Data Assimilation
- A05. 3DVAR and OI -

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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
- (10) Adaptive Inflations
- (11) 4D Variational Method (4DVAR)

Today's goals

- **Lecture**
  - what is the 3D-Var?
  - what is the cost function?
  - maximum likelihood vs. minimum variance
  - how can we get a reasonable **B**?

- **Training Course**
  - to implement 3DVAR
  - hints to develop KF
  - some tips for KF

Review:
Max. Likelihood Estimation

(復習: 最尤推定)

Maximum Likelihood Estimation

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forecast	$x_1 = x^{tru} + \varepsilon_1$	(1) unbias	$\langle x_1 \rangle = \langle x_2 \rangle = x^{tru}$
observation	$x_2 = x^{tru} + \varepsilon_2$	(2) uncorr.	$\langle \varepsilon_1 \varepsilon_2 \rangle = 0$

Likelihood　Prior (uniform, i.e., no prior info)

$$\underbrace{p(x|x_{1,2})}_{\text{Posterior}} = \frac{p(x_{1,2}|x)\,p(x)}{p(x_{1,2})}$$

Bayesian Estimates

constant (since they are given)

$$maximize \quad p(x|x_{1,2}) \Leftrightarrow maximize \quad p(x_{1,2}|x)$$

$$\Leftrightarrow maximize \quad \underline{p(x_1|x) \cdot p(x_2|x)}$$

to maximize likelihood

Maximum Likelihood Estimation

forecast $x_1 = x^{tru} + \varepsilon_1$ (1) unbias $\langle x_1 \rangle = \langle x_2 \rangle = x^{tru}$

observation $x_2 = x^{tru} + \varepsilon_2$ (2) uncorr. $\langle \varepsilon_1 \varepsilon_2 \rangle = 0$

$$maximize \quad p(x_1|x) \cdot p(x_2|x)$$

Suppose x_1 & x_2 follow Gaussian PDF $N(x, \sigma)$

$$p(x_i|x) = \frac{1}{\sqrt{2\pi\sigma_i^2}} \exp\left[-\frac{(x_i - x)^2}{2\sigma_i^2}\right]$$

$$maximize \quad p(x_1|x) \cdot p(x_2|x)$$

$$\Leftrightarrow maximize \quad \frac{1}{\sqrt{2\pi\sigma_1^2}} \frac{1}{\sqrt{2\pi\sigma_2^2}} \exp\left[-\frac{(x_1 - x)^2}{2\sigma_1^2} - \frac{(x_2 - x)^2}{2\sigma_2^2}\right]$$

$$\Leftrightarrow minimize \quad J(x) = \frac{(x_1 - x)^2}{\sigma_1^2} + \frac{(x_2 - x)^2}{\sigma_2^2}$$

Maximum Likelihood Estimation

forecast $x_1 = x^{tru} + \varepsilon_1$

observation $x_2 = x^{tru} + \varepsilon_2$

(1) unbias $\langle x_1 \rangle = \langle x_2 \rangle = x^{tru}$

(2) uncorr. $\langle \varepsilon_1 \varepsilon_2 \rangle = 0$

$$minimize \quad J(x) = \frac{(x_1 - x)^2}{\sigma_1^2} + \frac{(x_2 - x)^2}{\sigma_2^2}$$

$$\frac{\partial J}{\partial x} = -2\frac{(x_1 - x)}{\sigma_1^2} - 2\frac{(x_2 - x)}{\sigma_2^2} = 0$$

analysis of maximum likelihood estimates

$$\boxed{x^a = \frac{\sigma_2^2}{\sigma_1^2 + \sigma_2^2} x_1 + \frac{\sigma_1^2}{\sigma_1^2 + \sigma_2^2} x_2}$$

3DVAR

Assumption & Definition

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Assumption (1) : unbiased error

$$\mathbf{x}^b = \mathbf{x}^{tru} + \boldsymbol{\varepsilon}^b \qquad \langle \boldsymbol{\varepsilon}^b \rangle = 0$$

$$\mathbf{x}^a = \mathbf{x}^{tru} + \boldsymbol{\varepsilon}^a \qquad \langle \boldsymbol{\varepsilon}^a \rangle = 0$$

$$\mathbf{y}^o = \underbrace{\mathbf{y}^{tru}}_{H(\mathbf{x}^{tru})} + \boldsymbol{\varepsilon}^o \qquad \langle \boldsymbol{\varepsilon}^o \rangle = 0$$

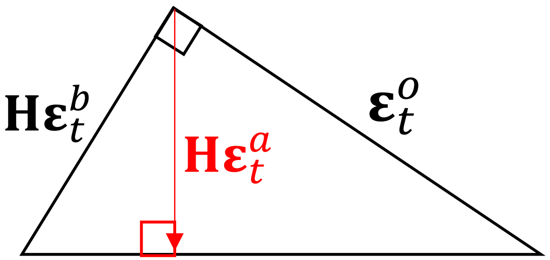
Assumption (2) : uncorrelated error

$$\langle \mathbf{H}\boldsymbol{\varepsilon}_t^b (\boldsymbol{\varepsilon}_t^o)^T \rangle = \langle (\boldsymbol{\varepsilon}_t^o)^T \mathbf{H}\boldsymbol{\varepsilon}_t^b \rangle = 0$$

since background and obs errors are independent

$$\langle \mathbf{H}\boldsymbol{\varepsilon}_t^a (\boldsymbol{\varepsilon}_t^o)^T \rangle \neq 0$$

$$\langle \boldsymbol{\varepsilon}_t^b (\boldsymbol{\varepsilon}_t^a)^T \rangle \neq 0$$



$\mathbf{x}$	model state	$\in \mathbb{R}^n$
$\boldsymbol{\varepsilon}$	error	
$\mathbf{y}$	observation	$\in \mathbb{R}^p$
$M(\,)$	nonlinear model	
$\mathbf{M}$	Jacobian of M	$\in \mathbb{R}^{n\times n}$
$\mathbf{K}$	Kalman gain	$\in \mathbb{R}^{n\times p}$
$H(\,)$	nonlin. obs. operator	
$\mathbf{H}$	Jacobian of H	$\in \mathbb{R}^{p\times n}$
$\mathbf{P}$	model error covariance	$\in \mathbb{R}^{n\times n}$
$\mathbf{R}$	obs. error covariance	$\in \mathbb{R}^{p\times p}$
n	# of model vars.	
p	# of observations	
m	# of ensemble	
tru	truth	
b	background	
a	analysis	
t	time	
o	observation	
$<>$	expectation	

Multidimensional Extension

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Scalar

Suppose x_1 & x_2 follow Gaussian PDF $N(x, \sigma)$

$$p(x_i|x) = \frac{1}{\sqrt{2\pi\sigma_i^2}} \exp\left[-\frac{(x_i - x)^2}{2\sigma_i^2}\right]$$

➔ $maximize \quad p(x_1|x) \cdot p(x_2|x)$

Multi-dims.

Suppose $\mathbf{x}_t^b$ follow $N(\mathbf{x}, \mathbf{B})$

$$p^b(\mathbf{x}_t^b|\mathbf{x}) \propto \exp[-\frac{1}{2}(\mathbf{x} - \mathbf{x}_t^b)^T \mathbf{B}^{-1}(\mathbf{x} - \mathbf{x}_t^b)]$$

Suppose $\mathbf{y}_t^o$ follow $N(H(\mathbf{x}), \mathbf{R})$

$$p^o(\mathbf{y}_t^o|\mathbf{x}) \propto \exp[-\frac{1}{2}(H(\mathbf{x}) - \mathbf{y}_t^o)^T \mathbf{R}^{-1}(H(\mathbf{x}) - \mathbf{y}_t^o)]$$

Joint Probability

$$p^b(\mathbf{x}_t^b|\mathbf{x}) \cdot p^o(\mathbf{y}_t^o|\mathbf{x}) \propto \exp[-J(\mathbf{x})]$$

$maximize \ \ p^b(\mathbf{x}_t^b|\mathbf{x}) \cdot p^o(\mathbf{y}_t^o|\mathbf{x})$
$\Leftrightarrow \quad minimize \ J(\mathbf{x})$

$$J(\mathbf{x}) = \frac{1}{2}(\mathbf{x} - \mathbf{x}_t^b)^T \mathbf{B}^{-1}(\mathbf{x} - \mathbf{x}_t^b) + \frac{1}{2}(H(\mathbf{x}) - \mathbf{y}_t^o)^T \mathbf{R}^{-1}(H(\mathbf{x}) - \mathbf{y}_t^o)$$

Variational DA

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$$J(\mathbf{x}) = \frac{1}{2}(\mathbf{x}-\mathbf{x}_t^b)^T\mathbf{B}^{-1}(\mathbf{x}-\mathbf{x}_t^b) + \frac{1}{2}(H(\mathbf{x})-\mathbf{y}_t^o)^T\mathbf{R}^{-1}(H(\mathbf{x})-\mathbf{y}_t^o)$$

$$\mathbf{x} = \mathbf{x}_t^b + \delta\mathbf{x} \quad \& \quad H\left(\mathbf{x}_t^b+\delta\mathbf{x}\right) \approx H\left(\mathbf{x}_t^b\right) + \mathbf{H}\delta\mathbf{x}$$

$$J(\delta\mathbf{x}) = \frac{1}{2}(\delta\mathbf{x})^T\mathbf{B}^{-1}(\delta\mathbf{x}) + \frac{1}{2}(\mathbf{H}\delta\mathbf{x}-\mathbf{d}_t^{o-b})^T\mathbf{R}^{-1}(\mathbf{H}\delta\mathbf{x}-\mathbf{d}_t^{o-b})$$

$$\mathbf{d}_t^{o-b} = \mathbf{y}_t^o - H\left(\mathbf{x}_t^b\right)$$

d: innovation, departure

gradient

$$\frac{\partial J(\delta\mathbf{x})}{\partial(\delta\mathbf{x})} = \mathbf{B}^{-1}\delta\mathbf{x} + \mathbf{H}^T\mathbf{R}^{-1}\left(\mathbf{H}\delta\mathbf{x}-\mathbf{d}_t^{o-b}\right) = \underline{\mathbf{0}}$$

necessary condition

$$\Leftrightarrow (\mathbf{B}^{-1}+\mathbf{H}^T\mathbf{R}^{-1}\mathbf{H})\delta\mathbf{x} = \mathbf{H}^T\mathbf{R}^{-1}\mathbf{d}_t^{o-b}$$

$$\Leftrightarrow \delta\mathbf{x} = \mathbf{A}\mathbf{H}^T\mathbf{R}^{-1}\mathbf{d}_t^{o-b}$$

$$\Leftrightarrow \mathbf{x}_t^a - \mathbf{x}_t^b = \delta\mathbf{x} = \mathbf{K}_t\mathbf{d}_t^{o-b}$$

B, P^b: background error covariance
A, P^a: analysis error covariance

Variational DA (cont'd)

Proof of Kalman Gain

$$
\begin{aligned}
\mathbf{K}_t &= (\mathbf{B}^{-1} + \mathbf{H}^T\mathbf{R}^{-1}\mathbf{H})^{-1}\mathbf{H}^T\mathbf{R}^{-1} \\
&= (\mathbf{B}^{-1} + \mathbf{H}^T\mathbf{R}^{-1}\mathbf{H})^{-1}\underline{\mathbf{H}^T\mathbf{R}^{-1}(\mathbf{R} + \mathbf{H}\mathbf{B}\mathbf{H}^T)}(\mathbf{R} + \mathbf{H}\mathbf{B}\mathbf{H}^T)^{-1} \\
&= (\mathbf{B}^{-1} + \mathbf{H}^T\mathbf{R}^{-1}\mathbf{H})^{-1}(\underline{\mathbf{H}^T + \mathbf{H}^T\mathbf{R}^{-1}\mathbf{H}\mathbf{B}\mathbf{H}^T})(\mathbf{R} + \mathbf{H}\mathbf{B}\mathbf{H}^T)^{-1} \\
&= \cancel{(\mathbf{B}^{-1} + \mathbf{H}^T\mathbf{R}^{-1}\mathbf{H})^{-1}}\cancel{(\mathbf{B}^{-1} + \mathbf{H}^T\mathbf{R}^{-1}\mathbf{H})}\mathbf{B}\mathbf{H}^T(\mathbf{R} + \mathbf{H}\mathbf{B}\mathbf{H}^T)^{-1} \\
&= \mathbf{B}\mathbf{H}^T(\mathbf{R} + \mathbf{H}\mathbf{B}\mathbf{H}^T)^{-1}
\end{aligned}
$$

Proof of Analysis Error Cov.

$$
\begin{aligned}
(\mathbf{B}^{-1} + \mathbf{H}^T\mathbf{R}^{-1}\mathbf{H})^{-1} &= \mathbf{B} - [\mathbf{I} - (\mathbf{B}^{-1} + \mathbf{H}^T\mathbf{R}^{-1}\mathbf{H})^{-1}\mathbf{B}^{-1}]\mathbf{B} \\
&= \mathbf{B} - \underline{(\mathbf{B}^{-1} + \mathbf{H}^T\mathbf{R}^{-1}\mathbf{H})^{-1}}[(\cancel{\mathbf{B}^{-1}} + \underline{\mathbf{H}^T\mathbf{R}^{-1}}\mathbf{H}) - \cancel{\mathbf{B}^{-1}}]\mathbf{B} \\
&= \mathbf{B} - \mathbf{K}\mathbf{H}\mathbf{B} = (\mathbf{I} - \mathbf{K}\mathbf{H})\mathbf{B} = \mathbf{A}
\end{aligned}
$$

Important Equations

Kalman Gain

$$\mathbf{K}_t = \mathbf{B}\mathbf{H}^T(\mathbf{R} + \mathbf{H}\mathbf{B}\mathbf{H}^T)^{-1} = \mathbf{A}\mathbf{H}^T\mathbf{R}^{-1}$$

Analysis Error Covariance

$$\mathbf{A} = (\mathbf{I} - \mathbf{K}\mathbf{H})\mathbf{B} \iff \mathbf{A}^{-1} = \mathbf{B}^{-1} + \mathbf{H}^T\mathbf{R}^{-1}\mathbf{H}$$

Analysis Update Equation

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

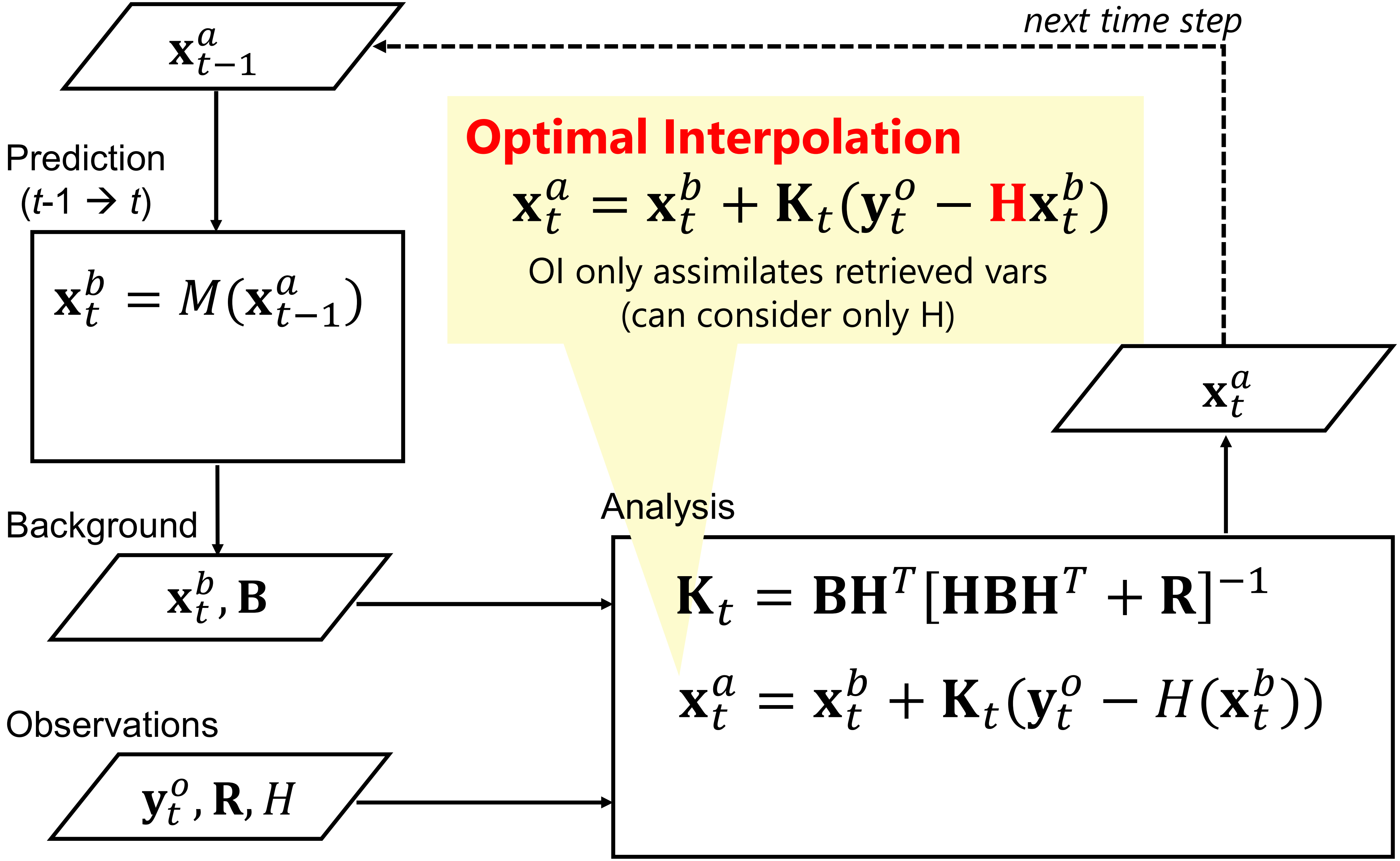
$$\iff \mathbf{A}^{-1}\mathbf{x}_t^a = \mathbf{B}^{-1}\mathbf{x}_t^b + \mathbf{H}^T\mathbf{R}^{-1}\mathbf{y}_t^o$$

$$\mathbf{A}\left[\mathbf{B}^{-1}\mathbf{x}_t^b + \mathbf{H}^T\mathbf{R}^{-1}\mathbf{y}_t^o\right]$$

$$= \mathbf{A}[\mathbf{A}^{-1} - \mathbf{H}^T\mathbf{R}^{-1}\mathbf{H}]\mathbf{x}_t^b + \mathbf{A}\mathbf{H}^T\mathbf{R}^{-1}\mathbf{y}_t^o$$

$$= \mathbf{x}_t^b + \mathbf{A}\mathbf{H}^T\mathbf{R}^{-1}\left[\mathbf{y}_t^o - \mathbf{H}\mathbf{x}_t^b\right] = \mathbf{x}_t^a$$

3DVAR


next time step
$\mathbf{x}_{t-1}^{a}$
Prediction
(t-1 → t)
$\mathbf{x}_t^b = M(\mathbf{x}_{t-1}^a)$
Background
$\mathbf{x}_t^b, \mathbf{B}$
Observations
$\mathbf{y}_t^o, \mathbf{R}, H$
Optimal Interpolation
$\mathbf{x}_t^a = \mathbf{x}_t^b + \mathbf{K}_t(\mathbf{y}_t^o - \mathbf{H}\mathbf{x}_t^b)$
OI only assimilates retrieved vars
(can consider only H)
Analysis
$\mathbf{K}_t = \mathbf{B}\mathbf{H}^T[\mathbf{H}\mathbf{B}\mathbf{H}^T + \mathbf{R}]^{-1}$
$\mathbf{x}_t^a = \mathbf{x}_t^b + \mathbf{K}_t(\mathbf{y}_t^o - H(\mathbf{x}_t^b))$
$\mathbf{x}_t^a$

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Training Course

DA Study w/ 40-variable Lorenz-96

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Lorenz-96 model (Lorenz 1996)

For j=1,…,N, $X_j = X_{j+N}$

$$dX_j / dt = \underbrace{(X_{j+1} - X_{j-2})X_{j-1}}_{\text{Advection term}} \underbrace{- X_j}_{\text{Dissipation term}} + \underbrace{F}_{\text{Forcing term}}$$

力学系モデル・データ同化基礎技術の速習コース

Training Course of Dynamical Model and Data Assimilation

January 31, 2020, Shunji Kotsuki

updated 2020/03/19, 2020/06/29, 2021/07/15

目的： 簡易力学モデル Lorenz の 40 変数モデル（以下 L96; Lorenz 1996）を使って複数のデータ同化手法を自ら実装し、様々な実験を行う。データ同化システムを実際に、0 からコーディングすることで、力学モデリングやデータ同化に関する実践的な「使える」基礎技術を体得する。

Purpose: Using the 40-variable dynamical a.k.a. Lorenz-96 (L96; Lorenz 1996), we are going to perform various experiments with multiple data assimilation (DA) methods. By actually coding a data assimilation system from scratch, you will acquire practically "usable" basic techniques related to mechanical modeling and data assimilation.

Text Books

① Training Description

pswd: ceres

Education | Kotsuki Lab.(小槻研究

https://kotsuki-lab.com/internal-pages/

Kotsuki Lab.

Environmental Prediction Science, Kotsuki Laboratory, Center for Environmental Remote Sensing (CEReS), Chiba University
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教育コンテンツについて

- 研究室として整備している教育コンテンツの一部を公開しています。
- 問合せなどありましたら、こちら(kotsuki.lab(at)gmail.com)までご連絡ください。
- また、不適切な記述や誤りなど、お気づきの点がありましたら、こちらもご指摘いただけると有難いです。

Python プログラミング教材

地球科学数値計算・pythonマニュアル・入門編 (in Japanese & English)

- 2020年現在、プログラミングの学び初めに最も適したプログラムはpythonです。
- 研究室で新規加入メンバー向けに作成してきたマニュアルで、鋭意UPDATE中です。
- PythonMannual_v20210928.dox

Data Assimilation Training Course (in Japanese & English)

- KotsukiLab_L96Training_v20210916.zip
- currently unpublic. please send an email to (kotsuki.lab(at)gmail.com) to get the password for

力学系モデル・データ同化基礎技術の速習コース

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January 31, 2020, Shunji Kotsuki
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Purpose: Using the 40-variable dynamical a.k.a. Lorenz-96 (L96; Lorenz 1996), we are going to perform various experiments with multiple data assimilation (DA) methods. By actually coding a data assimilation system from scratch, you will acquire practically "usable" basic techniques related to mechanical modeling and data assimilation.

方法： 以下の課題を自ら実装し、解決していく。使用言語やプラットフォームは問わない。研究室の MTG において、各自が進捗を報告し、問題点を解消していく。質問は MTG の他も、居室で適宜受け付ける。使用言語については、特に拘りがなければ、行列演算の容易な python が扱いやすい。また、単精度ではなく倍精度でコーディングする事。でないと、既往研究と比較して正しく動作しているか確認できない。

Method: Implement and solve the following problems yourself. Any programing languages or platforms can be used in this exercise. At the Kotsuki Lab. mtg, each personnel will report the progress, and try to solve the problems. Questions are accepted during the MTG as well as at the office when necessary. As for the programing language, python, which is easy to perform matrix operations, is recommended unless specific language is preferred. Also, you should code in double precision instead of single precision. Otherwise, confirming whether performing properly or not compared to the previous studies will not be possible.

- https://kotsuki-lab.com/internal-pages/

Basic Task 5

Basic Task 5

5．３次元変分法と KF の比較実験を行う。この際、観測分布・観測密度への依存性を調べる。

5. Perform a comparative experiment between the 3D variational method and KF. At this time, the dependence on the observation distribution and observation density is investigated.

3DVAR (Full Observations)

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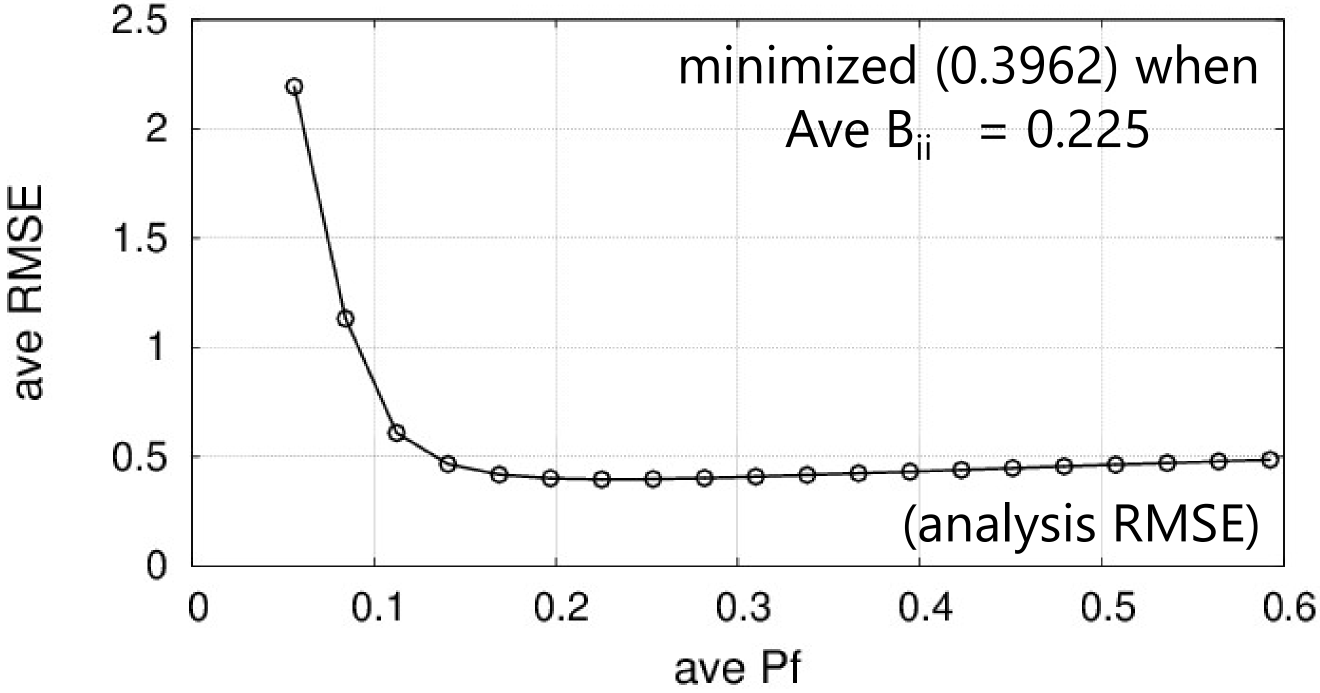
when B is diagonal matrix.

$$B = \begin{pmatrix} b_{11} & & & & \\ & \ddots & & 0 & \\ & & b_{ii} & & \\ & 0 & & \ddots & \\ & & & & b_{nn} \end{pmatrix}$$

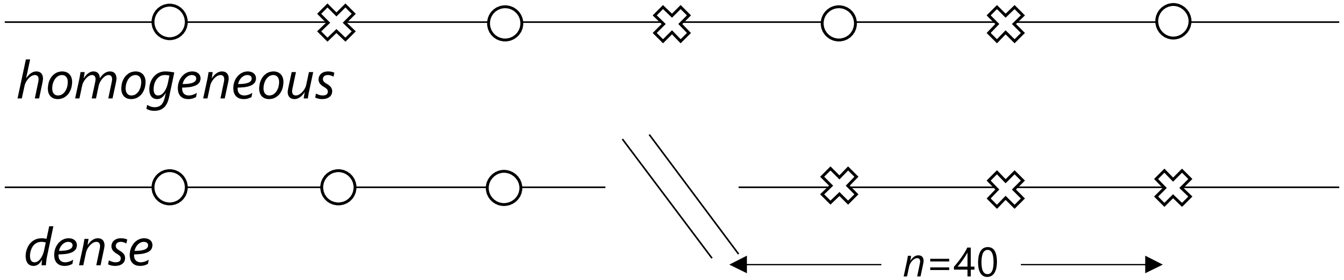
Time-mean RMSE



Sensitivity to Obs. Network

Case 1: Num. Obs. = X

Case 2: Num. Obs. = X



Full Observations

$n=40$, $p=40$

$$\mathbf{H} = \begin{pmatrix} 1 & 0 & 0 & 0 & & 0 \\ 0 & 1 & 0 & 0 & & 0 \\ 0 & 0 & 1 & 0 & \cdots & 0 \\ 0 & 0 & 0 & 1 & & 0 \\ & & \vdots & & \ddots & \\ 0 & 0 & 0 & 0 & & 1 \end{pmatrix}$$

20 Obs (Case1)

$n=40$, $p=20$

$$\mathbf{H} = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & \\ 0 & 0 & 1 & 0 & 0 & \\ 0 & 0 & 0 & 0 & 1 & \cdots \\ 0 & 0 & 0 & 0 & 0 & \\ 0 & 0 & 0 & 0 & 0 & \\ & & \vdots & & & \ddots \end{pmatrix}$$

20 Obs (Case2)

$n=40$, $p=20$

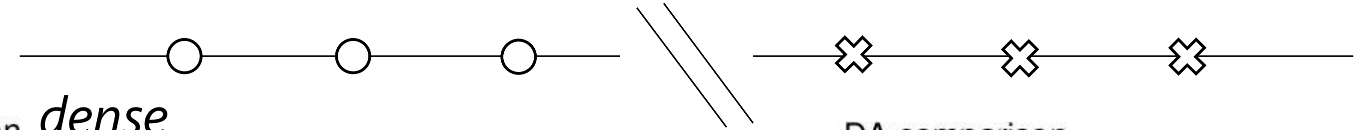
$$\mathbf{H} = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & \\ 0 & 1 & 0 & 0 & 0 & \\ 0 & 0 & 1 & 0 & 0 & \cdots \\ 0 & 0 & 0 & 1 & 0 & \\ 0 & 0 & 0 & 0 & 1 & \\ & & \vdots & & & \ddots \end{pmatrix}$$

Sensitivity to Obs. Network

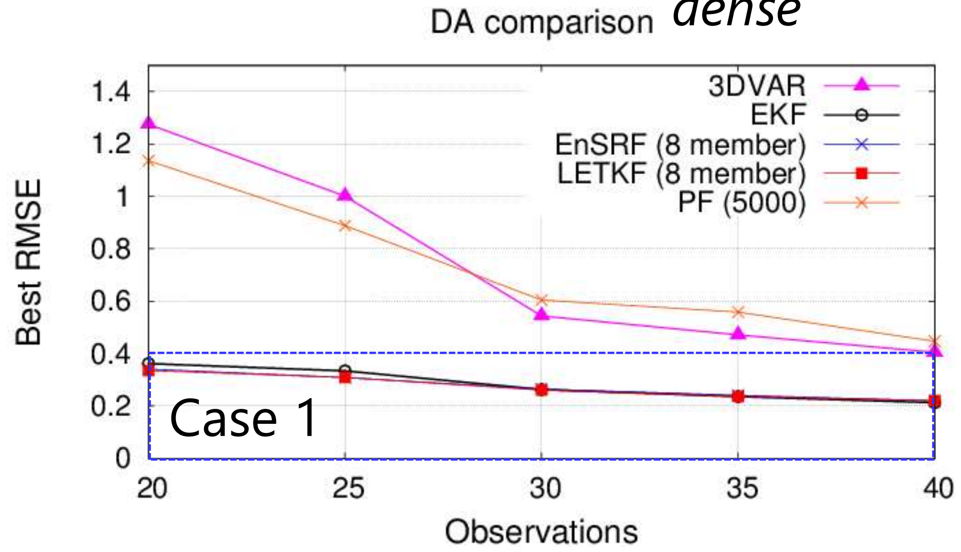
Case 1: Num. Obs. = X

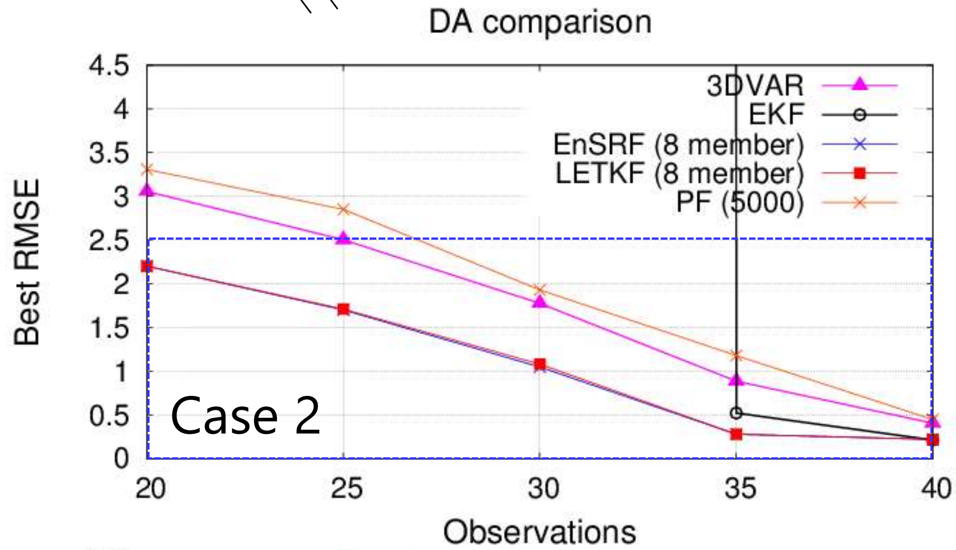
homogeneous

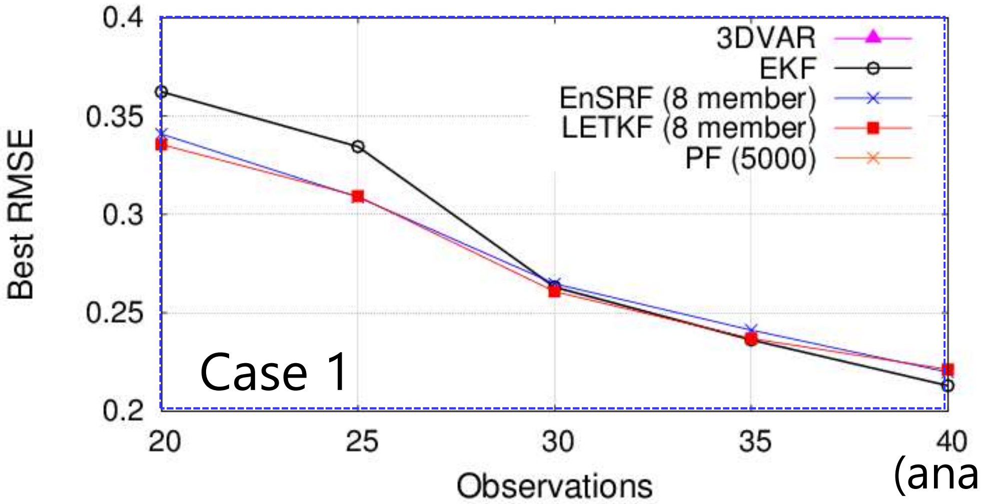
Case 2: Num. Obs. = X

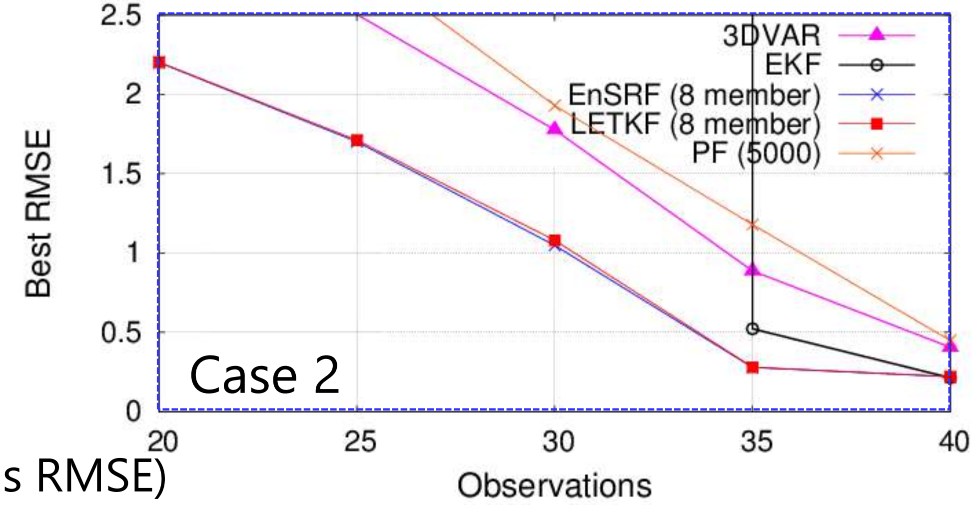


dense









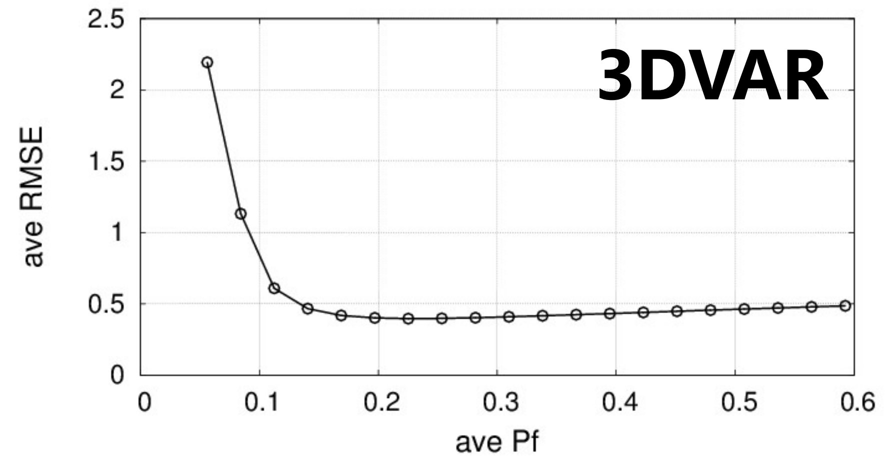
(analysis RMSE)

Hints to Develop KF & 3DVAR

(1) Steps for KF & 3DVAR

	KF	3DVAR
State Prediction	$\mathbf{x}_t^b = M(\mathbf{x}_{t-1}^a)$	
Background Error Cov.	$\mathbf{P}_t^b = \mathbf{M}\mathbf{P}_{t-1}^a\mathbf{M}^T$	**B** (static)
Kalman Gain	$\mathbf{K}_t = \mathbf{P}_t^b\mathbf{H}^T\left[\mathbf{H}\mathbf{P}_t^b\mathbf{H}^T + \mathbf{R}\right]^{-1}$	
State Analysis	$\mathbf{x}_t^a = \mathbf{x}_t^b + \mathbf{K}_t(\mathbf{y}_t^o - H(\mathbf{x}_t^b))$	
Analysis Error Cov.	$\mathbf{P}_t^a = [\mathbf{I} - \mathbf{K}_t\mathbf{H}]\mathbf{P}_t^b$	

Starting with 3DVAR is a good strategy, followed by KF



Thank you for your attention!

Presented by Shunji Kotsuki
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Further information is available at
https://kotsuki-lab.com/

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