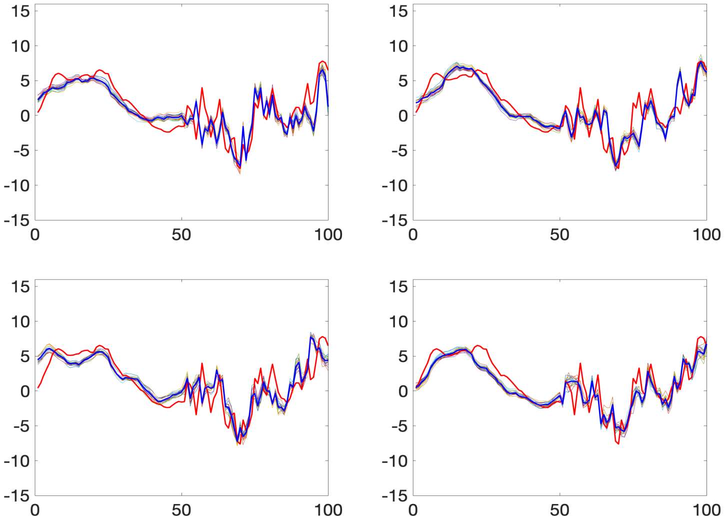
EnKF results with $M = 19$ ensemble members, time $t = 3$



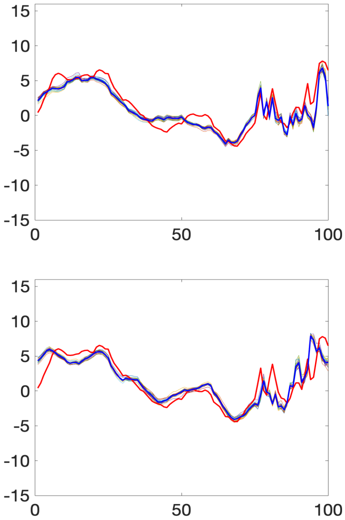
EnKF results with $M = 19$ ensemble members, time $t = 6$



EnKF results with $M = 19$ ensemble members, time $t = 10$

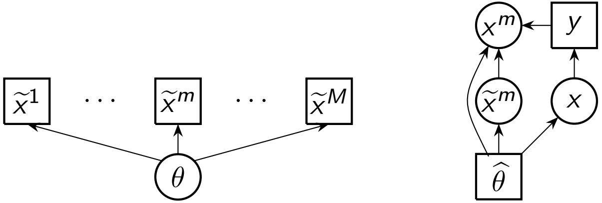


EnKF results with $M = 19$ ensemble members, time $t = 15$



Issues with the EnKF

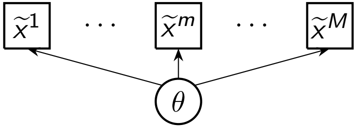
⋆ Recall: Underlying models for the EnKF updating of $\widetilde{x}^m$ to x^m

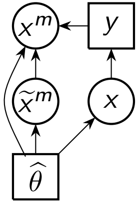


⋆ Issues:
- uncertainty in $\widehat{\theta}$ is ignored
  + Myrseth and Omre (2010), Tsyrulnikov and Rakitko (2017)
- the information in y about θ is ignored
  + discussed in Myrseth and Omre (2010)
- the information in $\widetilde{x}^m$ is used two times
  + and inconsistently?

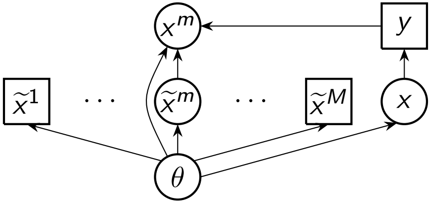
Propose new model for the updating step

⋆ Recall: Standard EnKF model for updating $\widetilde{x}^m$ to x^m





⋆ Propose to base update on a merged model



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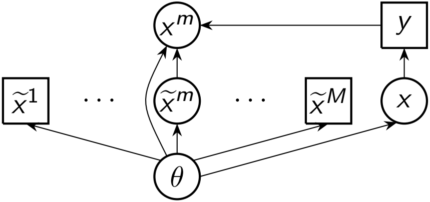

- ⋆ Assumed model:

$$\widetilde{x}^1, \ldots, \widetilde{x}^M, x|\theta \overset{\text{iid}}{\sim} \mathsf{N}(\mu, \Sigma)$$

$$\theta = (\mu, \Sigma) \sim \mathsf{NIW}(\mu_0, \lambda, \Psi, \nu)$$

$$y|x \sim \mathsf{N}(Hx, R)$$

- ⋆ Require: $x^m|\widetilde{x}^{-m}, y \quad \overset{\text{d}}{=} \quad x|\widetilde{x}^{-m}, y$

Class of possible of update procedures

- ⋆ Require: $x^m | \widetilde{x}^{-m}, y \quad \stackrel{\mathsf{d}}{=} \quad x | \widetilde{x}^{-m}, y$
- ⋆ Class of possible solutions:

$$\theta = (\mu, \Sigma) \sim f(\theta | \widetilde{x}^{-m}, y)$$
$$x^m = B(\widetilde{x}^m - \mu) + \mu + K(y - H\mu) + \varepsilon$$

where

$$\varepsilon \sim \mathrm{N}(0, S) \quad \text{and} \quad S = (\mathbb{I} - KH)\Sigma - B\Sigma B^T \geq 0$$

Class of possible of update procedures

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- Three special cases:
  - $S = 0$: square root filter, many possible B's
  - $B = \mathbb{I} - KH$: ensemble Kalman filter update
  - $B = 0$: sample x^m independently of $\widetilde{x}^m$

Class of possible of update procedures

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- Class of possible solutions:

$$\begin{aligned} \theta &= (\mu, \Sigma) \sim f(\theta|\widetilde{x}^{-m}, y) \\ x^m &= B(\widetilde{x}^m - \mu) + \mu + K(y - H\mu) + \varepsilon \end{aligned}$$

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- Three special cases:
  - $S = 0$: square root filter, many possible B's
  - $B = \mathbb{I} - KH$: ensemble Kalman filter update
  - $B = 0$: sample x^m independently of $\widetilde{x}^m$
- What is "the best" (B, S)?

Optimality criterion

- ⋆ What is the best (B, S)?
- ⋆ If the assumed model is correct:
  - all allowed choices of (B, S) are equally good!
- ⋆ If the assumed model is wrong:
  - all allowed choices of (B, S) are wrong
  - wants an update procedure that is robust
- ⋆ Intuition: Should do small changes

$$x^m = B(\widetilde{x}^m - \mu) + \mu + K(y - H\mu) + \varepsilon$$

- ⋆ Our optimality criterion: want to minimise

$$\mathrm{E}\left[(x^m - \widetilde{x}^m)^T (x^m - \widetilde{x}^m) \middle| \widetilde{x}^{-m}, y\right]$$

with respect to B and S, under the restriction

$$S = (\mathbb{I} - KH)\Sigma - B\Sigma B^T \geq 0$$

- ⋆ The solution can be found analytically

Optimal solution

- ⋆ Recall: Update procedure:

$$\theta = (\mu, \Sigma) \sim f(\theta | \widetilde{x}^{-m}, y)$$
$$x^m = B(\widetilde{x}^m - \mu) + \mu + K(y - H\mu) + \varepsilon$$

where

$$\varepsilon \sim \mathrm{N}(0, S) \quad \text{and} \quad S = (\mathbb{I} - KH)\Sigma - B\Sigma B^T \geq 0$$

- ⋆ Optimal solution of (B, S):

$$S = 0 \quad \text{and} \quad B = U\Lambda^{\frac{1}{2}} F P^T D^{-\frac{1}{2}} V^T$$

where (using singular value decomposition)

$$\Sigma = VDV^T, \quad (\mathbb{I} - KH)\Sigma = U\Lambda U^T \quad \text{and} \quad \Lambda^{\frac{1}{2}} U^T \Sigma V D^{-\frac{1}{2}} = PGF^T$$

Resulting computational procedure

- ⋆ For $m = 1, \ldots, M$
    1. Sample $\theta = (\mu, \Sigma) \sim f(\theta | \widetilde{x}^{-m}, y)$
    2. From θ and y compute optimal weight matrix B
    3. Compute

$$x^m = B(\widetilde{x}^m - \mu) + \mu + K(y - H\mu)$$

Simulation example revisited

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- ⋆ State vector x_n is a vector of size 100
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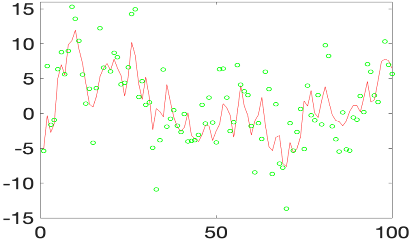
  - (non-linear example)
- ⋆ Prior for $\theta = (\mu, \Sigma)$: vague, the same for all time steps
- ⋆ Likelihood, $y_n | x_n \sim \mathrm{N}(x_n, 20\mathbb{I})$

$t = 1$



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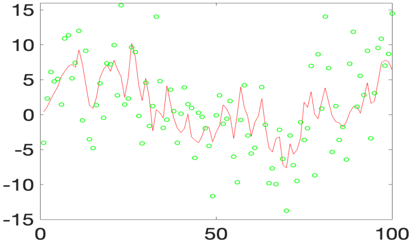

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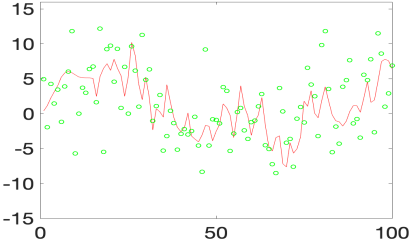
- ⋆ Prior for $\theta = (\mu, \Sigma)$: vague, the same for all time steps
- ⋆ Likelihood, $y_n | x_n \sim \mathrm{N}(x_n, 20\mathbb{I})$

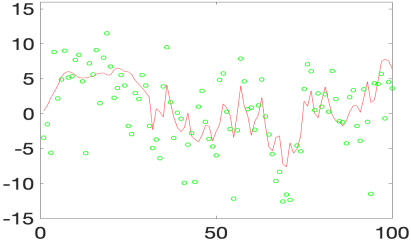
$t = 3$



Simulation example revisited

- ⋆ Use an example introduced in Myrseth and Omre (2010)
- ⋆ State vector x_n is a vector of size 100
- ⋆ $x_1 \sim \mathrm{N}(0, \Sigma)$, exponential correlation function
- ⋆ Forward function is deterministic
  - linear: smoothing for ten nodes
  - (non-linear example)
- ⋆ Prior for $\theta = (\mu, \Sigma)$: vague, the same for all time steps
- ⋆ Likelihood, $y_n | x_n \sim \mathrm{N}(x_n, 20\mathbb{I})$

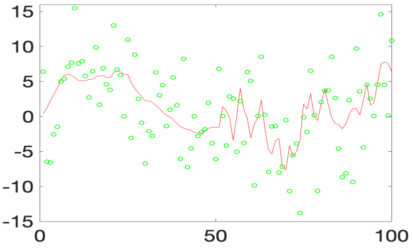
$t = 6$



Simulation example revisited

- ⋆ Use an example introduced in Myrseth and Omre (2010)
- ⋆ State vector x_n is a vector of size 100
- ⋆ $x_1 \sim \mathrm{N}(0, \Sigma)$, exponential correlation function
- ⋆ Forward function is deterministic
  - linear: smoothing for ten nodes
  - (non-linear example)
- ⋆ Prior for $\theta = (\mu, \Sigma)$: vague, the same for all time steps
- ⋆ Likelihood, $y_n | x_n \sim \mathrm{N}(x_n, 20\mathbb{I})$

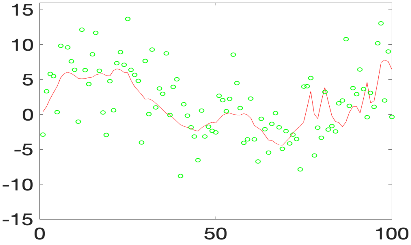
$t = 10$



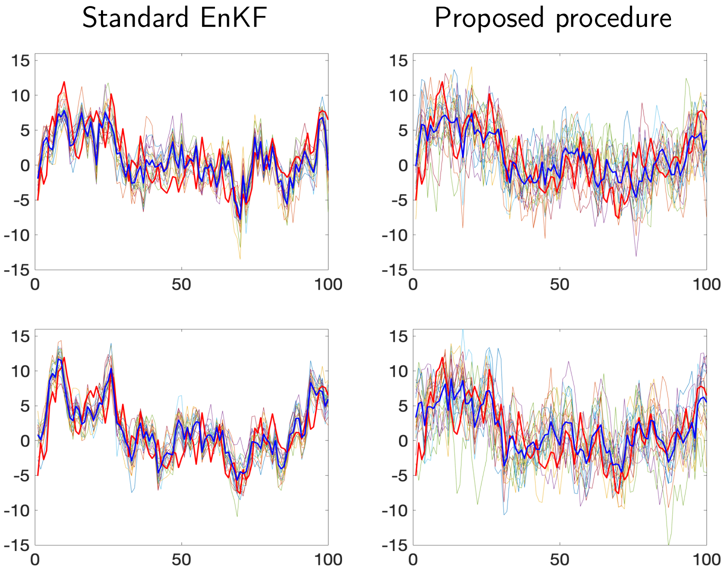
Simulation example revisited

- ⋆ Use an example introduced in Myrseth and Omre (2010)
- ⋆ State vector x_n is a vector of size 100
- ⋆ $x_1 \sim \mathrm{N}(0, \Sigma)$, exponential correlation function
- ⋆ Forward function is deterministic
  - – linear: smoothing for ten nodes
  - – (non-linear example)
- ⋆ Prior for $\theta = (\mu, \Sigma)$: vague, the same for all time steps
- ⋆ Likelihood, $y_n | x_n \sim \mathrm{N}(x_n, 20\mathbb{I})$

$t = 15$



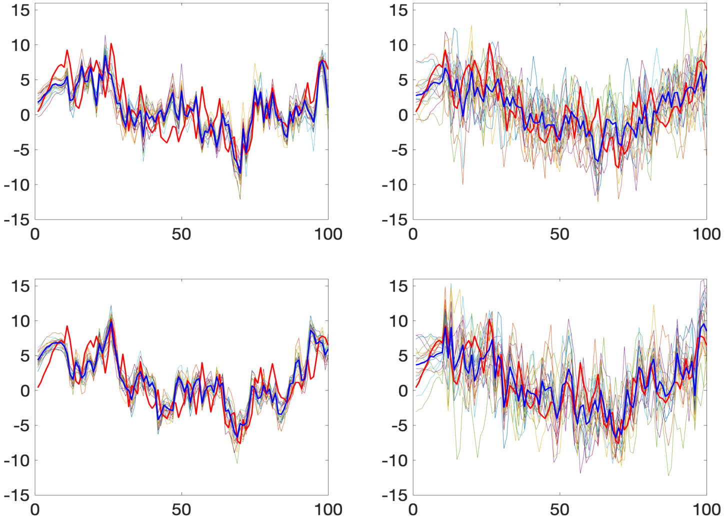
Results with $M = 19$, linear example, time $t = 1$



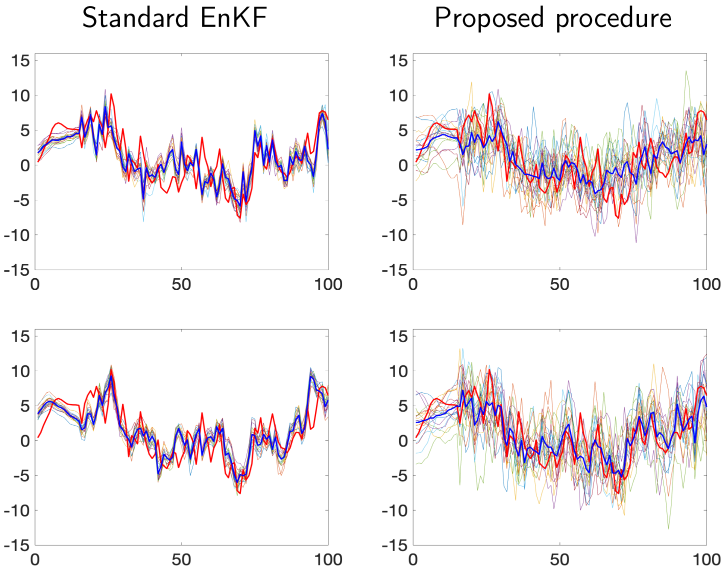
Results with $M = 19$, linear example, time $t = 2$

Standard EnKF

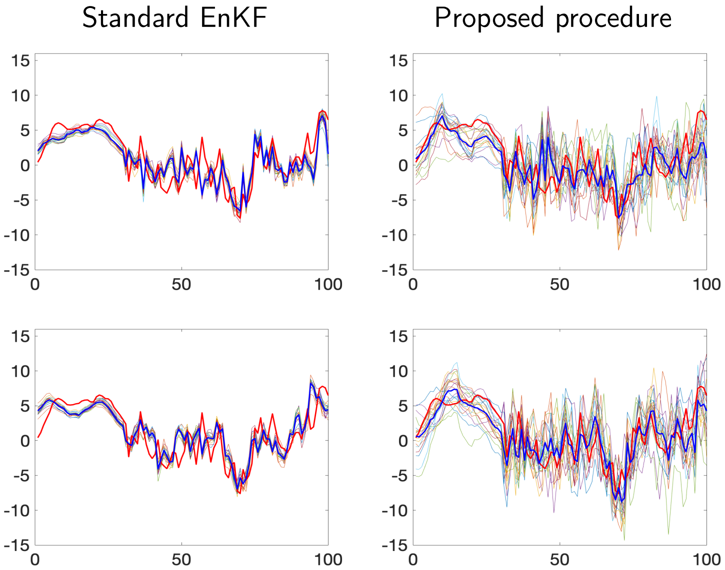
Proposed procedure



Results with $M = 19$, linear example, time $t = 3$

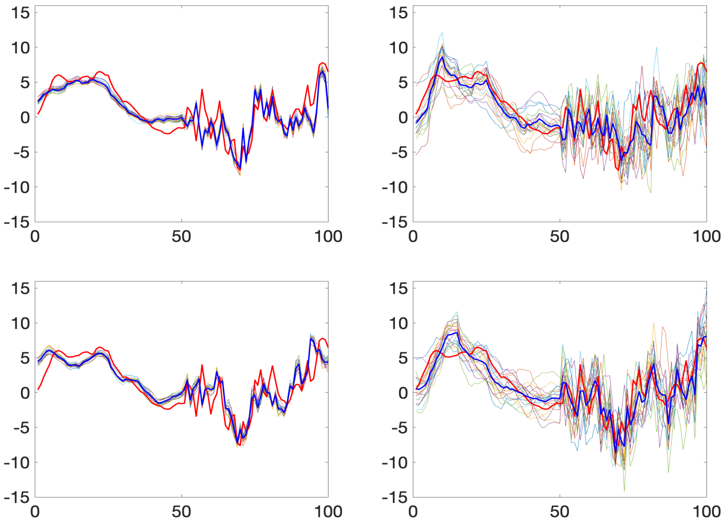


Results with $M = 19$, linear example, time $t = 6$

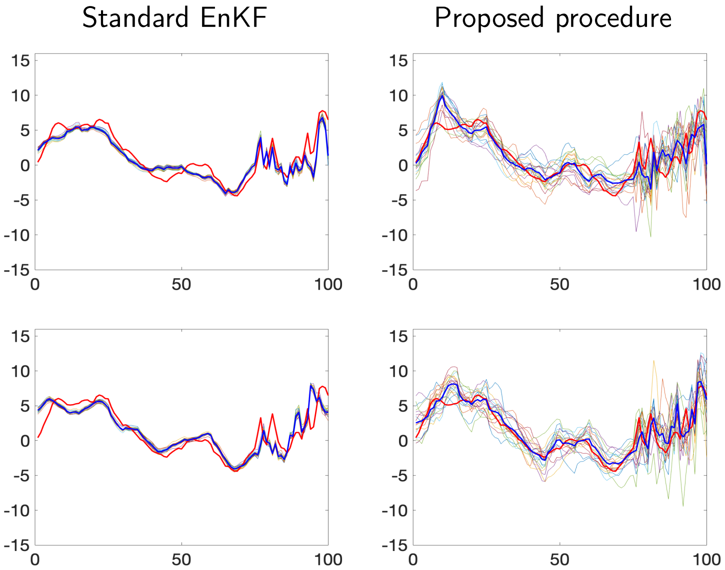


Results with $M = 19$, linear example, time $t = 10$

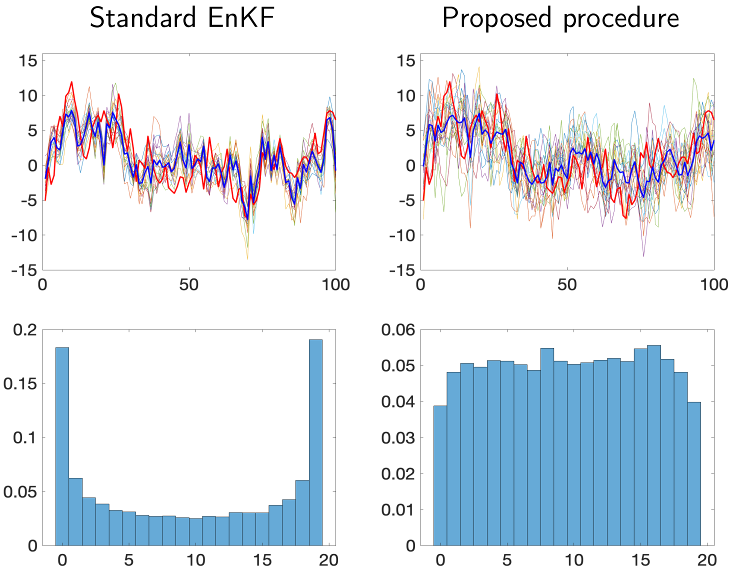
Standard EnKF | Proposed procedure



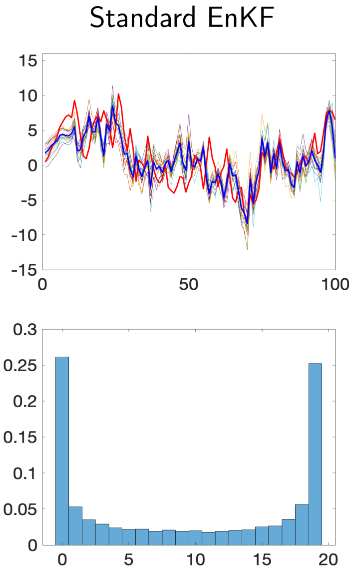
Results with $M = 19$, linear example, time $t = 15$



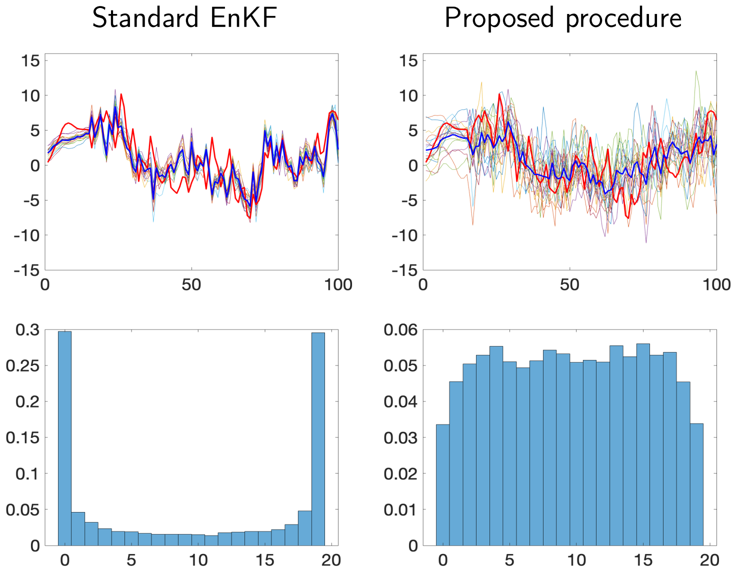
Results with $M = 19$, linear example, time $t = 1$



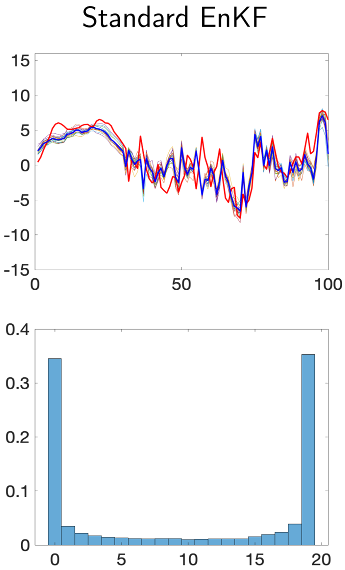
Results with $M = 19$, linear example, time $t = 2$



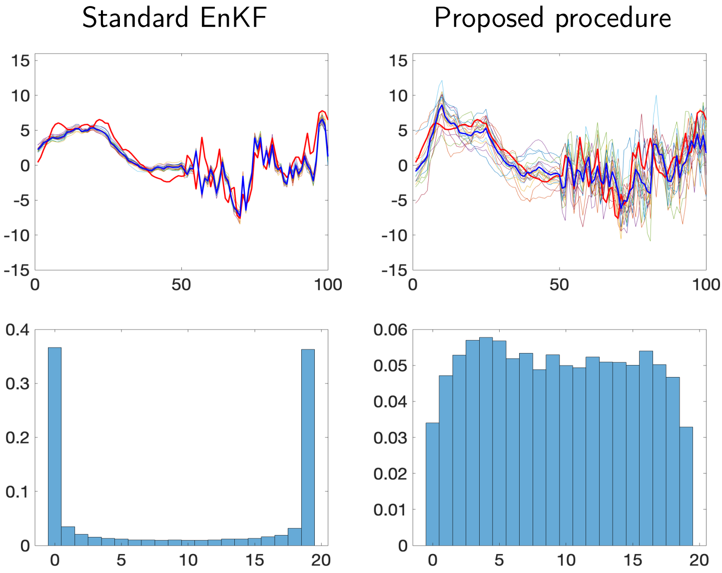
Results with $M = 19$, linear example, time $t = 3$



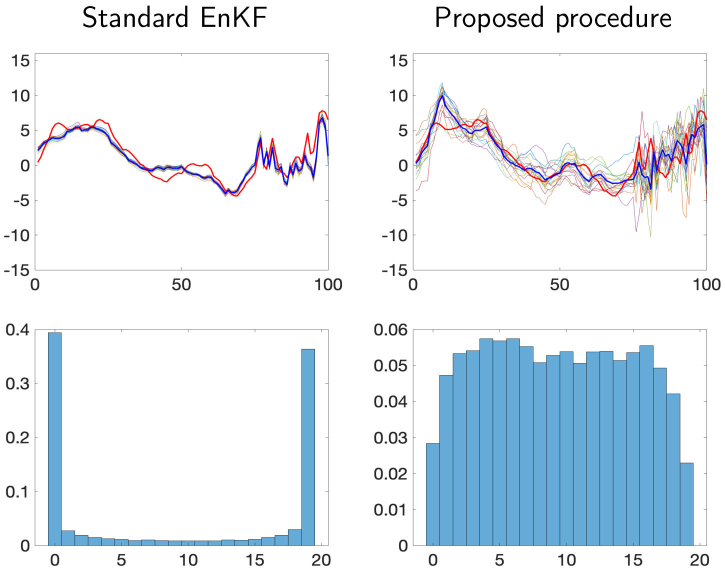
Results with $M = 19$, linear example, time $t = 6$



Results with $M = 19$, linear example, time $t = 10$



Results with $M = 19$, linear example, time $t = 15$



Closing remarks

- ⋆ Proposed procedure avoids variance underestimation
  - no need for variance inflation
- ⋆ Three changes in proposed update procedure
  - sample $\theta = (\mu, \Sigma)$
  - condition also on the new data y
  - do not condition on $\widetilde{x}^m$
- ⋆ Need more experience for non-linear models
- ⋆ The presented solution use matrices of full rank
  - not computationally feasible for high dimensional problems
  - ongoing work: formulate a sparse matrix variant of the proposed solution
- ⋆ We have also worked on generalising the idea underlying EnKF to a situation with categorical variables

References to our work

- ⋆ Loe, M.K. and Tjelmeland, H. (2021). A generalised and fully Bayesian framework for ensemble updating, `https://arxiv.org/abs/2103.14565`.
- ⋆ Loe, M.K. and Tjelmeland, H. (2020). Ensemble updating of binary state vectors by maximizing the expected number of unchanged components, *Scandinavian Journal of Statistics*, To appear, `https://doi.org/10.1111/sjos.12483`
- ⋆ Loe, M.K., Grana, D. and Tjelmeland, H. (2021). Geophysics-based fluid-facies predictions using ensemble updating of binary state vectors, *Mathematical Geosciences*, **53**, 325–347, `https://doi.org/10.1007/s11004-021-09922-4`
- ⋆ Loe, M.K. (2021). Ensemble updating for a state-space model with categorical variables, PhD thesis, NTNU, To appear.