Data Assimilation
- A06. Ensemble Kalman Filter-

Shunji Kotsuki

Environmental Prediction Science Laboratory
Center for Environmental Remote Sensing (CEReS), Chiba University
(shunji.kotsuki@chiba-u.jp)

A World Beyond Predictions
Environmental
Prediction
Science
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DA Lectures A (Basic Course)

- (1) Introduction and NWP
- (2) Deterministic Chaos and Lorenz-96 model
- (3) A toy model and Bayesian estimation
- (4) Kalman Filter (KF)
- (5) 3D Variational Method (3DVAR)
- (6) Ensemble Kalman Filter (PO method)
- (7) Serial Ens. Square Root Filter (Serial EnSRF)
- (8) Local Ens. Transform Kalman Filter (LETKF)
- (9) Innovation Statistics & Adaptive Inflation

Today’s Goal

- **Lecture: Ensemble Kalman Filter**
  - to introduce EnKF
  - to understand PO method
- **Training: Lorenz 96**
  - to implement PO method
  - to implement localization

Ensemble Kalman Filter (EnKF)

Why EnKF?

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Kalman Filter

$$\overleftarrow{\quad n \quad}\!\!\rightarrow \qquad \mathbf{P}_t^b \quad (n \times n)$$

Background error covariance cannot be stored on RAMfor high dimensional models such as NWP (n~O(10^{12}~10^{15}))

Ex) if $n=10^6$ ➔ 10^{12} x 8 byte = 8 TB

Ensemble Kalman Filter

$$\mathbf{P}_t^b \approx \frac{\delta\mathbf{X}_t^b\left(\delta\mathbf{X}_t^b\right)^T}{m-1}$$

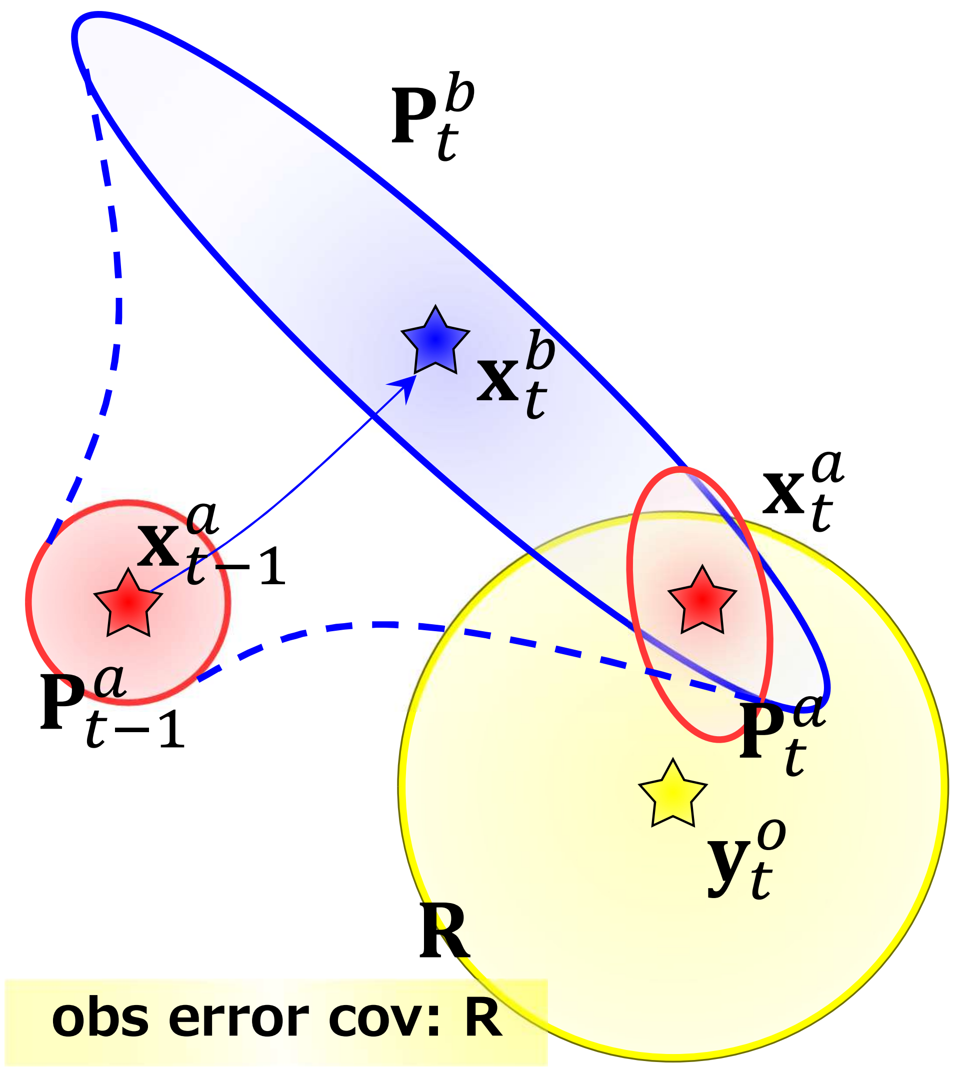
$$\delta\mathbf{X}_t^b \quad (n \times m)$$

An approximation of error covariance with ensemble perturbation matrix $\delta\mathbf{X}$.

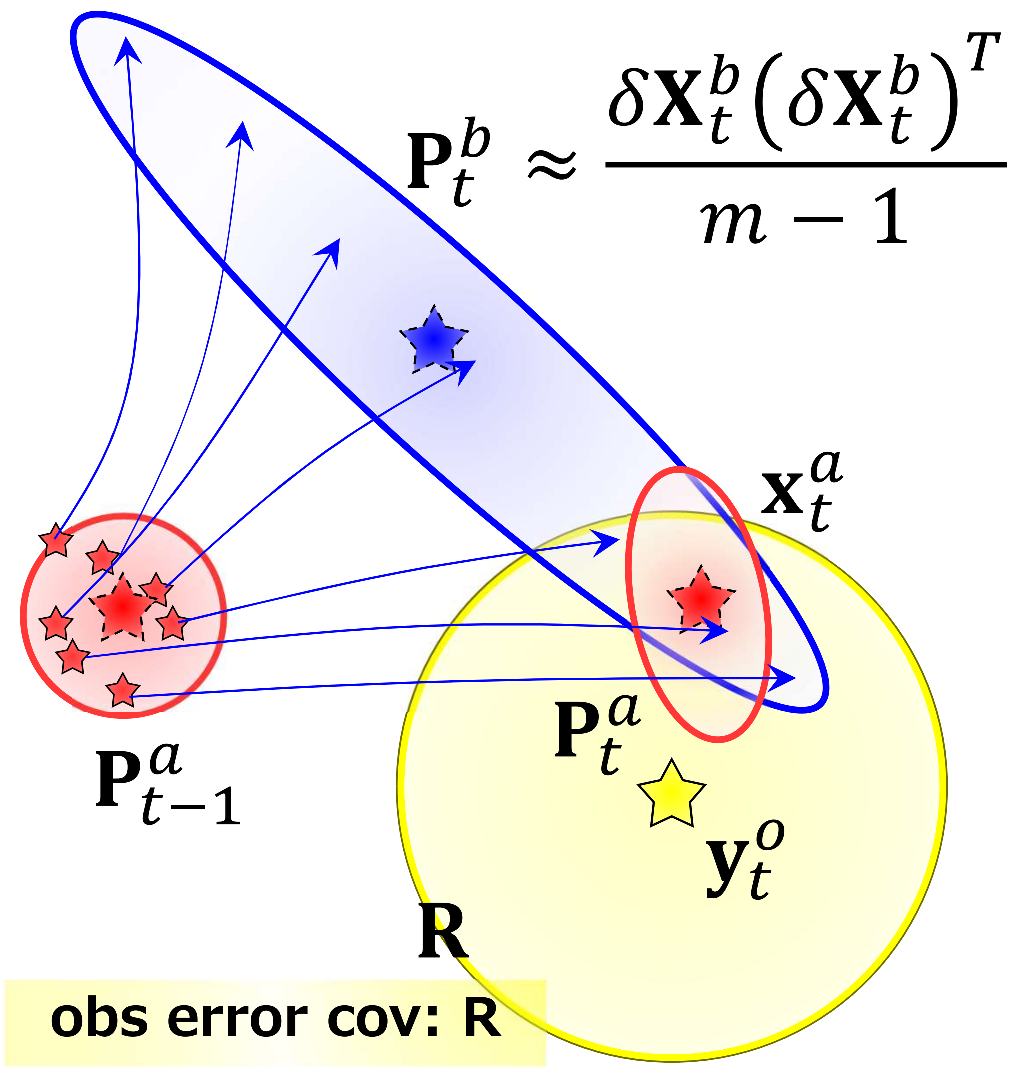
m: ensemble size

Conceptual Images

Kalman Filter



Ensemble Kalman Filter



Ensemble Forecasts

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Analysis Ensemble

$$\mathbf{X}_{t-1}^{a}=\left[\mathbf{x}_{t-1}^{a(1)},\mathbf{x}_{t-1}^{a(2)},\ldots,\mathbf{x}_{t-1}^{a(m)}\right]$$

Ensemble Forecasts

$$\mathbf{X}_{t}^{b}=\left[\mathbf{x}_{t}^{b(1)},\mathbf{x}_{t}^{b(2)},\ldots,\mathbf{x}_{t}^{b(m)}\right] \qquad where\ \mathbf{x}_{t}^{b(i)}=M\left(\mathbf{x}_{t-1}^{a(i)}\right)$$

for i = 1,…,m

Ensemble Mean

$$\bar{\mathbf{x}} \equiv \sum_{i=1}^{m}\mathbf{x}^{(i)}/m$$

Ensemble Perturbation

δ represents ensemble perturbation

$$\delta\mathbf{X}_{t}^{b}=\left[\mathbf{x}_{t}^{b(1)}-\bar{\mathbf{x}}_{t}^{b},\mathbf{x}_{t}^{b(2)}-\bar{\mathbf{x}}_{t}^{b},\ldots,\mathbf{x}_{t}^{b(m)}-\bar{\mathbf{x}}_{t}^{b}\right]$$

$$=\left[\delta\mathbf{x}_{t}^{b(1)},\delta\mathbf{x}_{t}^{b(2)},\ldots,\delta\mathbf{x}_{t}^{b(m)}\right]$$

$$\mathbf{Z}_{t}^{b}=\delta\mathbf{X}_{t}^{b}/\sqrt{m-1}$$

Approximation of $\mathbf{P}^b$

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Error Propagation in Ensemble Forecasts

$$\overline{M(\mathbf{x}_{t-1}^{a})} = \frac{1}{m}\sum_{i=1}^{m} M\left(\mathbf{x}_{t-1}^{a(i)}\right)$$

$$\delta\mathbf{x}_t^{b(i)} = M\left(\mathbf{x}_{t-1}^{a(i)}\right) - \overline{M(\mathbf{x}_{t-1}^{a})}$$

$$\approx \left[M(\bar{\mathbf{x}}_{t-1}^{a}) + \mathbf{M}\delta\mathbf{x}_{t-1}^{a(i)}\right] - \left[M(\bar{\mathbf{x}}_{t-1}^{a}) + \cancel{\left\langle \mathbf{M}\delta\mathbf{x}_{t-1}^{a(i)} \right\rangle}\right]$$

$$= \mathbf{M}\delta\mathbf{x}_{t-1}^{a(i)}$$

$$\mathbf{P}_t^b \approx \frac{1}{m-1}\delta\mathbf{X}_t^b\left(\delta\mathbf{X}_t^b\right)^T$$

$$= \frac{1}{m-1}\mathbf{M}\delta\mathbf{X}_{t-1}^{a}(\mathbf{M}\delta\mathbf{X}_{t-1}^{a})^T = \mathbf{M}\mathbf{P}_{t-1}^{a}\mathbf{M}^T$$

Ensemble forecasts can be used for approximating propagation of error covariance !

Ensemble Kalman Filter

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Ensemble Perturbation in Observation Space

$$\mathbf{Y}_t^b \equiv \mathbf{H}\mathbf{Z}_t^b \approx \left[H\left(\mathbf{X}_t^b\right) - \overline{H\left(\mathbf{X}_t^b\right)} \cdot \mathbf{1}\right] / \sqrt{m-1}$$

i.e. no **H** is needed

Error Covariance Approximation

$$\mathbf{P}_t^b \approx \mathbf{Z}_t^b\left(\mathbf{Z}_t^b\right)^T = \delta\mathbf{X}_t^b\left(\delta\mathbf{X}_t^b\right)^T/(m-1) \qquad \mathbf{H}\mathbf{P}_t^b\mathbf{H}^T \approx \mathbf{Y}_t^b(\mathbf{Y}_t^b)^T$$

Kalman Gain

$$\mathbf{K}_t = \mathbf{P}_t^b\mathbf{H}^T\left[\mathbf{H}\mathbf{P}_t^b\mathbf{H}^T + \mathbf{R}\right]^{-1}$$

We can choose inverse computation depending on *p* and *m*.

$$\approx \mathbf{Z}_t^b(\mathbf{Y}_t^b)^T\Big[\underbrace{\mathbf{Y}_t^b(\mathbf{Y}_t^b)^T+\mathbf{R}}_{p\ \mathrm{x}\ p}\Big]^{-1} = \mathbf{Z}_t^b\Big[\underbrace{\mathbf{I} + (\mathbf{Y}_t^b)^T\mathbf{R}^{-1}\mathbf{Y}_t^b}_{m\ \mathrm{x}\ m}\Big]^{-1}(\mathbf{Y}_t^b)^T\mathbf{R}^{-1}$$

※ usually **R** is diagonal (i.e., no obs error corr.)

$$\mathbf{Z}_t^b(\mathbf{Y}_t^b)^T\left[\mathbf{Y}_t^b(\mathbf{Y}_t^b)^T+\mathbf{R}\right]^{-1}$$

$$= \mathbf{Z}_t^b\left[\mathbf{I} + (\mathbf{Y}_t^b)^T\mathbf{R}^{-1}\mathbf{Y}_t^b\right]^{-1}\left[\mathbf{I} + (\mathbf{Y}_t^b)^T\mathbf{R}^{-1}\mathbf{Y}_t^b\right](\mathbf{Y}_t^b)^T\left[\mathbf{Y}_t^b(\mathbf{Y}_t^b)^T+\mathbf{R}\right]^{-1}$$

$$= \mathbf{Z}_t^b\left[\mathbf{I} + (\mathbf{Y}_t^b)^T\mathbf{R}^{-1}\mathbf{Y}_t^b\right]^{-1}(\mathbf{Y}_t^b)^T\left[\mathbf{I} + \mathbf{R}^{-1}\mathbf{Y}_t^b(\mathbf{Y}_t^b)^T\right]\left[\mathbf{Y}_t^b(\mathbf{Y}_t^b)^T+\mathbf{R}\right]^{-1}$$

$$= \mathbf{Z}_t^b\left[\mathbf{I} + (\mathbf{Y}_t^b)^T\mathbf{R}^{-1}\mathbf{Y}_t^b\right]^{-1}(\mathbf{Y}_t^b)^T\mathbf{R}^{-1}\cancel{\left[\mathbf{R} + \mathbf{Y}_t^b(\mathbf{Y}_t^b)^T\right]}\cancel{\left[\mathbf{Y}_t^b(\mathbf{Y}_t^b)^T+\mathbf{R}\right]^{-1}}$$

KF

Prediction (state)

$$\mathbf{x}_t^b = M(\mathbf{x}_{t-1}^a)$$

Prediction of Error Cov. (explicitly)

$$\mathbf{P}_t^b = \mathbf{M}\mathbf{P}_{t-1}^a\mathbf{M}^T(+\mathbf{Q})$$

Kalman Gain

$$\mathbf{K}_t = \mathbf{P}_t^b\mathbf{H}^T\left[\mathbf{H}\mathbf{P}_t^b\mathbf{H}^T + \mathbf{R}\right]^{-1}$$

Analysis (state)

$$\mathbf{x}_t^a = \mathbf{x}_t^b + \mathbf{K}_t(\mathbf{y}_t^o - H(\mathbf{x}_t^b))$$

Analysis Error Covariance

$$\mathbf{P}_t^a = [\mathbf{I} - \mathbf{K}_t\mathbf{H}]\mathbf{P}_t^b$$

EnKF

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Ensemble Prediction (state)

$$\mathbf{x}_t^{b(i)} = M\left(\mathbf{x}_{t-1}^{a(i)}\right) \quad \text{for } i = 1,\ldots,m$$

Prediction of Error Covariance (implicitly)

$$\mathbf{P}_t^b \approx \mathbf{Z}_t^b\left(\mathbf{Z}_t^b\right)^T$$

Kalman Gain

$$\mathbf{K}_t = \mathbf{Z}_t^b(\mathbf{Y}_t^b)^T\left[\mathbf{Y}_t^b(\mathbf{Y}_t^b)^T + \mathbf{R}\right]^{-1}$$

$$= \mathbf{Z}_t^b\left[\mathbf{I} + (\mathbf{Y}_t^b)^T\mathbf{R}^{-1}\mathbf{Y}_t^b\right]^{-1}(\mathbf{Y}_t^b)^T\mathbf{R}^{-1}$$

Analysis (state)

$$\mathbf{x}_t^a = \mathbf{x}_t^b + \mathbf{K}_t(\mathbf{y}_t^o - H(\mathbf{x}_t^b))$$

Analysis Error Covariance

(1) Stochastic: PO method
(2) Deterministic: Square Root Filter (SRF)
(e.g., serial EnSRF, EAKF, LETKF)

PO Method (stochastic)

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Analysis of Ensemble

$$\boldsymbol{\varepsilon}_t^o \sim N(0, \mathbf{R})$$

randomly drawn perturbation
➔ perturbed observation

$$\mathbf{x}_t^{a(i)} = \mathbf{x}_t^{b(i)} + \mathbf{K}_t(\mathbf{y}_t^o + \boldsymbol{\varepsilon}_t^o - H(\mathbf{x}_t^{b(i)}))$$

Why do we need perturbation?

if w/o perturbation (to take ave. from both sides)

$$\delta\mathbf{x}_t^{a(i)} \approx \delta\mathbf{x}_t^{b(i)} - \mathbf{K}_t\mathbf{H}\delta\mathbf{x}_t^{b(i)}$$

$$\Leftrightarrow \delta\mathbf{X}_t^a \approx (\mathbf{I} - \mathbf{K}_t\mathbf{H})\delta\mathbf{X}_t^b$$

$$\mathbf{K}_t\mathbf{R}\mathbf{K}_t^T = \mathbf{K}_t\langle\boldsymbol{\varepsilon}_t^o(\boldsymbol{\varepsilon}_t^o)^T\rangle\mathbf{K}_t^T$$

$$\mathbf{P}_t^a \approx \delta\mathbf{X}_t^a(\delta\mathbf{X}_t^a)^T/(m-1)$$

$$= (\mathbf{I} - \mathbf{K}_t\mathbf{H})\mathbf{P}_t^b(\mathbf{I} - \mathbf{K}_t\mathbf{H})^T$$

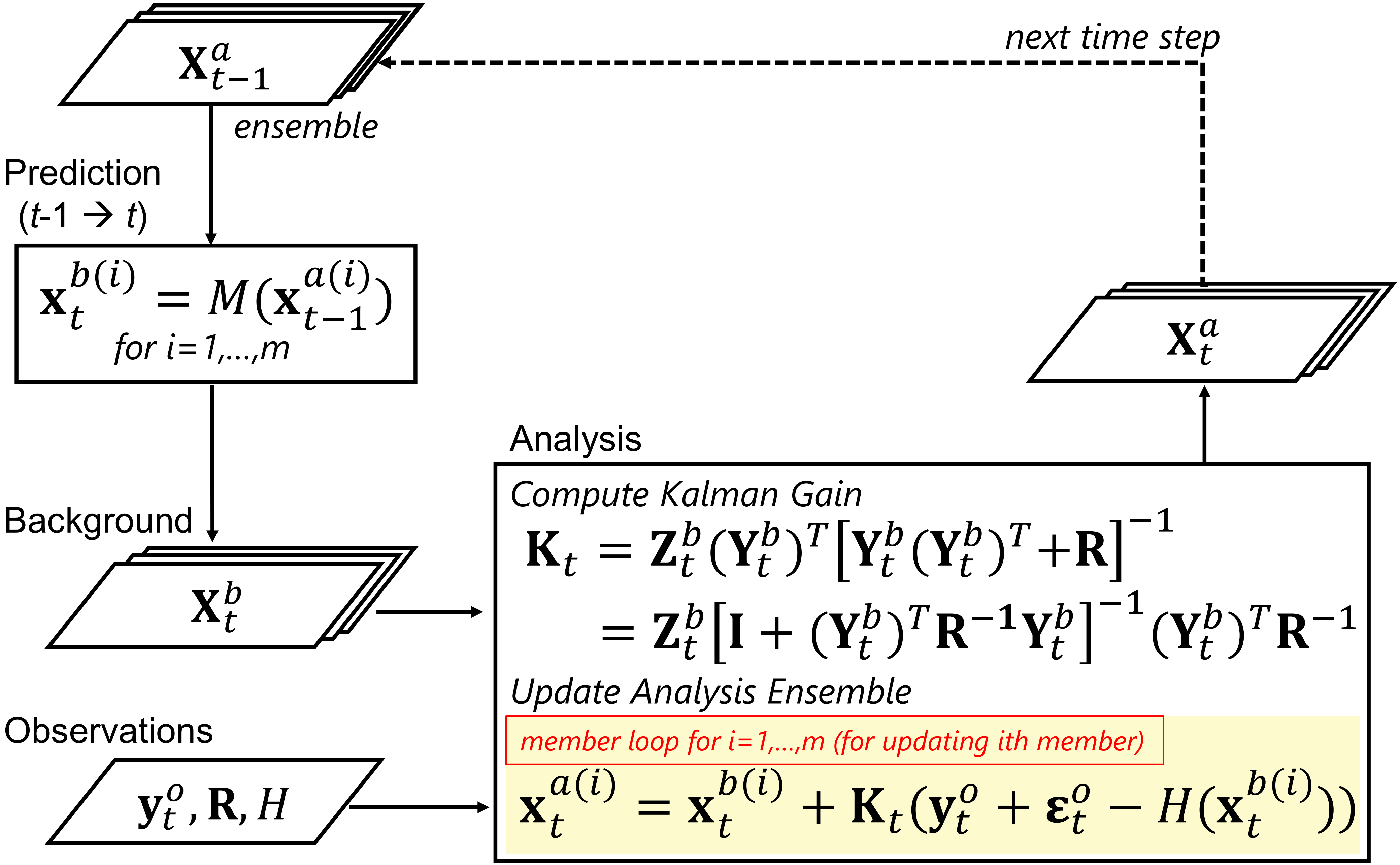
Analysis error covariance is underestimated if without perturbation!

Burgers et al. (1998)

Analysis error covariance should be (cf. 4th lecture)

$$\mathbf{P}_t^a = (\mathbf{I} - \mathbf{K}\mathbf{H})\mathbf{P}_t^b(\mathbf{I} - \mathbf{K}\mathbf{H})^T + \mathbf{K}\mathbf{R}\mathbf{K}^T$$

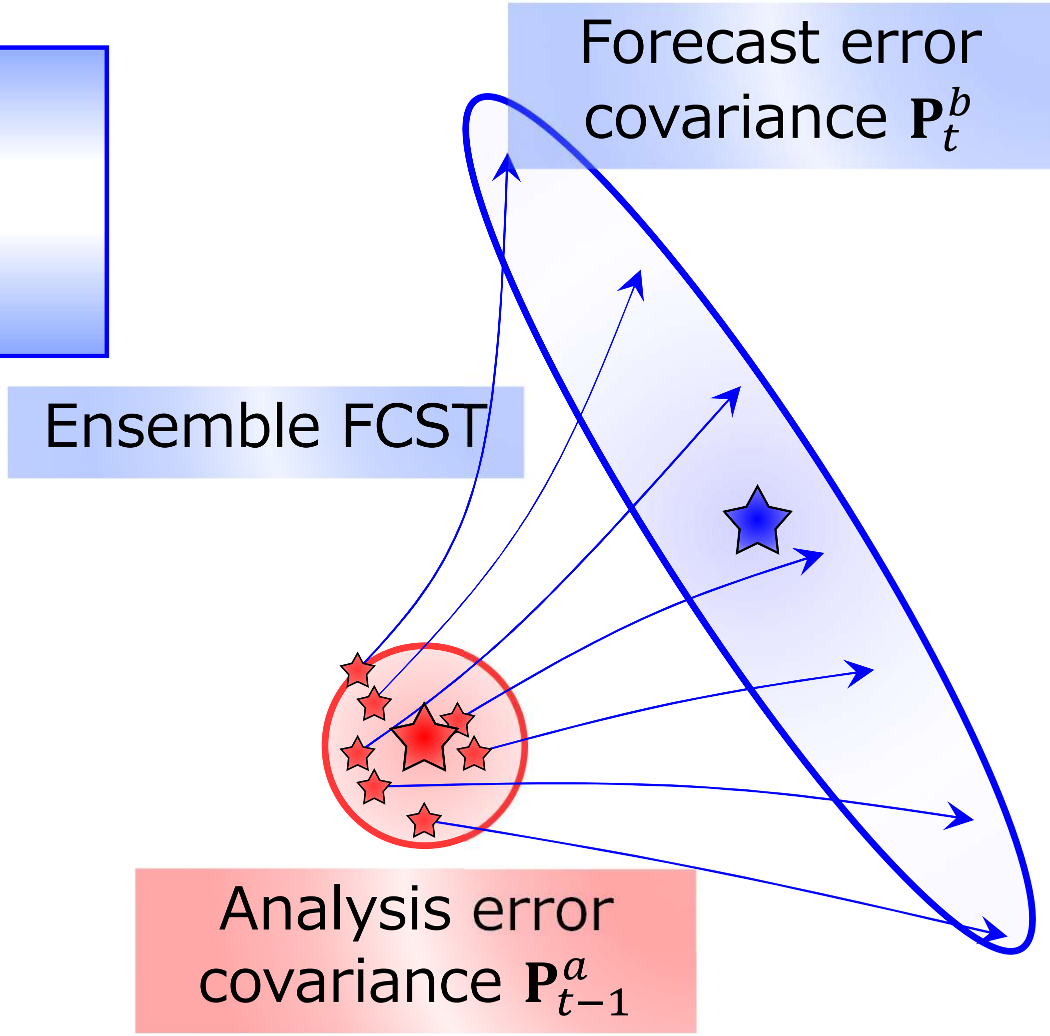
EnKF (PO) Algorithm



Ensemble Kalman Filter

$$\mathbf{X}_t^b = M(\mathbf{X}_{t-1}^a)$$

$$\mathbf{P}_t^b = \mathbf{Z}_t^b \left(\mathbf{Z}_t^b\right)^T$$



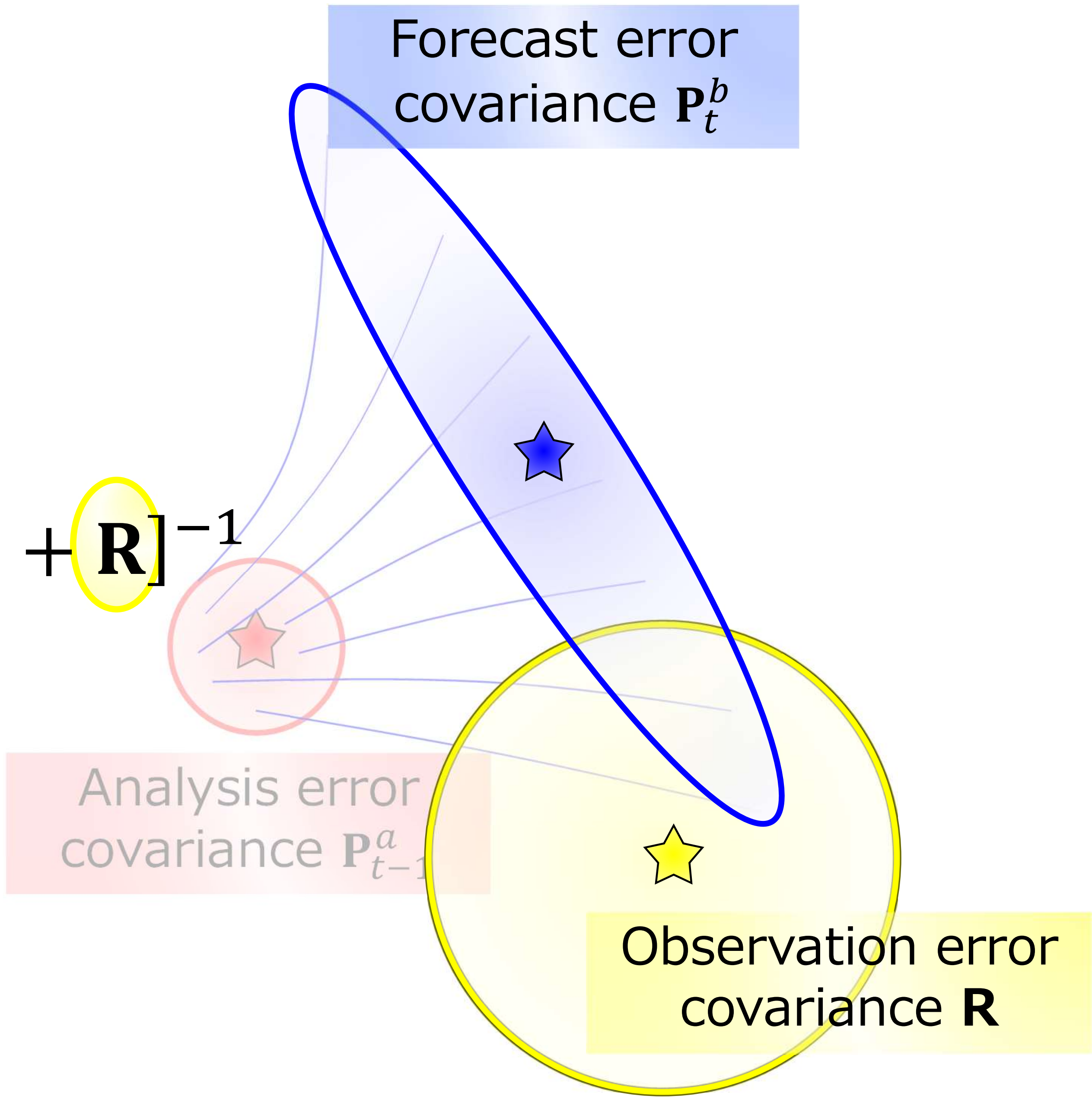
$$\mathbf{Z}_t^b = \delta \mathbf{X}_t^b / \sqrt{m-1}$$

Ensemble Kalman Filter

$$\mathbf{X}_t^b = M(\mathbf{X}_{t-1}^a)$$

$$\mathbf{P}_t^b = \mathbf{Z}_t^b(\mathbf{Z}_t^b)^T$$

$$\mathbf{K}_t = \mathbf{P}_t^b\mathbf{H}^T[\mathbf{H}\mathbf{P}_t^b\mathbf{H}^T + \mathbf{R}]^{-1}$$



Ensemble Kalman Filter

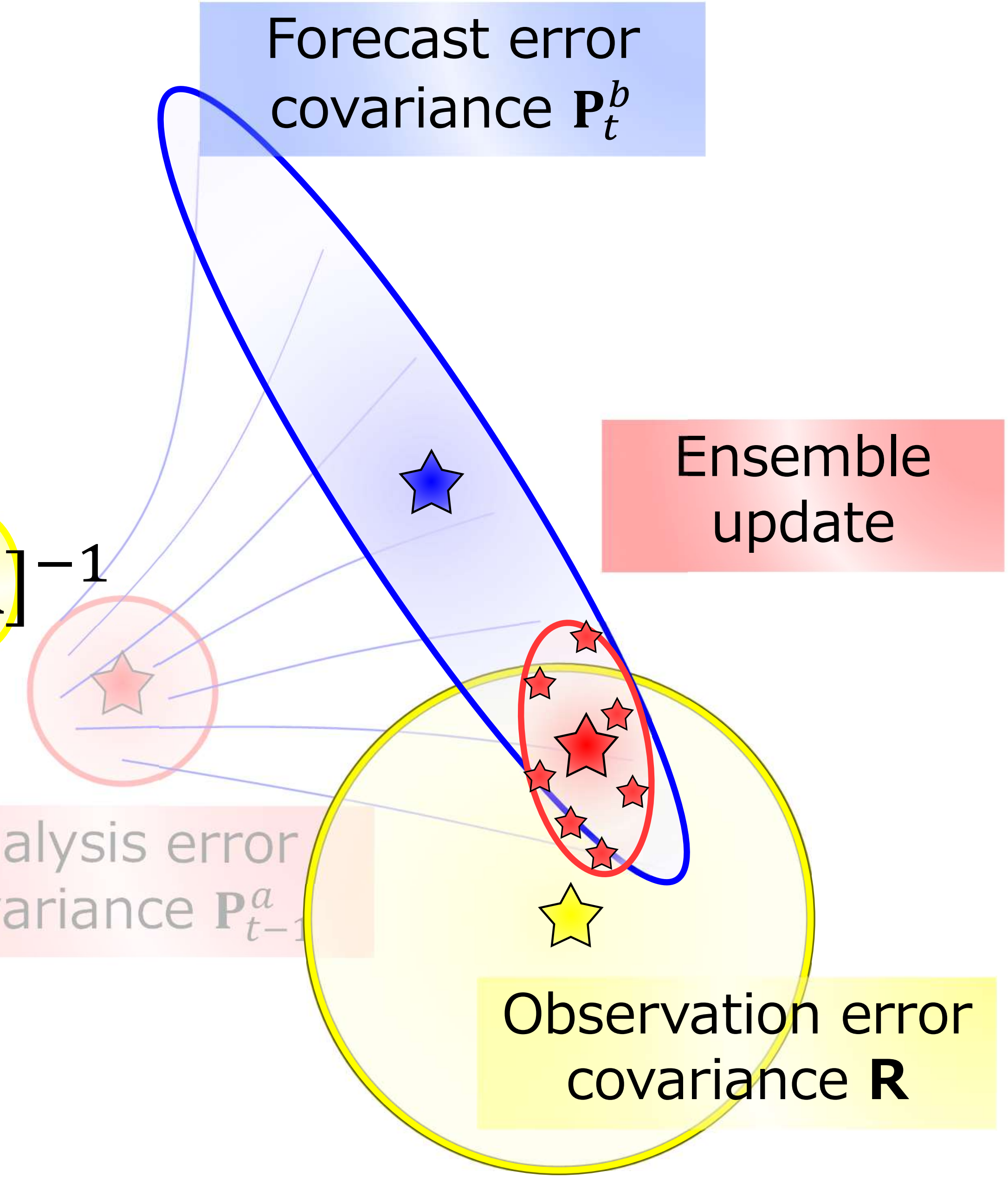
$$\mathbf{X}_t^b = M(\mathbf{X}_{t-1}^a)$$

$$\mathbf{P}_t^b = \mathbf{Z}_t^b(\mathbf{Z}_t^b)^T$$

$$\mathbf{K}_t = \mathbf{P}_t^b\mathbf{H}^T[\mathbf{H}\mathbf{P}_t^b\mathbf{H}^T + \mathbf{R}]^{-1}$$

$$\mathbf{X}_t^a = \mathbf{X}_t^b + \mathbf{K}(\mathbf{y}_t^o - \mathbf{H}\mathbf{X}_t^b)$$

$$\mathbf{P}_t^a = \mathbf{Z}_t^a(\mathbf{Z}_t^a)^\mathrm{T}$$



Ensemble Kalman Filter

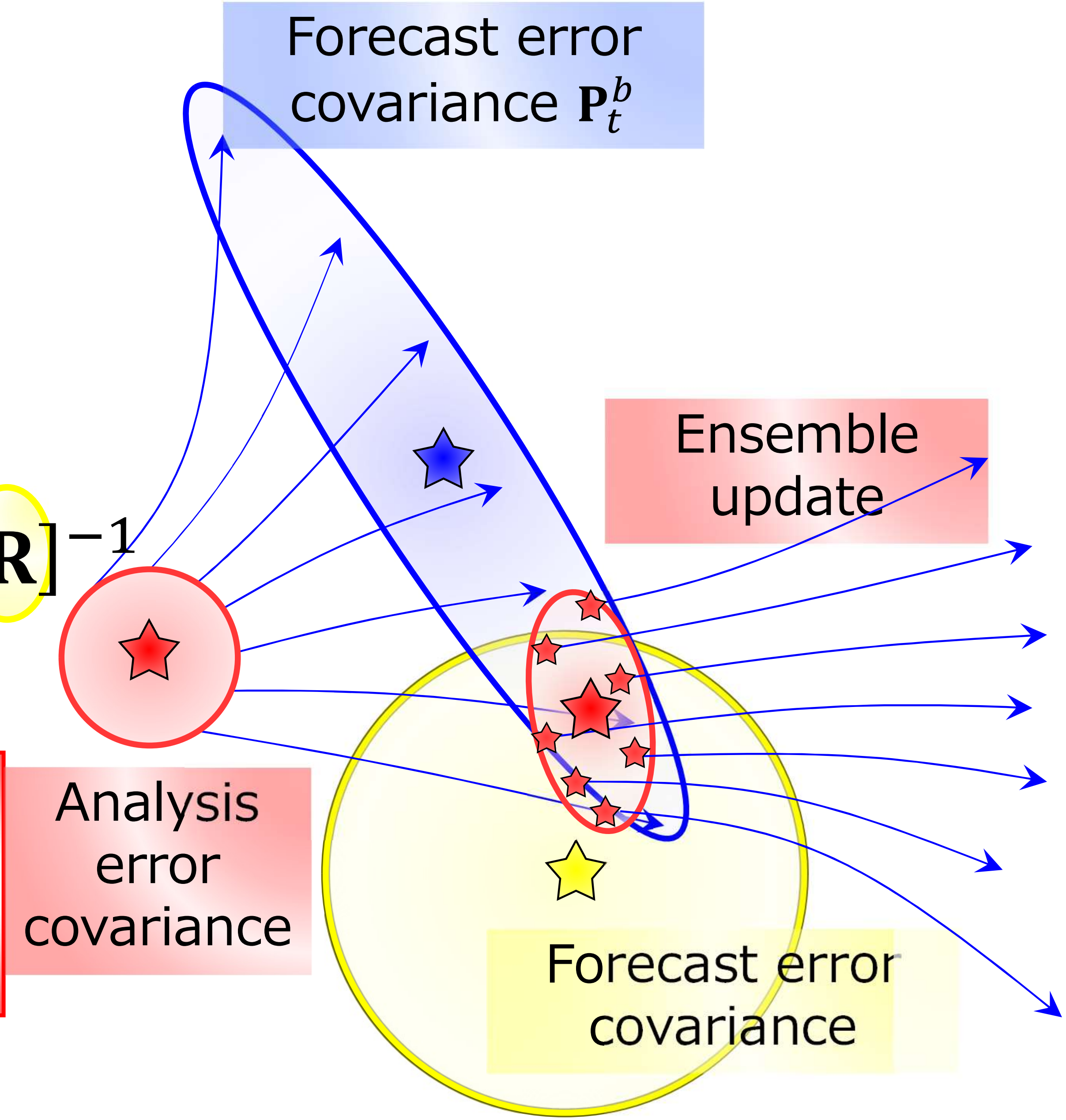
$$\mathbf{X}_t^b = M(\mathbf{X}_{t-1}^a)$$

$$\mathbf{P}_t^b = \delta\mathbf{Z}_t^b\left(\delta\mathbf{Z}_t^b\right)^T$$

$$\mathbf{K}_t = \mathbf{P}_t^b\mathbf{H}^T[\mathbf{H}\mathbf{P}_t^b\mathbf{H}^T + \mathbf{R}]^{-1}$$

$$\mathbf{X}_t^a = \mathbf{X}_t^b + \mathbf{K}(\mathbf{y}_t^o - \mathbf{H}\mathbf{X}_t^b)$$

$$\mathbf{P}_t^a = \mathbf{Z}_t^a(\mathbf{Z}_t^a)^\mathrm{T}$$



Basic Task 5

Basic Task 5

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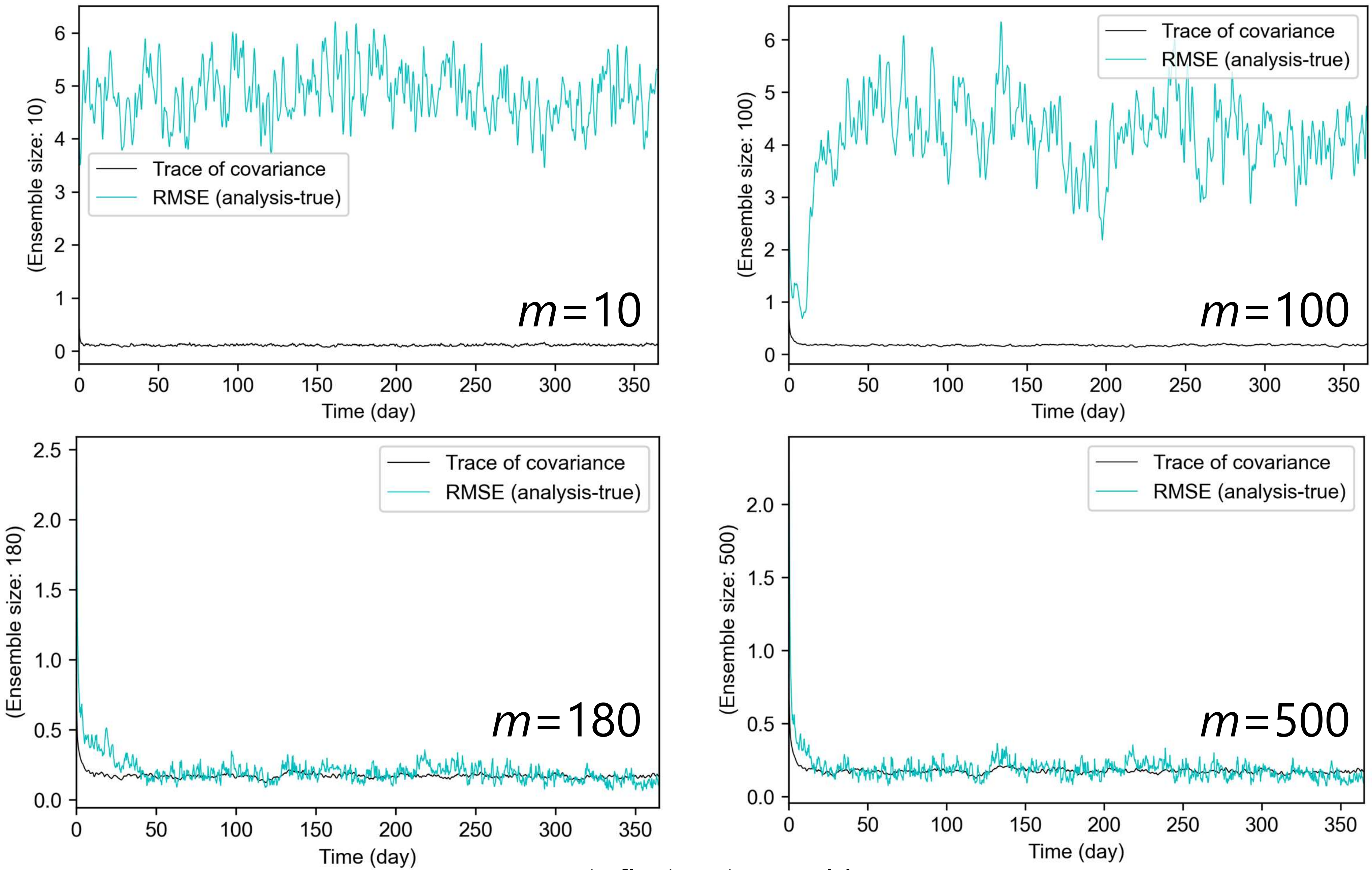
6．EnKF を実装し、KF と比較する。Whitaker and Hamill (2002)による Serial EnSRF, Bishop et al. (2001)による ETKF、Hunt et al. (2007)による LETKF、PO 法などの解法がある。2 つ以上実装すること。

ヒント）気象分野の EnKF では、上述の手法が良く用いられている。カナダでは PO 法、米国気象局では Serial EnSRF、ドイツ・日本では LETKF など。小槻研で研究を進める場合、LETKF を用いた研究をしていくことが想定されるため、LETKF の実装には取り組んで欲しい。

6. Implement EnKF and compare with KF. There are solutions such as Serial EnSRF by Whitaker and Hamill (2002), ETKF by Bishop et al. (2001), LETKF and PO method by Hunt et al. (2007). Implement at least two or more.

Hint) The above methods are often used in EnKF in the meteorological field. PO method in Canada, Serial EnSRF in the US Meteorological Bureau, LETKF in Germany and Japan, etc. When proceeding with research at Kotsuki Lab, it is expected that research using LETKF will be carried out, so I would like you to work on the implementation of LETKF at least.

EnKF (PO) w/o Localization



no inflation is used here

Treatments

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(1) Perturbed Observations

$$\mathbf{x}_t^{a(i)} = \mathbf{x}_t^{b(i)} + \mathbf{K}_t(\mathbf{y}_t^o + \boldsymbol{\varepsilon}_t^{o(i)} - H(\mathbf{x}_t^{b(i)}))$$

for i=1,…,m

this error should be modified so that $\sum_{i=1}^{m} \boldsymbol{\varepsilon}_t^{o(i)} = 0$

$$\Leftrightarrow \bar{\mathbf{x}}_t^a = \bar{\mathbf{x}}_t^b + \mathbf{K}_t(\mathbf{y}_t^o - \overline{H(\mathbf{x}_t^b)})$$

(2) Variance Inflation

$$\mathbf{P}_{inf}^b = (1+\delta)^2 \cdot \mathbf{P}^b$$

$$\Leftrightarrow \delta\mathbf{X}_{inf}^b = (1+\delta) \cdot \delta\mathbf{X}^b$$

(3) Localization

Localization Function

Gaspari Cohn Function

$$r = \frac{d}{\sqrt{10/3}\,\sigma}$$

tuning parameter

$$L(r) = \begin{cases} 1 - \frac{1}{4}r^5 + \frac{1}{2}r^4 + \frac{5}{8}r^3 - \frac{5}{3}r^2 & (r \le 1) \\ \frac{1}{12}r^5 - \frac{1}{2}r^4 + \frac{5}{8}r^3 + \frac{5}{3}r^2 \\ -5r + 4 - \frac{2}{3}r^{-1} & (1 < r \le 2) \\ 0 & (2 < r) \end{cases}$$

d: distance b/w grids
σ: localization length scale

Gaspari and Cohn (1999)

usually used in PO and serial EnSRF

Gaussian Function

$$L(d) = \begin{cases} \exp(-\frac{d^2}{2\sigma^2}) & d < 2\sqrt{10/3}\sigma \\ 0 & else \end{cases}$$

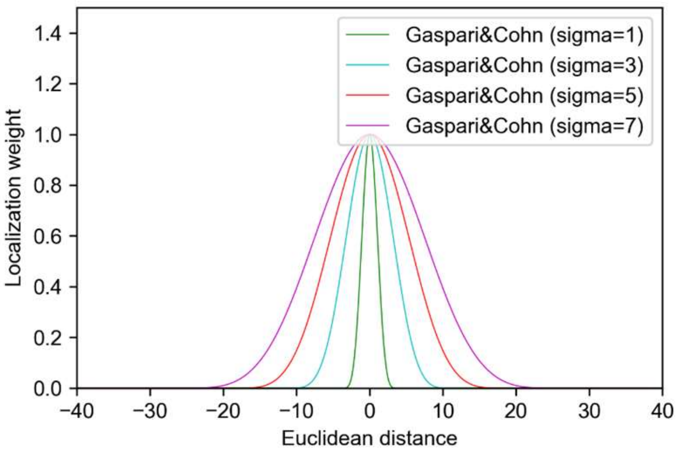
tuning parameter

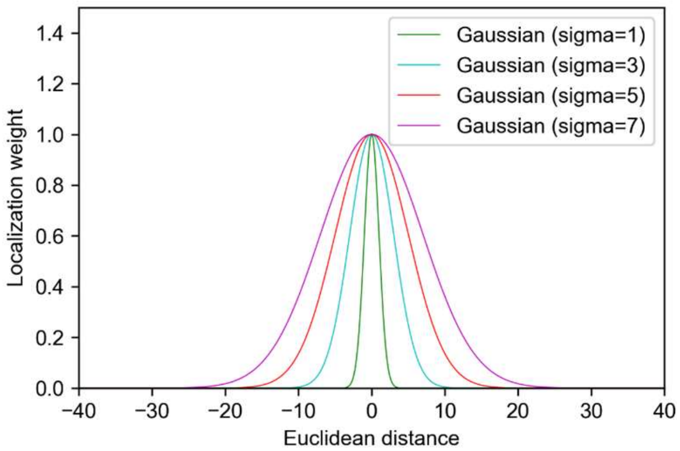
d: distance b/w grids
σ: localization length scale

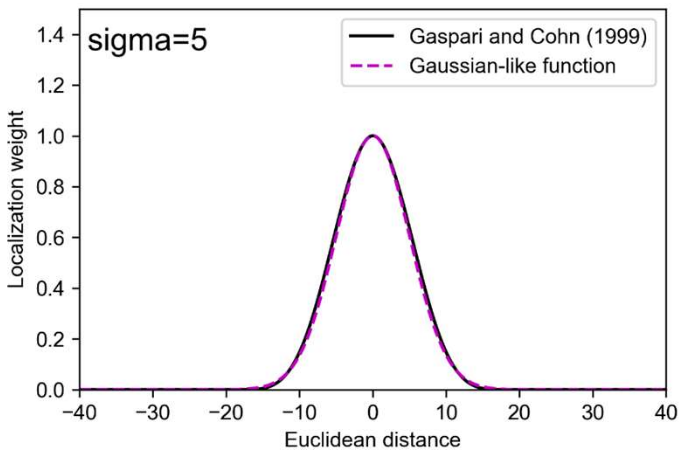
usually used in LETKF

Localization Function

Localization Function

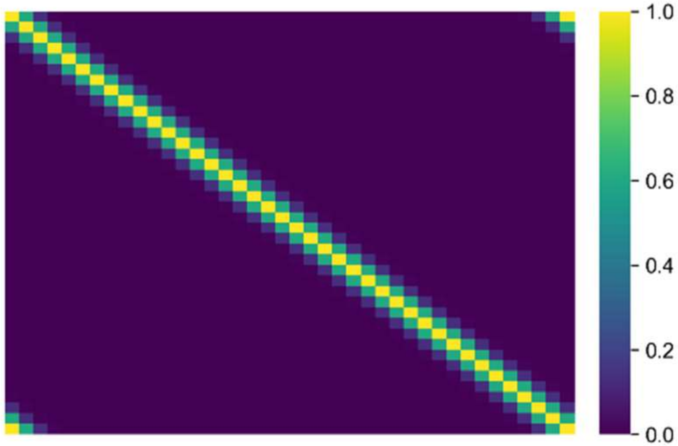




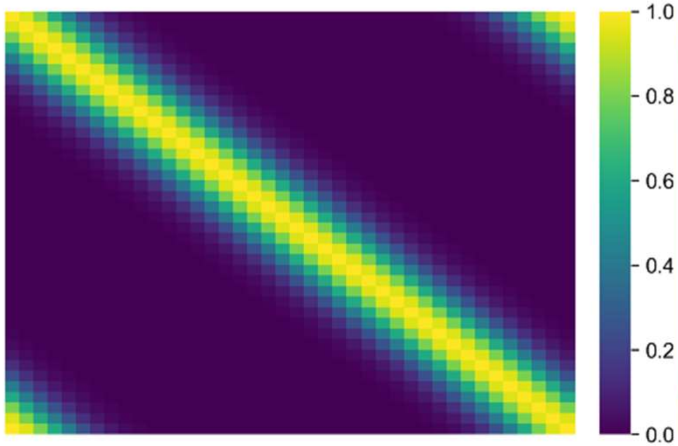


Localization Matrix (Gaussian Function)

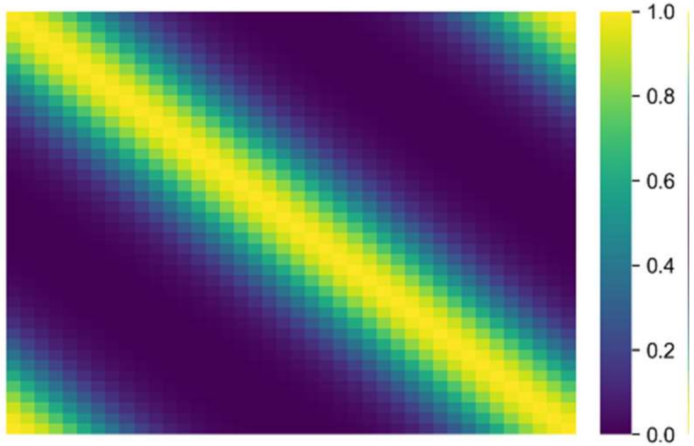
$\sigma = 1$



$\sigma = 3$



$\sigma = 5$



Localization in PO method

Kalman Gain

$$\mathbf{K}_t = \mathbf{Z}_t^b(\mathbf{Y}_t^b)^T\left[\mathbf{Y}_t^b(\mathbf{Y}_t^b)^T + \mathbf{R}\right]^{-1}$$

$$\mathbf{P}_t^b\mathbf{H}^T = \mathbf{L} \circ \mathbf{Z}_t^b(\mathbf{Y}_t^b)^T$$

$\mathbf{L}$ ($\in \mathbb{R}^{n\times p}$) : Localization Matrix

$\circ$: Shur product
also known as Hadamard product
or, element-wise product

未解決メモ:
Yb YbT は 局所化掛けなくて良いのか？

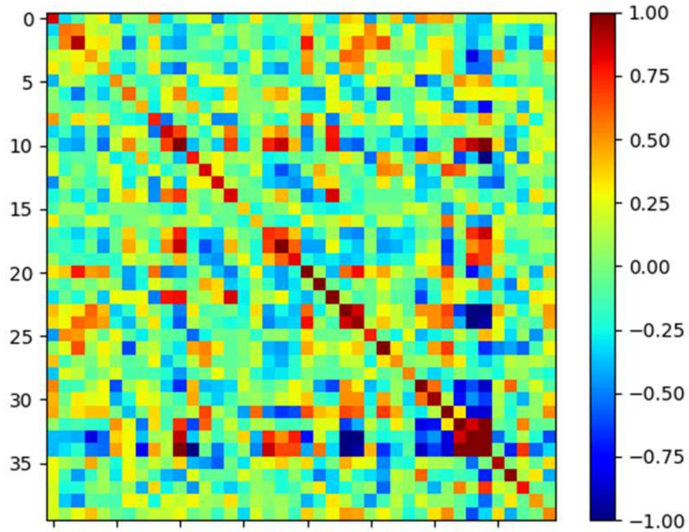
covariance localization (EnKF)

Empirical treatment for
(1) reducing sampling noise
(2) increasing the rank

$$\mathbf{P}^b \rightarrow \mathbf{L} \circ \mathbf{P}^b$$

$\circ$: Schur product

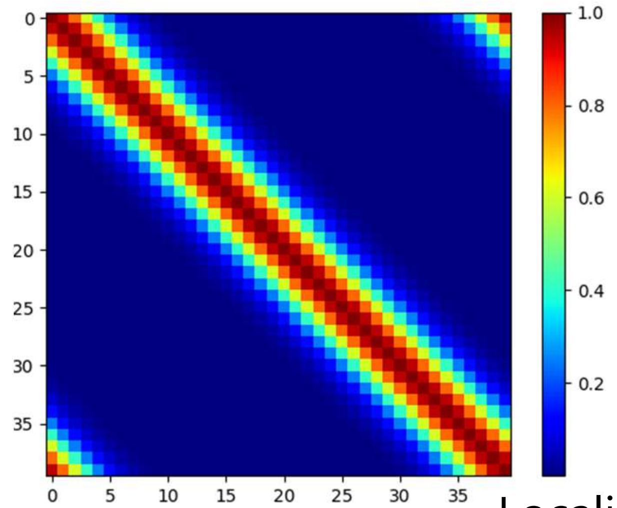
$$\mathbf{P}^b \approx \frac{1}{m-1}\delta\mathbf{X}^b\left(\delta\mathbf{X}^b\right)^{\mathrm{T}}$$



Sampled error covariance
(ensemble approximation)

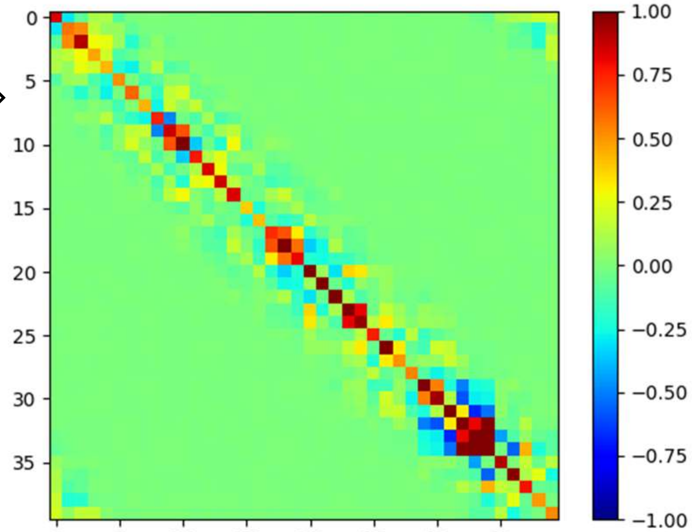
localization

$\mathbf{L}$



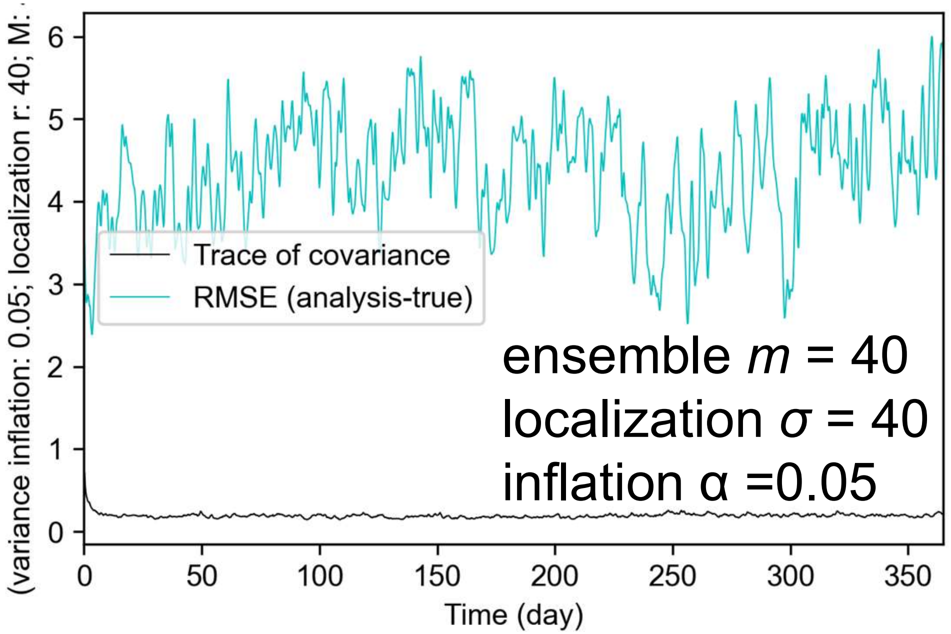
Localization Function

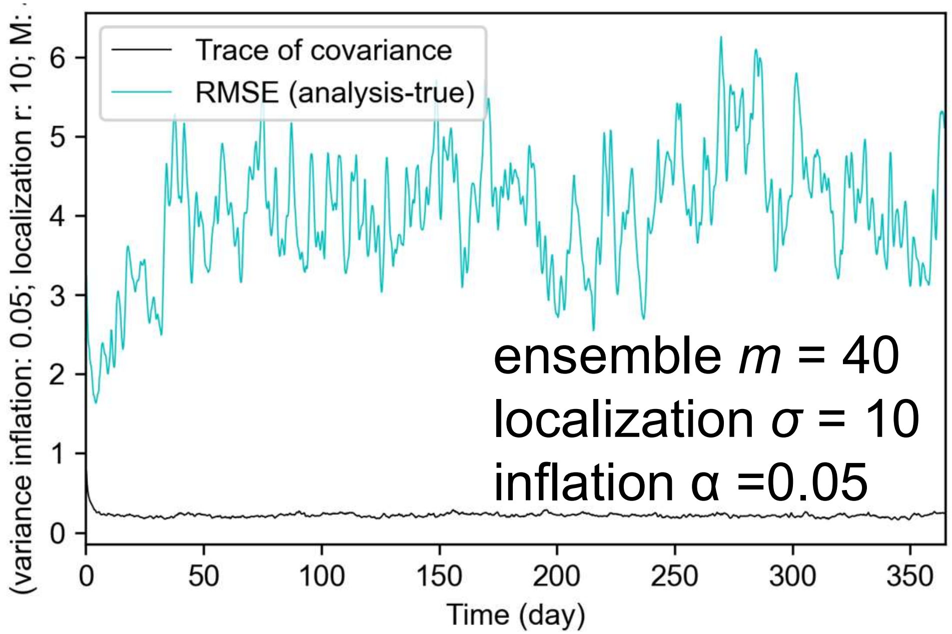
$$\mathbf{L} \circ \mathbf{P}^b$$

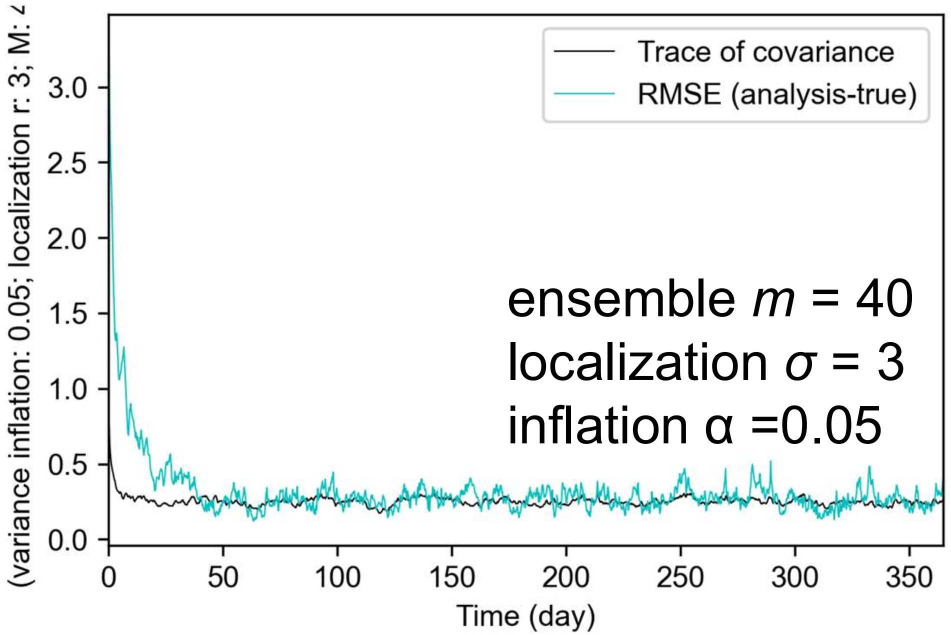


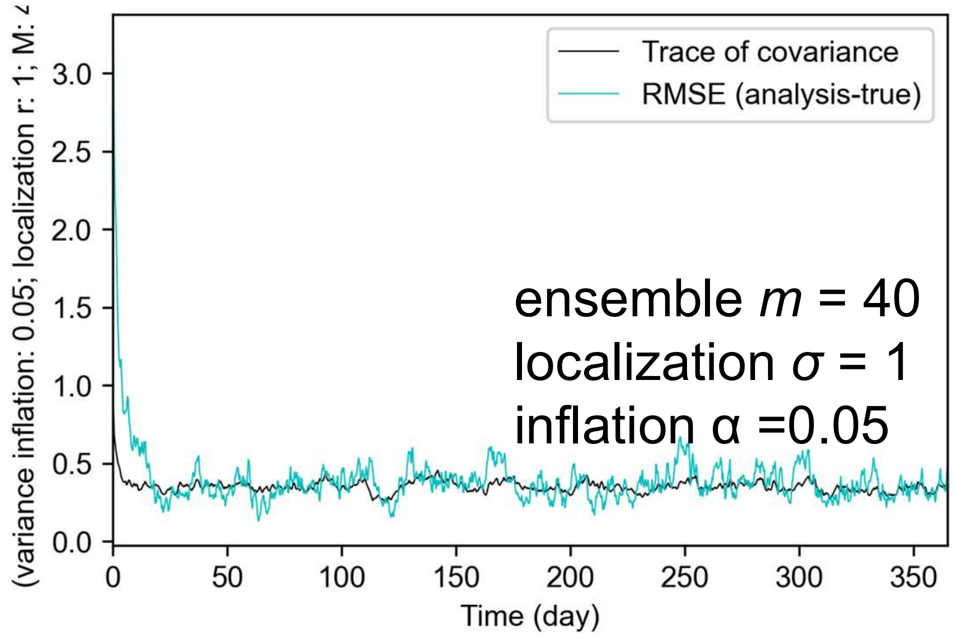
Error Cov. w/ Localization

EnKF (PO) w/ Localization









Thank you for your attention!

Presented by Shunji Kotsuki
(shunji.kotsuki@chiba-u.jp)

Further information is available at
https://kotsuki-lab.com/

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