Data Assimilation
- 8. LETKF -

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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

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- **Lecture: LETKF**
  - to introduce ETKF
  - to introduce LETKF
- **Training: Lorenz 96**
  - to implement LETKF into L96

Ensemble Kalman Filter (EnKF)

KF

EnKF

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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

Ensemble Prediction (state)

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

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)

Square Root Filter (SRF)

SRF assumes the following update w/o adding perturbation in obs.

$$\mathbf{Z}_t^a = \mathbf{Z}_t^b \mathbf{W}$$

$\mathbf{W}$ ($\in \mathbb{R}^{m\times m}$): Ensemble Ptb. Transform Matrix

and compute **W** that satisfies

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

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

However, SRF cannot determine $\mathbf{W}$ deterministically.
For example, for $\mathbf{U}$ that satisfies $\mathbf{U}\mathbf{U}^T = \mathbf{I}$,
a new matrix $\mathbf{S} = \mathbf{W}\mathbf{U}$ can be also a ptb. transform matrix since

$$\mathbf{P}_t^a = \mathbf{Z}_t^b \mathbf{W} (\mathbf{Z}_t^b \mathbf{W})^T = \mathbf{Z}_t^b \mathbf{W}\mathbf{U} (\mathbf{Z}_t^b \mathbf{W}\mathbf{U})^T = \mathbf{Z}_t^b \mathbf{S} (\mathbf{Z}_t^b \mathbf{S})^T$$

Question: how can we determine **W**?

Ensemble Transform Kalman Filter

Data Assimilation

model space

$\mathbf{P}^b$

$\mathbf{P}^a$

projection

$\mathbf{H}$

observation space

$\mathbf{R}$

standard Kalman filter

Kalman Gain

$$\mathbf{K} = \mathbf{P}^b\mathbf{H}^T\left(\mathbf{H}\mathbf{P}^b\mathbf{H}^T + \mathbf{R}\right)^{-1} = \mathbf{P}^a\mathbf{H}^T\mathbf{R}^{-1}$$

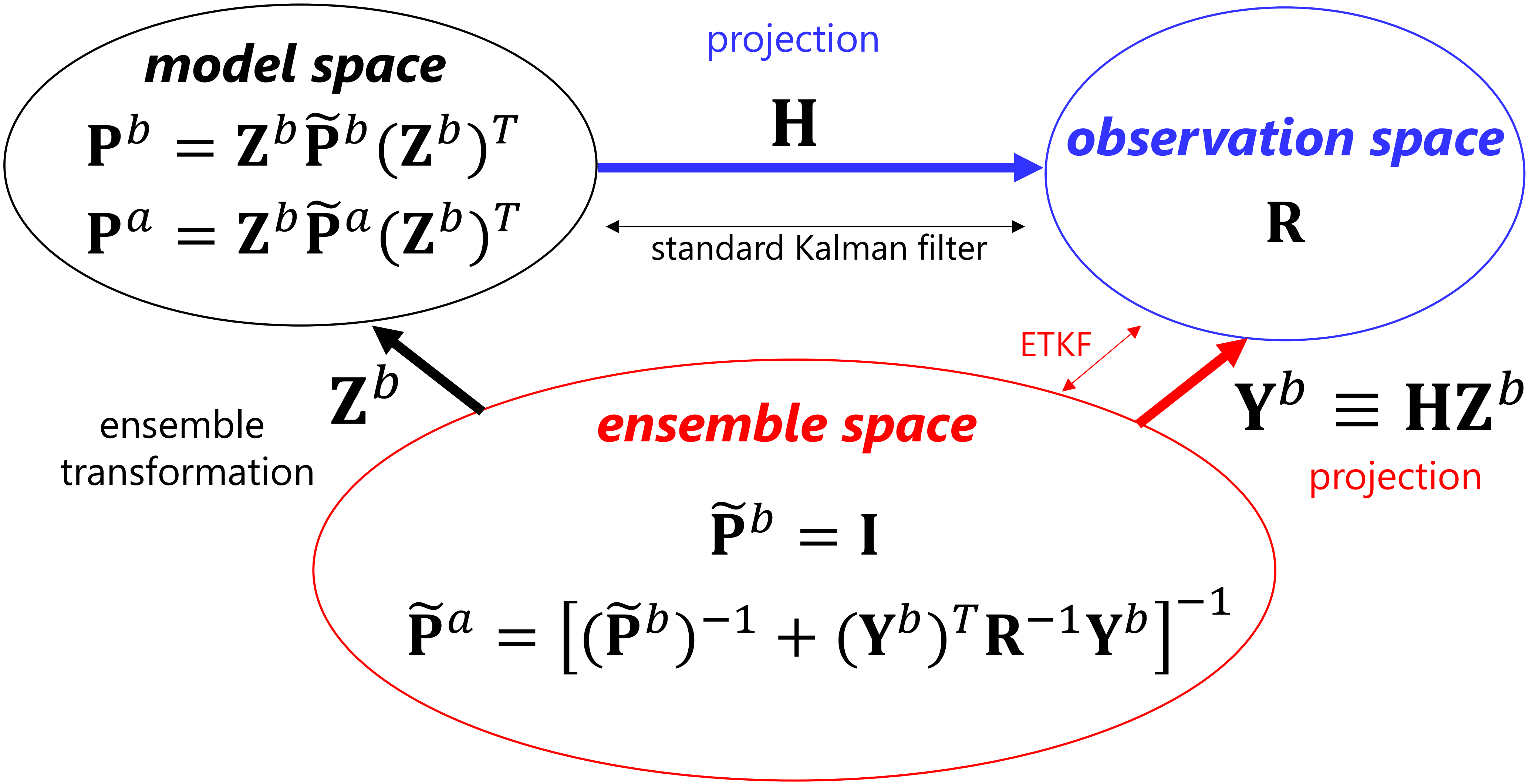
Analysis Error Covariance

$$\mathbf{P}^a = (\mathbf{I} - \mathbf{K}\mathbf{H})\mathbf{P}^b \Leftrightarrow (\mathbf{P}^a)^{-1} = (\mathbf{P}^b)^{-1} + \mathbf{H}^T\mathbf{R}^{-1}\mathbf{H}$$

Analysis Update Equation

$$\mathbf{x}^a = \mathbf{x}^b + \mathbf{K}\mathbf{d}^{o-b} = \mathbf{P}^a\left[(\mathbf{P}^b)^{-1}\mathbf{x}^b + \mathbf{H}^T\mathbf{R}^{-1}\mathbf{y}^o\right]$$

Ensemble Transform KF



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

Bishop et al. (2001; MWR)
Figure adopted from Kotsuki et al. (2020; QJRMS)

ETKF (Ens. Trans. KF)

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ETKF considers (m-1)-dimensional subspace (ensemble space) spanned by $\mathbf{Z}^b$

$$\mathbf{P}^b = \mathbf{Z}^b \widetilde{\mathbf{P}}^b \left(\mathbf{Z}^b\right)^T \qquad \mathbf{P}^a = \mathbf{Z}^b \widetilde{\mathbf{P}}^a \left(\mathbf{Z}^b\right)^T$$

① Background Error Cov.

$$\mathbf{P}^b = \frac{1}{m-1}\mathbf{X}^b\left(\mathbf{X}^b\right)^T \quad \Rightarrow \quad \widetilde{\mathbf{P}}^b = \mathbf{I}$$

② Analysis Error Cov.

$$\mathbf{P}^a = \frac{1}{m-1}\mathbf{X}^a\left(\mathbf{X}^a\right)^T \quad \Rightarrow \quad \mathbf{Z}^a = \underline{\mathbf{Z}^b\left[\widetilde{\mathbf{P}}^a\right]}^{1/2}$$

③ Analysis Increment

$$\delta\bar{\mathbf{x}}^a = \mathbf{K}\mathbf{d}^{o-b} = \mathbf{P}^a\mathbf{H}^T\mathbf{R}^{-1}\mathbf{d}^{o-b}$$
$$= \underline{\mathbf{Z}^b\widetilde{\mathbf{P}}^a\left(\mathbf{Y}^b\right)^T\mathbf{R}^{-1}\mathbf{d}^{o-b}}$$

④ Analysis Equation

$$\left(\widetilde{\mathbf{P}}^a\right)^{-1} = \left(\widetilde{\mathbf{P}}^b\right)^{-1} + \left(\mathbf{Y}^b\right)^T\mathbf{R}^{-1}\mathbf{Y}^b$$
$$\Leftrightarrow \widetilde{\mathbf{P}}^a = \left[\mathbf{I} + \left(\mathbf{Y}^b\right)^T\mathbf{R}^{-1}\mathbf{Y}^b\right]^{-1}$$

$$\mathbf{Y}^b \equiv \mathbf{H}\mathbf{Z}^b$$

Eigenvalue Decomposition

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A World Beyond Predictions

Analysis Equations

mean $\delta\bar{\mathbf{x}}^a = \mathbf{Z}^b\widetilde{\mathbf{P}}^a\left(\mathbf{Y}^b\right)^T\mathbf{R}^{-1}\mathbf{d}^{o-b} = \mathbf{Z}^b\mathbf{w}$

perturbation $\mathbf{Z}^a = \mathbf{Z}^b\left(\widetilde{\mathbf{P}}^a\right)^{1/2} = \mathbf{Z}^b\mathbf{W}$

$\mathbf{w} \in \mathbb{R}^m$: weight vector
$\mathbf{W} \in \mathbb{R}^{m\times m}$: weight matrix

Eigenvalue Decomposition

$$\left(\widetilde{\mathbf{P}}^a\right)^{-1} = \boxed{\mathbf{I} + \left(\mathbf{Y}^b\right)^T\mathbf{R}^{-1}\mathbf{Y}^b = \mathbf{\Lambda}\mathbf{D}\mathbf{\Lambda}^T}$$

$$\Rightarrow \widetilde{\mathbf{P}}^a = \mathbf{\Lambda}\mathbf{D}^{-1}\mathbf{\Lambda}^T \;\&$$

$$\Rightarrow \left(\widetilde{\mathbf{P}}^a\right)^{1/2} = \mathbf{\Lambda}\mathbf{D}^{-1/2}\mathbf{\Lambda}^T$$

$\mathbf{\Lambda} \in \mathbb{R}^{m\times m}$: eigenvectors
$\mathbf{D} \in \mathbb{R}^{m\times m}$: eigenvalues (diagonal)

Hunt et al. (2007)'s approach requiring $O(m^3)$

$rank\left(\mathbf{I} + \left(\mathbf{Y}^b\right)^T\mathbf{R}^{-1}\mathbf{Y}^b\right)$ is always m because of adding $\mathbf{I} \in \mathbb{R}^{m\times m}$.

Analysis Update Equation

$$\mathbf{X}^a = \bar{\mathbf{x}}^a \cdot \mathbf{1} + \sqrt{m-1}\,\mathbf{Z}^a$$

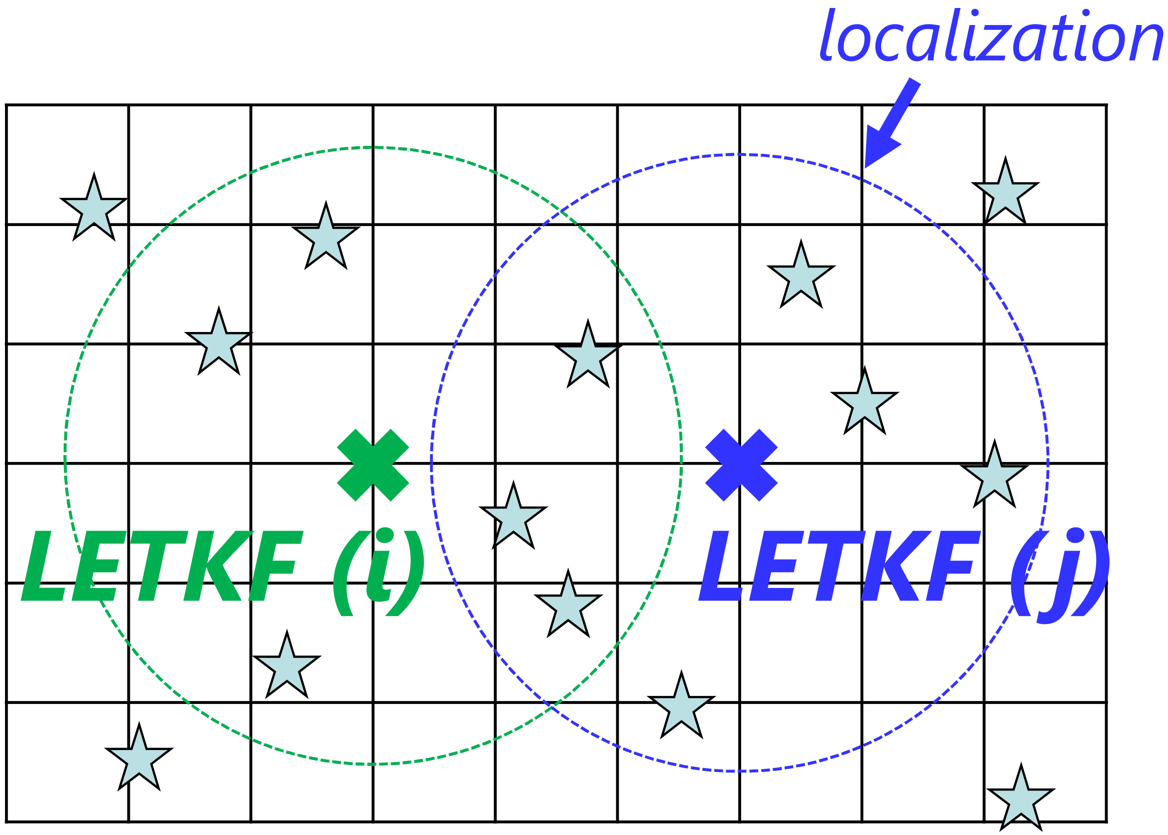
$$= \left(\bar{\mathbf{x}}^b + \mathbf{Z}^b\mathbf{w}\right) \cdot \mathbf{1} + \sqrt{m-1}\,\mathbf{Z}^b\mathbf{W} = \bar{\mathbf{x}}^b \cdot \mathbf{1} + \mathbf{Z}^b\mathbf{T}$$

$\mathbf{1} \equiv [1,1,\ldots,1]$: row vector with ones.
$\mathbf{T} \in \mathbb{R}^{m\times m}$: transform matrix of the ETKF

where $\mathbf{T} \equiv \mathbf{w}\cdot\mathbf{1} + \mathbf{W} = \left[\widetilde{\mathbf{P}}^a\left(\mathbf{Y}^b\right)^T\mathbf{R}^{-1}\mathbf{d}^{o-b}\cdot\mathbf{1} + \sqrt{m-1}\,\left(\widetilde{\mathbf{P}}^a\right)^{1/2}\right]$

ETKF → LETKF (Local ETKF)

Adopted from
Kotsuki et al. (2020; QJRMS)



☆ : observations

✖ : analysis grid points of the LETKF

- The LETKF computes the transform matrix **T** at every model grid point by assimilating surrounding obs within a prescribed localization cutoff radius.
- And the LETKF updates analysis ensemble at every model grid point

R-localization

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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

R-localization (to reduce impacts of obs far from anl. grid point)

$$(R_{loc})_{ii} \leftarrow R_{ii}\, L(d)^{-1}$$

Localized obs error variance of ith observation

Localized R is used for

Eigenvalue decomposition $$(\widetilde{\mathbf{P}}^a)^{-1} = \mathbf{I} + \left(\mathbf{Y}^b\right)^T \mathbf{R}_{loc}^{-1} \mathbf{Y}^b = \mathbf{\Lambda} \mathbf{D} \mathbf{\Lambda}^T$$

mean update equation $$\delta\bar{\mathbf{x}}^a = \mathbf{Z}^b \widetilde{\mathbf{P}}^a \left(\mathbf{Y}^b\right)^T \mathbf{R}_{loc}^{-1} \mathbf{d}^{o-b}$$

Symmetric Square Root

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SRF including ETKF assumes the following update equation.

$$\mathbf{Z}_t^a = \mathbf{Z}_t^b \mathbf{W}$$

We cannot determine **W** uniquely

Symmetric Square Root

The symmetric square root matric $(\widetilde{\mathbf{P}}^a)^{1/2}$ can be determined deterministically!

$$\mathbf{Z}^a = \mathbf{Z}^b (\widetilde{\mathbf{P}}^a)^{1/2}$$ where $$(\widetilde{\mathbf{P}}^a)^{1/2} = \mathbf{\Lambda} \mathbf{D}^{-1/2} \mathbf{\Lambda}^T$$

Importance

- Since the LETKF generates analysis ens. perturbations as $\mathbf{Z}^a = \mathbf{Z}^b \mathbf{W}$ at all model grid points independently, the smooth transition of **W** in space is essential not to produce imbalanced analysis ensemble. The symmetric of $\mathbf{W} = (\widetilde{\mathbf{P}}^a)^{1/2}$ ensures a spatially smooth transition of $(\widetilde{\mathbf{P}}^a)^{1/2}$ from one grid point to the next (Hunt et al. 2007).
- The symmetric square root matrix also ensures the analysis ensemble perturbations are consistent with the background ensemble perturbations because it minimizes the mean square distance b/w $(\widetilde{\mathbf{P}}^a)^{1/2}$ and $\mathbf{I}$.

Kotsuki and Bishop (2021)

Characteristics

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$$\left(\widetilde{\mathbf{P}}^a\right)^{-1} = \left[\mathbf{I} + \left(\mathbf{Y}^b\right)^T \mathbf{R}^{-1}\mathbf{Y}^b\right] = \mathbf{\Lambda}\mathbf{D}\mathbf{\Lambda}^T$$

Eigenvalue decomposition

$$\mathbf{Z}^a = \mathbf{Z}^b\left(\widetilde{\mathbf{P}}^a\right)^{1/2} = \mathbf{Z}^b\mathbf{W}$$

$$\left(\widetilde{\mathbf{P}}^a\right)^{1/2} = \mathbf{\Lambda}\mathbf{D}^{-1/2}\mathbf{\Lambda}^T$$

sum of ptb. = 0

$$\sum_{i(j)=1}^{p}\left(\mathbf{Y}^b\right)_{k,i(j)} = 0 \Leftrightarrow \sum_{i(j)=1}^{m}\left[\left(\mathbf{Y}^b\right)^T\mathbf{R}^{-1}\mathbf{Y}^b\right]_{i,j} = 0$$

$$\Leftrightarrow \sum_{i(j)=1}^{m}\left(\widetilde{\mathbf{P}}^a\right)^{-1}_{i,j} = 1 \Leftrightarrow \sum_{i(j)=1}^{m}\left(\widetilde{\mathbf{P}}^a\right)^{1/2}_{i,j} = (1)^{-1/2} \Leftrightarrow \sum_{i(j)=1}^{m}\mathbf{W}_{i,j} = 1$$

$$\left(\widetilde{\mathbf{P}}^a\right)^{-1} = \mathbf{I} + \left(\mathbf{Y}^b\right)^T\mathbf{R}^{-1}\mathbf{Y}^b$$

Posterior perturbation $\mathbf{Z}^a$ is given by linear combination of prior members.

$$\left[\left(\mathbf{Y}^b\right)^T\mathbf{R}^{-1}\mathbf{Y}^b\right]_{i,j} = \sum_{k=1}^{p}\sum_{l=1}^{p}\left(\mathbf{Y}^b\right)_{k,i}\left(\mathbf{R}^{-1}\right)_{k,l}\left(\mathbf{Y}^b\right)_{l,j}$$

LETKF

$\mathbf{X}^a_{t-1}$

ensemble

Prediction (t-1 → t)

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

for i=1,...,m

Background

$\mathbf{X}^b_t$

Observations

$\mathbf{y}^o_t, \mathbf{R}, H$

next time step

$\mathbf{X}^a_t$

Analysis

(1) Preparation Step

$$\mathbf{Z}^b_t, \mathbf{Y}^b_t \equiv \mathbf{H}\mathbf{Z}^b_t, \mathbf{d}^{o-b}_t = \mathbf{y}^o_t - H(\overline{\mathbf{x}}^b_t)$$

(2) Local Analysis

grid loop for i=1,...,n (for updating ith grid points)

(2.1) Eigenvalue Decomposition

$$(\widetilde{\mathbf{P}}^a)^{-1} = \mathbf{I} + \left(\mathbf{Y}^b\right)^T \mathbf{R}^{-1}_{loc}\mathbf{Y}^b = \mathbf{\Lambda}\mathbf{D}\mathbf{\Lambda}^T$$

$$\Rightarrow \widetilde{\mathbf{P}}^a = \mathbf{\Lambda}\mathbf{D}^{-1}\mathbf{\Lambda}^T \;\&\; (\widetilde{\mathbf{P}}^a)^{1/2} = \mathbf{\Lambda}\mathbf{D}^{-1/2}\mathbf{\Lambda}^T$$

(2.2) Update Ensemble

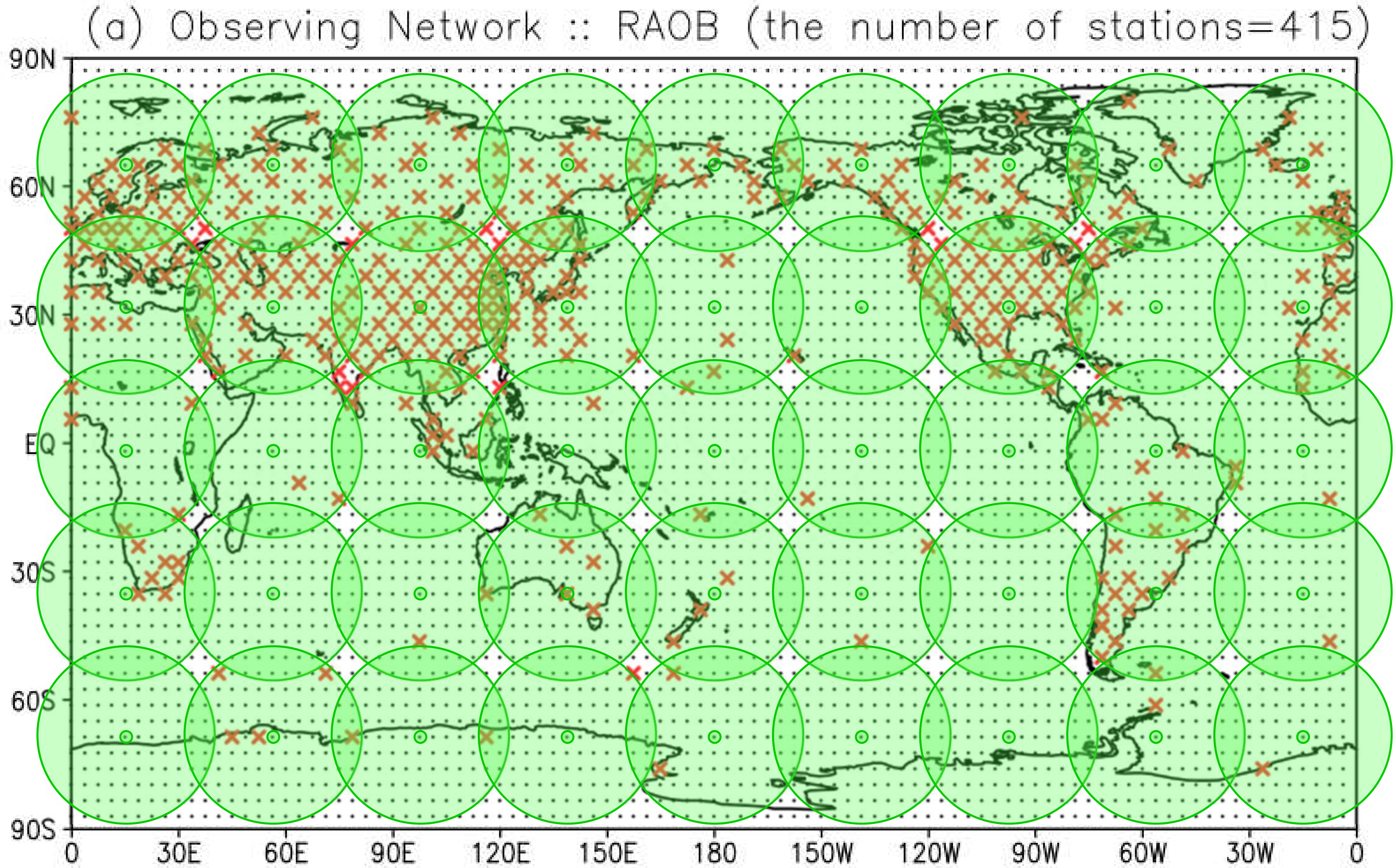
$$\mathbf{X}^a_t = \mathbf{X}^b_t + \mathbf{Z}^b\mathbf{T}$$

$$\mathbf{T} = \left[\widetilde{\mathbf{P}}^a\left(\mathbf{Y}^b_t\right)^T \mathbf{R}^{-1}_{loc}\mathbf{d}^{o-b}_t \cdot \mathbf{1} + \sqrt{m-1}\,(\widetilde{\mathbf{P}}^a)^{1/2}\right]$$

(3) Collect analysis ens of all model grid points to obtain $\mathbf{X}^a_t$ for subsequent forecasts

LETKF

・: model grid points
×: observing station



LETKF can be parallelized for model grid points

Basic Task 5

Basic Task 5

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.

Techniques for LETKF

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Gaussian Function

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

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

tuning parameter

$$(R_{loc})_{ii} \leftarrow R_{ii}\, L(d)^{-1}$$

localized obs error variance of ith observation

Localization

$$\mathbf{X}_t^a = \mathbf{X}_t^b + \mathbf{Z}^b\mathbf{T}$$

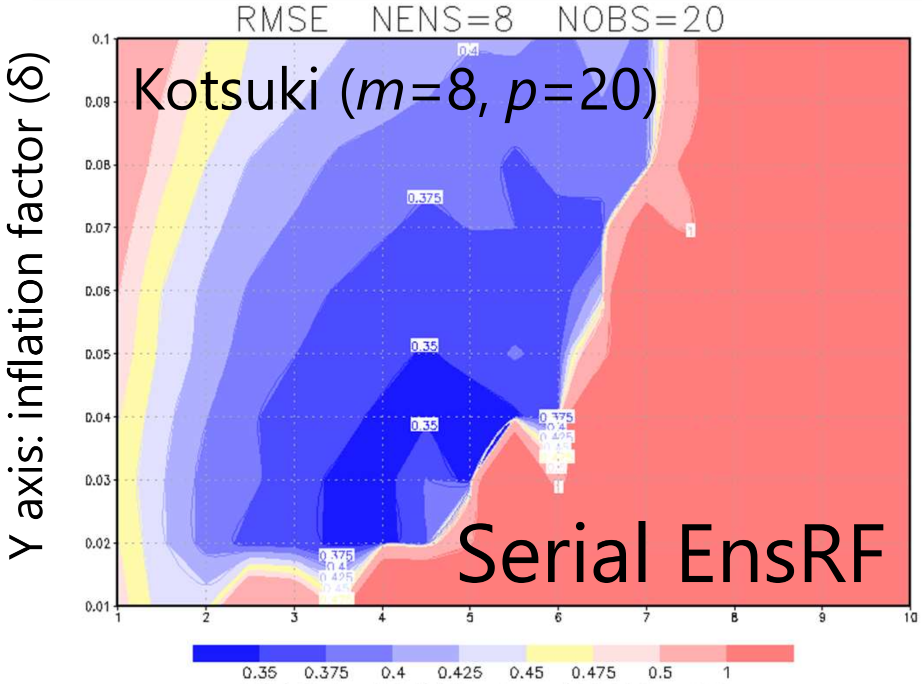
$$\mathbf{T} = \left[\widetilde{\mathbf{P}}^a \left(\mathbf{Y}_t^b\right)^T \mathbf{R}_{loc}^{-1}\mathbf{d}_t^{o-b} \cdot \mathbf{1} + \sqrt{m-1}\,(\widetilde{\mathbf{P}}^a)^{1/2}\right]$$

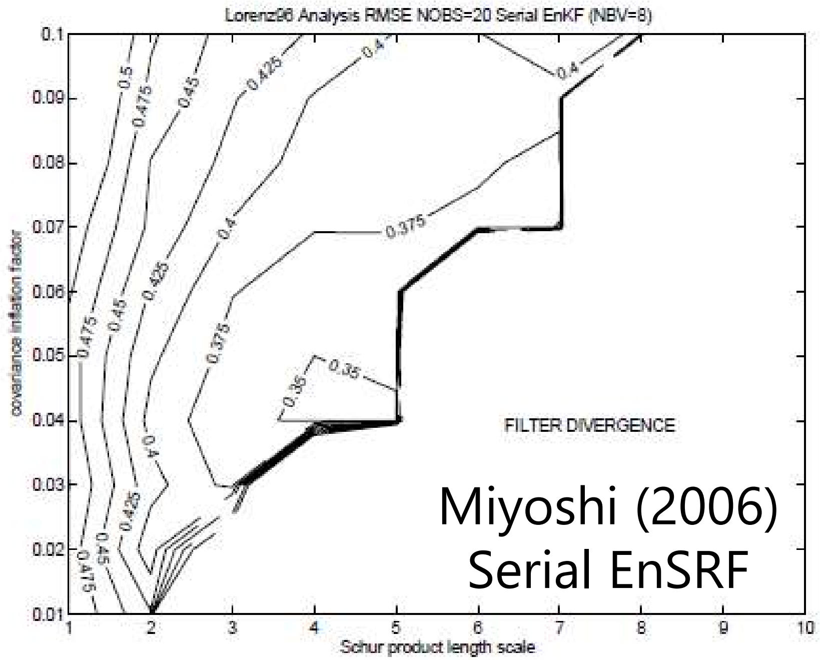
where EVD is solved by $(\widetilde{\mathbf{P}}^a)^{-1} = \mathbf{I} + \left(\mathbf{Y}^b\right)^T \mathbf{R}_{loc}^{-1}\mathbf{Y}^b = \mathbf{\Lambda}\mathbf{D}\mathbf{\Lambda}^T$

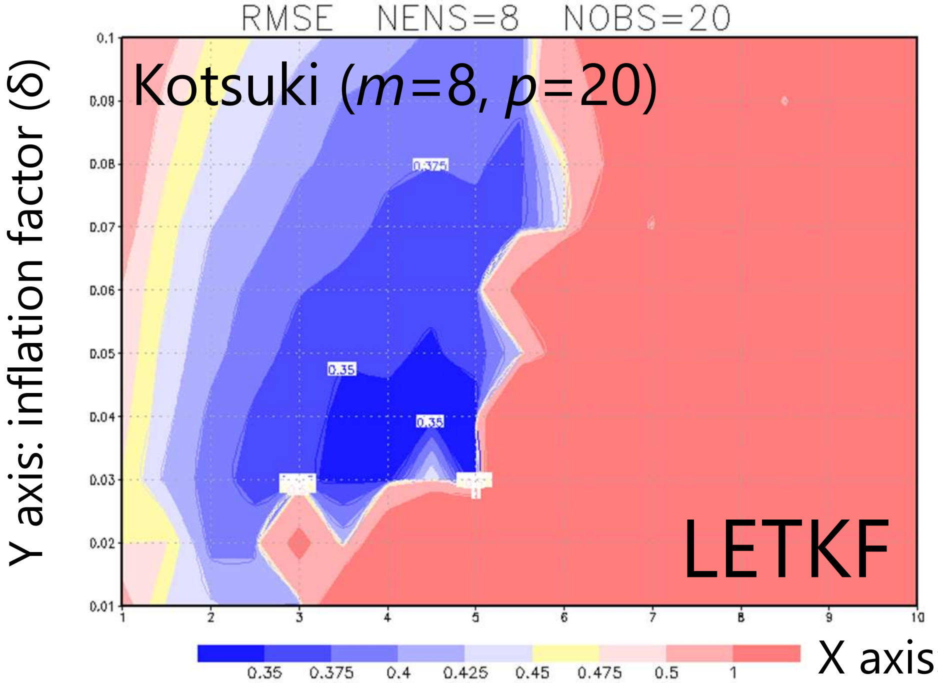
Inflation

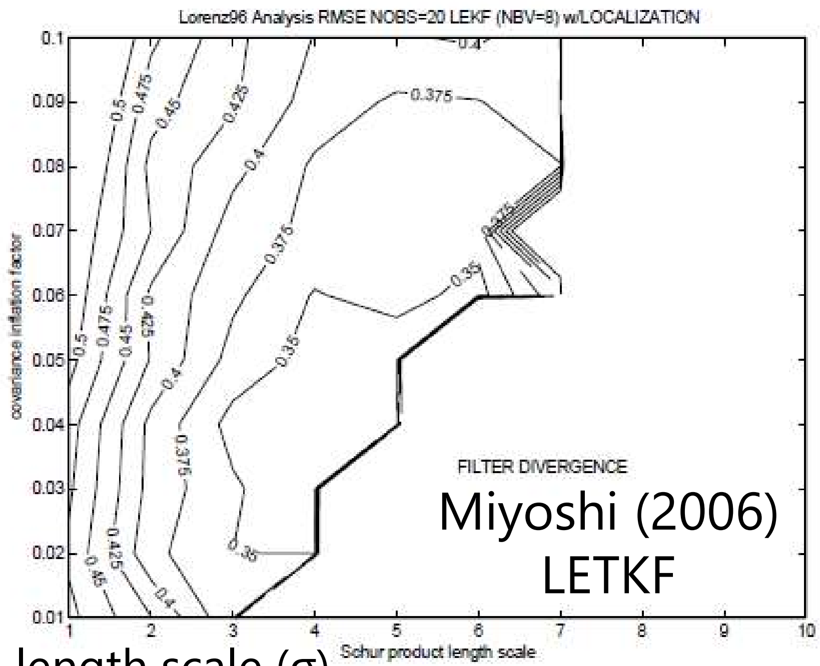
$$\delta\mathbf{X}_{inf}^b = (1+\delta)\delta\mathbf{X}^b$$

Analysis RMSE (Serial EnSRF vs. LETKF)







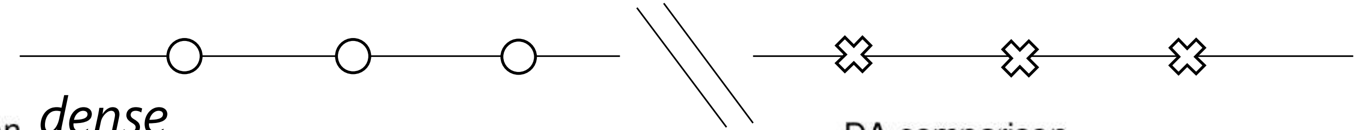


X axis: localization length scale (σ)

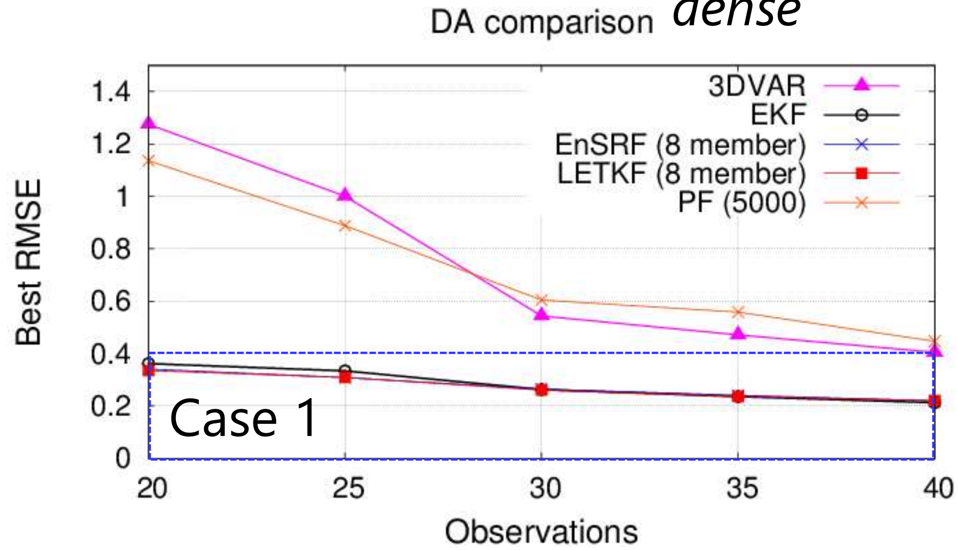
Sensitivity to Obs. Network

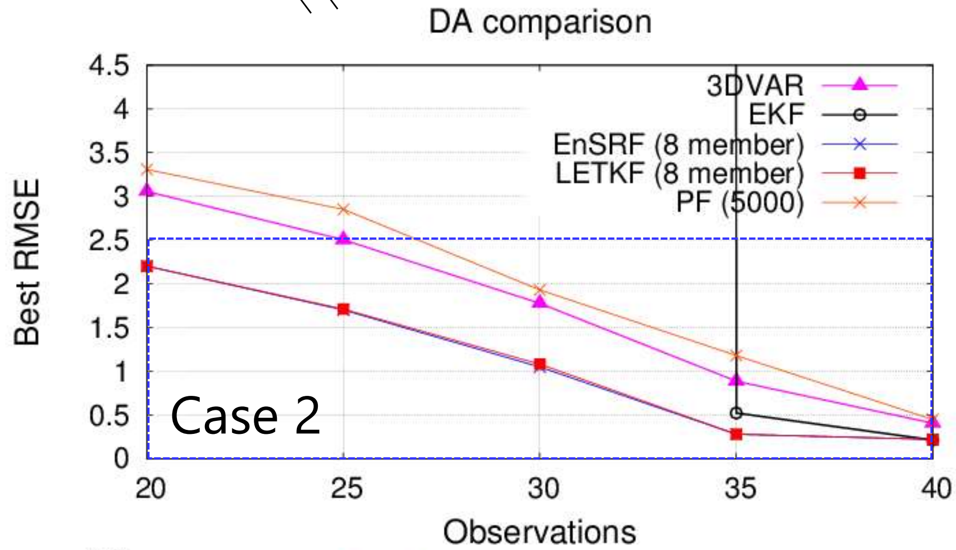
Case 1: Num. Obs. = X 

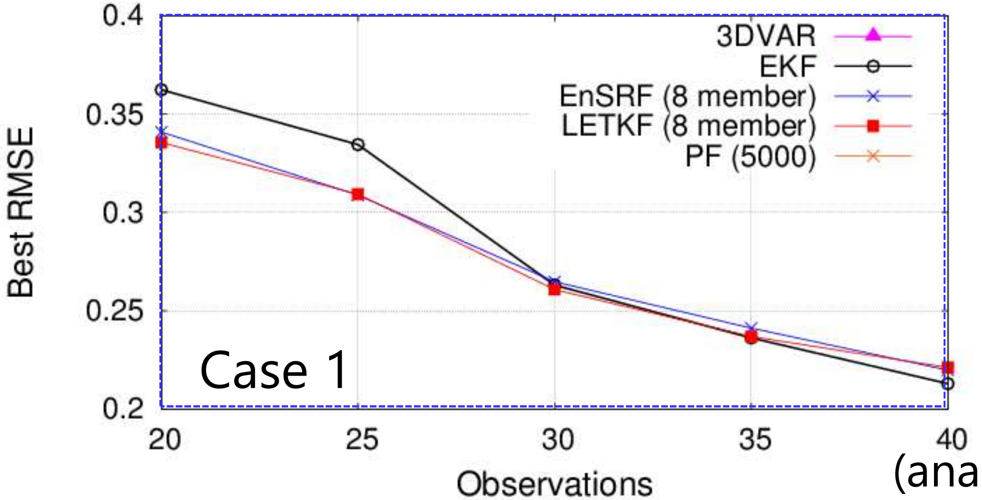
homogeneous

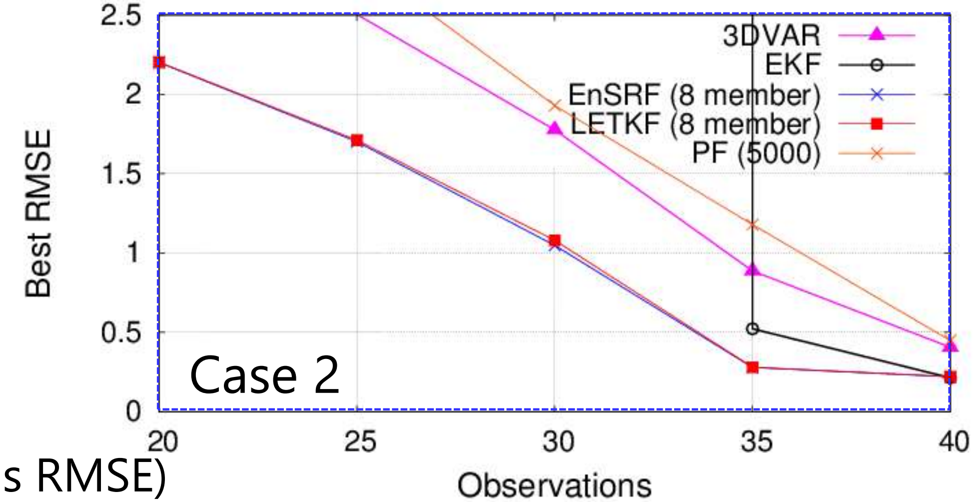
Case 2: Num. Obs. = X 

dense





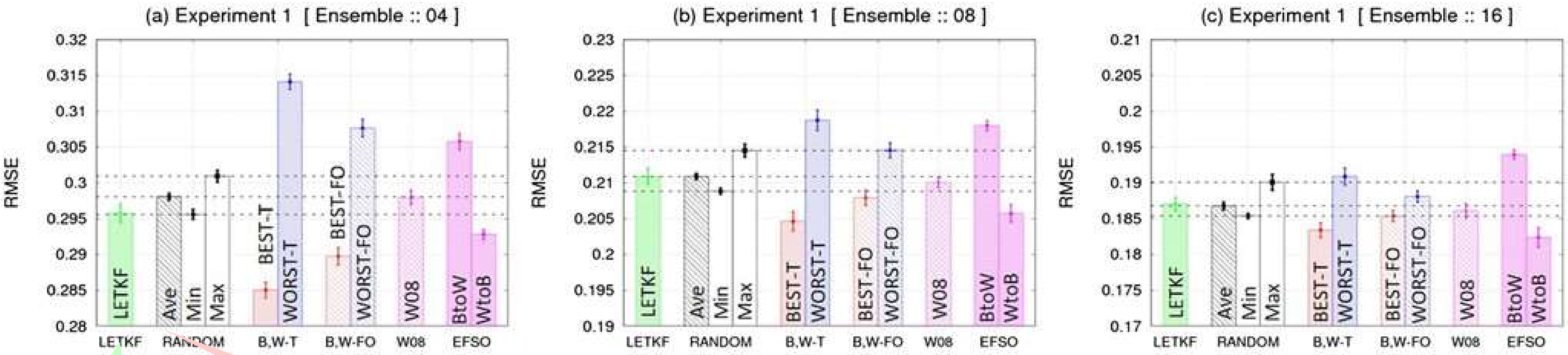




(analysis RMSE)

Kotsuki et al. (2017)

Analysis RMSE with 40 observations w/ L96 (w/ best loc. scale)



LETKF

Serial EnSRF

Kotsuki, S., Greybush, S., and Miyoshi, T. (2017):
Can we optimize the assimilation order in the serial ensemble Kalman filter? A study with the Lorenz-96 model. *Mon. Wea. Rev.*, 145, 4977-4995.

Thank you for your attention!

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

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