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Approximation of Forecast Covariances in the Ensemble Kalman Filter

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Evaluation of Ensemble Kalman Filter

Qualitative and quantitative description of the effects of sampling variability on the forecast and analysis covariance for different ensemble Kalman filters.

Outline of the Talk

- Introduction and statement of the problem
- Effects in the EnKF
  - Forecast difference
  - Analysis difference
- Effects in the EnKF with tapering
  - Forecast difference
  - Analysis difference
- Optimal taper matrices
- Optimal covariance boosting
- Conclusions and open questions

Kalman Filter

Given the state-space model

$$\begin{aligned} \mathbf{y}_t &= \mathbf{H}_t\mathbf{x}_t + \mathbf{w}_t & \mathbf{w}_t &\sim \mathcal{N}_m(\mathbf{0}, \mathbf{R}_t) \\ \mathbf{x}_t &= \mathbf{G}_t\mathbf{x}_{t-1} + \mathbf{v}_t & \mathbf{v}_t &\sim \mathcal{N}_n(\mathbf{0}, \mathbf{Q}_t) \end{aligned}$$

the Kalman filter uses the iterative quantities

$$\begin{aligned} \mathbf{P}_t^f &= \mathbf{G}_t\mathbf{P}_{t-1}^a\mathbf{G}_t^\mathsf{T} + \mathbf{Q}_t \\ \mathbf{K}_t &= \mathbf{P}_t^f\mathbf{H}_t^\mathsf{T}(\mathbf{H}_t\mathbf{P}_t^f\mathbf{H}_t^\mathsf{T} + \mathbf{R}_t)^{-1} \\ \mathbf{P}_t^a &= (\mathbf{I} - \mathbf{K}_t\mathbf{H}_t^\mathsf{T})\mathbf{P}_t^f \end{aligned}$$

to filter the state $\mathbf{x}_t$ given the observations $\mathbf{y}_t, \ldots, \mathbf{y}_0$.

Approximations to Covariance matrices

The forecast covariance matrix $\mathbf{P}_t^f$ is often approximated with $\widetilde{\mathbf{P}}_t^f$:

1. $\mathbf{P}_t^f$ is estimated with N ensembles
   $\rightsquigarrow$ $\widetilde{\mathbf{P}}_t^f = \widehat{\mathbf{P}}_t^f$: the ensemble Kalman filter (EnKF)
2. $\mathbf{P}_t^f$ is estimated with N ensembles and tapered with $\mathbf{C}$
   $\rightsquigarrow$ $\widetilde{\mathbf{P}}_t^f = \widehat{\mathbf{P}}_t^f \circ \mathbf{C}$

We want to quantify the effect of the approximation with

$\left\Vert \mathbf{P}_t^f - \widetilde{\mathbf{P}}_t^f \right\Vert$	$\left\Vert \mathbf{P}_t^a - \widetilde{\mathbf{P}}_t^a \right\Vert$	
forecast	analysis	difference

We suppose $\mathbf{H} = \mathbf{I}$ and $\mathbf{R} = \mathbf{I}$ ($\rightsquigarrow$ $\widetilde{\mathbf{P}}_t^a = (\widetilde{\mathbf{P}}_t^f + \mathbf{I})^{-1}$) and we consider only one-step forecasts ($\rightsquigarrow$ drop subscript t).

Goal of the Study

What is the dependence of

$$\left\Vert \mathbf{P}^f - \widetilde{\mathbf{P}}^f \right\Vert \qquad \left\Vert (\mathbf{P}^f + \mathbf{I})^{-1} - (\widetilde{\mathbf{P}}^f + \mathbf{I})^{-1} \right\Vert$$

with

$$\widetilde{\mathbf{P}}^f = \widehat{\mathbf{P}}^f \qquad \text{or} \qquad \widetilde{\mathbf{P}}^f = \widehat{\mathbf{P}}^f \circ \mathbf{C}$$

on ensemble size N, state dimension n and eigenvalues of λ_i of $\mathbf{P}^f$?

Associated questions:

- how big has the ensemble size N to be?
- what is an optimal taper matrix $\mathbf{C}$?

Statistical Approach

Most calculations can be summarized by

- Choose a norm: $\|\mathbf{A}\| = \mathrm{tr}(\mathbf{A}^\mathsf{T}\mathbf{A})^{1/2}$
- Use the eigenvalue/eigenvector decomposition of $\mathbf{P}^f$:

$$\mathbf{P}^f = \Gamma\Lambda\Gamma^\mathsf{T}$$

  Γ contains the eigenvectors
  $\Lambda = \mathrm{diag}(\lambda_1, \ldots, \lambda_n)$ contains the eigenvalues

- Simplify the norm to an expression containing $\{\lambda_i\}$, N:

$$\begin{aligned}\left\|\mathbf{P}^f\right\|^2 &= \mathrm{tr}(\mathbf{P}^{f\mathsf{T}}\mathbf{P}^f) = \mathrm{tr}(\Gamma^\mathsf{T}\mathbf{P}^f\Gamma\Gamma^\mathsf{T}\mathbf{P}^f\Gamma)\\ &= \mathrm{tr}(\Lambda\Lambda) = \sum_{i=1}^{n} \lambda_i^2\end{aligned}$$

EnKF 123: Forecast Covariance

Straightforward analysis leads to

$$\mathsf{E}\left\|\mathbf{P}^f - \widehat{\mathbf{P}}^f\right\|^2 = \frac{2}{N}\sum_i \lambda_i^2 + \frac{2}{N}\sum_{i<j}\lambda_i\lambda_j$$

Remarks:

- we do not need Gaussianity,
- off-diagonal terms dominate,
- for polynomial spectra $\lambda_i = \sigma^2 i^{-\theta}$ we get the asymptotic results $(n \to \infty)$

$$\approx \frac{\sigma^4}{(2\theta-1)N} + \frac{\sigma^4}{(\theta-1)^2 N}$$

EnKF 123: Analysis Covariance

We cannot evaluate $\mathrm{tr}\big((\widehat{\mathbf{P}}^f + \mathbf{I})^{-1}\big)$.

If there is a matrix norm such that $\|\Lambda\mathbf{D} - \widehat{\Lambda}\mathbf{D}\| < 1$, then the following expansion holds

$$\left\|\mathbf{P}^a - \widehat{\mathbf{P}}^a\right\|^2 = \sum_{i=2}^{\infty}(i-1)\,\mathrm{tr}\Big((\Lambda\mathbf{D} - \widehat{\Lambda}\mathbf{D})^i\mathbf{D}^2\Big)$$

To use the third order approximation

$$\left\|\mathbf{P}^a - \widehat{\mathbf{P}}^a\right\|^2 \approx \mathrm{tr}\Big((\Lambda\mathbf{D} - \widehat{\Lambda}\mathbf{D})^2\mathbf{D}^2\Big) - 2\,\mathrm{tr}\Big((\Lambda\mathbf{D} - \widehat{\Lambda}\mathbf{D})^3\mathbf{D}^2\Big)$$

we need to calculate

$$\mathsf{E}\big(\widehat{\lambda}_{ij}^2\big) \qquad \text{and} \qquad \mathsf{E}\big(\widehat{\lambda}_{ij}\widehat{\lambda}_{jk}\widehat{\lambda}_{ki}\big)$$

EnKF 123: Analysis Covariance

Evaluating the expressions, we have

$$\begin{aligned}\mathsf{E}\left\|\mathbf{P}^a - \widehat{\mathbf{P}}^a\right\|^2 \approx{}& \frac{1}{N}\Big(\sum_i \frac{\lambda_i^2}{(\lambda_i+1)^4} + \sum_{i,j}\frac{\lambda_i\lambda_j}{(\lambda_i+1)^3(\lambda_j+1)}\Big)\\ &- \frac{2}{N^2}\Big(\sum_i \frac{\lambda_i^3}{(\lambda_i+1)^5} + \sum_{i,j}\frac{\lambda_i\lambda_j^2}{(\lambda_i+1)^3(\lambda_j+1)^2}\\ &+ \sum_{i,j}\frac{2\lambda_i^2\lambda_j}{(\lambda_i+1)^4(\lambda_j+1)}\\ &+ \sum_{i,j,\ell}\frac{\lambda_i\lambda_j\lambda_\ell}{(\lambda_i+1)^3(\lambda_j+1)(\lambda_\ell+1)}\Big)\end{aligned}$$

For small N the expansion may not be informative.

EnKF with tapering 12: Forecast

The Schur product induced by the tapering implies

$$\mathsf{E}\left\|\mathbf{P}^f - \widehat{\mathbf{P}}^f \circ \mathbf{C}\right\|^2 = \mathrm{function}\big(\{\lambda_i\}, \{\gamma_{ij}\}, \{c_{ij}\}\big)$$

If $\mathbf{P}^f$ is diagonal we have

$$\mathsf{E}\left\|\mathbf{P}^f - \widetilde{\mathbf{P}}^f\right\|^2 = \sum_i \lambda_i^2(c_{ii}-1)^2 + \frac{1}{N}\sum_i c_{ii}^2\lambda_i^2 + \frac{1}{N}\sum_{i,j} c_{ij}^2\lambda_i\lambda_j$$

For non-correlation matrices we introduce a bias.

EnKF with tapering 12: Analysis

For the ‘analysis’ difference we encounter the same problems as above.

If $\mathbf{P}^f$ is diagonal we have the second order approximation

$$\begin{aligned}\mathsf{E}\left\|\mathbf{P}^f - \widetilde{\mathbf{P}}^f\right\|^2 ={}& \sum_i \frac{(c_{ii}-1)^2\lambda_i^2}{(\lambda_i+1)^4}\\ &+ \frac{1}{N}\sum_i \frac{c_{ii}^2\lambda_i^2}{(\lambda_i+1)^4} + \frac{1}{N}\sum_{i,j}\frac{c_{ij}^2\lambda_i\lambda_j}{(\lambda_i+1)^3(\lambda_j+1)}\end{aligned}$$

Optimal Taper C 12

We want to minimize

$$\mathsf{E}\left\| \mathbf{P}^f - \widehat{\mathbf{P}}^f \circ \mathbf{C} \right\|^2$$

with respect to all positive definite matrices $\mathbf{C}$

With $\mathbf{P}^f = (p_{ij})$, the optimal taper matrix $\mathbf{C} = (c_{ij})$ minimizes

$$\sum_{i,j} \Big(-2c_{ij}p_{ij}^2 + c_{ij}^2 \big(p_{ij}^2 + \frac{1}{N}(p_{ij}^2 + p_{ii}p_{jj}) \big) \Big)$$

Without further constraints it is impossible to find the optimum.

Note, the expression is in function of the elements of the forecast matrix and not of its spectrum.

Optimal Taper C 12

A naive approach is to minimize component-wise (equivalent to minimum without the constraint)

$$(\mathbf{C}_{\mathsf{min}})_{ij} = \frac{p_{ij}^2}{p_{ij}^2 + (p_{ij}^2 + p_{ii}p_{jj})/N}$$

But $\mathbf{C}_{\mathsf{min}}$ is

- not a correlation matrix
  $N/(N+2)$ on the diagonal
- not always positive definite
  depends on N

As $N \to \infty$, $(\mathbf{C}_{\mathsf{min}})_{ij} = \begin{cases} 1 & \text{if } p_{ij} \neq 0 \\ 0 & \text{if } p_{ij} = 0 \end{cases}$

Optimal Taper with isotropic $\mathbf{P}^f$ 12

Suppose we have an "isotropic" forecast matrix

$$(\mathbf{P}^f)_{ij} = p\big(|\mathbf{x}_i - \mathbf{x}_j|\big)$$

It is natural to minimize within "isotropic" taper matrices.

The minimization problem could be restated as

$$\min_{c(\cdot)} \mathsf{E} \int_{\ell_n}^{u_n} \omega(h)\big(p(h) - \widehat{p}(h)c(h)\big)^2 \, \mathsf{d}h$$

$$\iff$$

$$\min_{c(\cdot)} \int_{\ell_n}^{u_n} \omega(h)\Big(p(h)^2(c(h)-1)^2 - \frac{1}{N}(p(h)^2 + p(0)^2)c(h)^2\Big) \, \mathsf{d}h$$

Analytic solutions are only available in particular cases.

Optimal Taper with isotropic $\mathbf{P}^f$ 12

Suppose $p(h) = \alpha \exp(-\beta h)$, we minimize within the class of functions $\{\exp(\theta h)\}$.

With a weight function $\omega(h) \propto 1/h$,

$$\theta_{\mathsf{opt}} = \beta \cdot \frac{5 + \sqrt{9 + 8N}}{2(N-2)}$$

For other specific weight functions we also have

$$\theta_{\mathsf{opt}} = \mathcal{O}\big(\beta/\sqrt{N}\big)$$

Optimal Covariance Boosting 12

In order to avoid filter divergence, the covariance is boosted with ρ.

The optimal ρ is such that $\rho\widetilde{\mathbf{P}}^f$ mimics best the truth, i.e. minimizes the bias

$$\min_{\rho} \mathbf{B}(\rho) = \min_{\rho} \left| \mathsf{E}\Big((\rho\widetilde{\mathbf{P}}^f + \mathbf{I})^{-1} - (\mathbf{P}^f + \mathbf{I})^{-1} \Big) \right|$$

The bias is a matrix, we reduce it to

$$\mathsf{bias}(\rho) = \sum_{i,j} (\mathbf{B})_{ij}$$

Optimal Covariance Boosting 12

To find ρ_{opt} we apply same approximation techniques.

A second order approximation leads to a quadratic equation in ρ, which can be solved.

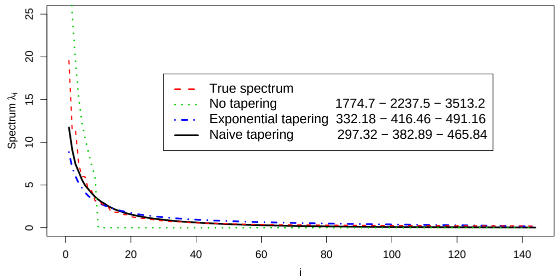
- For given $\mathbf{P}^f$, we can calculate the optimal boosting factor
- $\rho_{\mathsf{opt}} = \mathcal{O}\big(1/\sqrt{N}\big)$
- For small N, the second order approximation is of poor quality
- Same results hold with covariance tapering

Numerical Example 12

Suppose a regular 12×12 grid in $[0,1]^2$ and let

$$(\mathbf{P}^f)_{ij} = p\big(|i-j|\big) = \exp\big(-0.2|i-j|\big)$$

We consider ensemble size $N = 10$.
For 100 MC samples we calculated the spectrum.

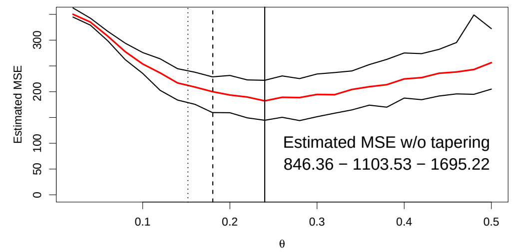


Numerical Example 12

Suppose a regular 10×10 grid in $[0,1]^2$ and let

$$p\big(|i-j|\big) = \exp\big(-0.2|i-j|\big) \quad c\big(|i-j|\big) = \exp\big(-\theta|i-j|\big)$$

For 100 MC samples we calculated the MSE of the spectrum in function of θ for ensemble size $N = 10$.



Conclusion

- Tapering the forecast matrix reduces significantely the error due to sampling variablility.
- There exists an optimal taper matrix:
  - which is not always practical, i.e. is not always positive definite,
  - the system is not sensitive with respect to the choice of the taper.

Further research

- Find optimal **C** for specific cases.
- Generalize to other matrices **H** and **R**.
- Apply to high dimensional problems.