Data Assimilation
- A09. Innovation Statistics -

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DA Lectures A (Basic Course)

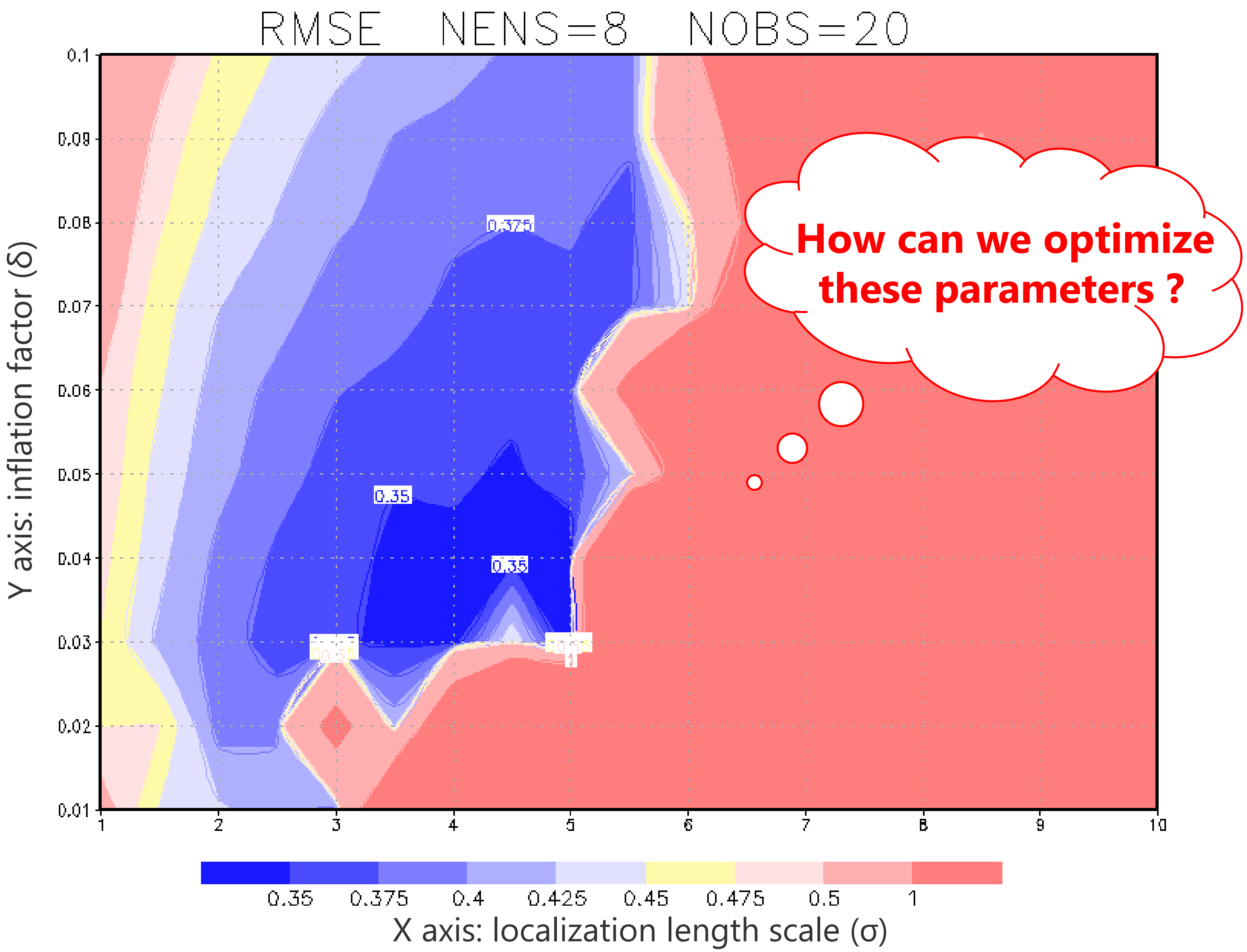
- (1) Introduction and NWP
- (2) Deterministic Chaos and Lorenz-96 model
- (3) A toy model and Bayesian estimation
- (4) Kalman Filter (KF)
- (5) 3D Variational Method (3DVAR)
- (6) Ensemble Kalman Filter (PO method)
- (7) Serial Ens. Square Root Filter (Serial EnSRF)
- (8) Local Ens. Transform Kalman Filter (LETKF)
- (9) Innovation Statistics
- (10) Adaptive Inflations
- (11) 4D Variational Method (4DVAR)

Today's Goal

- **Lecture: innovation statistics**
  - to introduce innovation statistics
  - to understand adaptive inflation

- **Training Course: Lorenz 96**
  - to implement adaptive inflation into L96

Motivation (1)



Innovation statistics

$$\mathbf{d}^{o-b} = \mathbf{y}^o - \mathbf{H}\mathbf{x}^b$$

$$\mathbf{d}^{o-a} = \mathbf{y}^o - \mathbf{H}\mathbf{x}^a$$

$$\mathbf{d}^{a-b} = \mathbf{H}\mathbf{x}^a - \mathbf{H}\mathbf{x}^b$$

b: background

a: analysis

o: observation

Desroziers' innovation statistics (Desroziers et al. 2005)

$$\left\langle \mathbf{d}^{o-b}(\mathbf{d}^{o-b})^T \right\rangle = \mathbf{HBH}^T + \mathbf{R}$$

$$\left\langle \mathbf{d}^{a-b}(\mathbf{d}^{o-b})^T \right\rangle \approx \mathbf{HBH}^T$$

$$\left\langle \mathbf{d}^{o-a}(\mathbf{d}^{o-b})^T \right\rangle \approx \mathbf{R}$$

$$\left\langle \mathbf{d}^{a-b}(\mathbf{d}^{o-a})^T \right\rangle \approx \mathbf{HAH}^T$$

Innovation Statistics (Derivations)

Innovation Statistics

Definition

$\langle \bullet \rangle$: Statistical Expectations

$$\boldsymbol{\varepsilon}^o = \mathbf{y}^o - \mathbf{y}^t, \qquad \boldsymbol{\varepsilon}^b = \mathbf{x}^b - \mathbf{x}^t, \qquad \boldsymbol{\varepsilon}^a = \mathbf{x}^a - \mathbf{x}^t$$

$$\mathbf{R} = \langle \boldsymbol{\varepsilon}^o (\boldsymbol{\varepsilon}^o)^T \rangle, \qquad \mathbf{B} = \mathbf{P}^b = \langle \boldsymbol{\varepsilon}^b (\boldsymbol{\varepsilon}^b)^T \rangle, \qquad \mathbf{A} = \mathbf{P}^a = \langle \boldsymbol{\varepsilon}^a (\boldsymbol{\varepsilon}^a)^T \rangle$$

Derivation from Kalman Gain

$\widetilde{\mathbf{B}}, \widetilde{\mathbf{R}}, \widetilde{\mathbf{A}}, \widetilde{\mathbf{K}}$ matrices used in DA (usually imperfect)

$$\mathbf{x}^a = \mathbf{x}^b + \widetilde{\mathbf{K}}\mathbf{d}^{o-b}, \qquad \widetilde{\mathbf{A}} = \left[\mathbf{I} - \widetilde{\mathbf{K}}\mathbf{H}\right]\widetilde{\mathbf{B}}$$

$$\mathbf{K} = \widetilde{\mathbf{B}}\mathbf{H}^T\left[\mathbf{H}\widetilde{\mathbf{B}}\mathbf{H}^T + \widetilde{\mathbf{R}}\right]^{-1} = \widetilde{\mathbf{A}}\mathbf{H}^T\widetilde{\mathbf{R}}^{-1}$$

$$\left\langle \mathbf{d}^{o-b} (\mathbf{d}^{o-b})^T \right\rangle = \mathbf{HBH}^T + \mathbf{R} \qquad \left\langle \mathbf{d}^{a-b} (\mathbf{d}^{o-b})^T \right\rangle \approx \mathbf{HBH}^T$$

$$\left\langle \mathbf{d}^{o-a} (\mathbf{d}^{o-b})^T \right\rangle \approx \mathbf{R} \qquad \left\langle \mathbf{d}^{a-b} (\mathbf{d}^{o-a})^T \right\rangle \approx \mathbf{HAH}^T$$

Derivations

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

$$\langle \mathbf{d}^{o-b} (\mathbf{d}^{o-b})^T \rangle = \mathbf{HBH}^T + \mathbf{R}$$

$$\mathbf{d}^{o-b} = \mathbf{y}^o - \mathbf{Hx}^b = \boldsymbol{\varepsilon}^o - \mathbf{H}\boldsymbol{\varepsilon}^b$$

$$\langle \mathbf{d}^{o-b} (\mathbf{d}^{o-b})^T \rangle = \left\langle \left(\boldsymbol{\varepsilon}^o - \mathbf{H}\boldsymbol{\varepsilon}^b\right)\left(\boldsymbol{\varepsilon}^o - \mathbf{H}\boldsymbol{\varepsilon}^b\right)^T \right\rangle = \mathbf{R} + \mathbf{HBH}^T$$

$$\langle \mathbf{d}^{a-b} (\mathbf{d}^{o-b})^T \rangle \approx \mathbf{HBH}^T$$

$$\mathbf{d}^{a-b} = \mathbf{Hx}^a - \mathbf{Hx}^b = \mathbf{H}\widetilde{\mathbf{K}}\mathbf{d}^{o-b}$$

$$\langle \mathbf{d}^{a-b} (\mathbf{d}^{o-b})^T \rangle = \left\langle \mathbf{H}\widetilde{\mathbf{K}} (\mathbf{d}^{o-b})\left(\mathbf{d}^{o-b}\right)^T \right\rangle = \mathbf{H}\widetilde{\mathbf{B}}\mathbf{H}^T\left(\mathbf{H}\widetilde{\mathbf{B}}\mathbf{H}^T + \widetilde{\mathbf{R}}\right)^{-1}(\mathbf{HBH}^T + \mathbf{R})$$

$$= \mathbf{HB}^e\mathbf{H}^T \approx \mathbf{HBH}^T$$

$$\langle \mathbf{d}^{o-a} (\mathbf{d}^{o-b})^T \rangle \approx \mathbf{R}$$

$$\begin{aligned} \mathbf{d}^{o-a} &= \mathbf{d}^{o-b} + \mathbf{d}^{b-a} \\ &= \mathbf{d}^{o-b} - \mathbf{H}\widetilde{\mathbf{K}}\mathbf{d}^{o-b} \\ &= \left(\mathbf{I} - \mathbf{H}\widetilde{\mathbf{K}}\right)\mathbf{d}^{o-b} \\ &= \widetilde{\mathbf{R}}\left(\mathbf{H}\widetilde{\mathbf{B}}\mathbf{H}^T + \widetilde{\mathbf{R}}\right)^{-1}\mathbf{d}^{o-b} \end{aligned}$$

$$\begin{aligned} &\langle \mathbf{d}^{o-a} (\mathbf{d}^{o-b})^T \rangle \\ &= \widetilde{\mathbf{R}}\left(\mathbf{H}\widetilde{\mathbf{B}}\mathbf{H}^T + \widetilde{\mathbf{R}}\right)^{-1}\left\langle \mathbf{d}^{o-b}\left(\mathbf{d}^{o-b}\right)^T \right\rangle \\ &= \widetilde{\mathbf{R}}\left(\mathbf{H}\widetilde{\mathbf{B}}\mathbf{H}^T + \widetilde{\mathbf{R}}\right)^{-1}(\mathbf{HBH}^T + \mathbf{R}) \\ &= \mathbf{R}^e \approx \mathbf{R} \end{aligned}$$

$$\mathbf{R}^e + \mathbf{HB}^e\mathbf{H}^T = \widetilde{\mathbf{R}}\left(\mathbf{H}\widetilde{\mathbf{B}}\mathbf{H}^T + \widetilde{\mathbf{R}}\right)^{-1}(\mathbf{HBH}^T + \mathbf{R}) + \mathbf{H}\widetilde{\mathbf{B}}\mathbf{H}^T\left(\mathbf{H}\widetilde{\mathbf{B}}\mathbf{H}^T + \widetilde{\mathbf{R}}\right)^{-1}(\mathbf{HBH}^T + \mathbf{R}) = \mathbf{R} + \mathbf{HBH}^T$$

Derivations (cont'd)

$$\left\langle \mathbf{d}^{a-b}(\mathbf{d}^{o-a})^T \right\rangle \approx \mathbf{HAH}^T$$

$$\mathbf{d}^{o-a} = \widetilde{\mathbf{R}}\left(\mathbf{H}\widetilde{\mathbf{B}}\mathbf{H}^T + \widetilde{\mathbf{R}}\right)^{-1}\mathbf{d}^{o-b}$$

$$\begin{aligned}
\left\langle \mathbf{d}^{a-b}(\mathbf{d}^{o-a})^T \right\rangle &= \left\langle \mathbf{H}\widetilde{\mathbf{K}}\mathbf{d}^{o-b}\left(\widetilde{\mathbf{R}}\left(\mathbf{H}\widetilde{\mathbf{B}}\mathbf{H}^T + \widetilde{\mathbf{R}}\right)^{-1}\mathbf{d}^{o-b}\right)^T \right\rangle \\
&= \mathbf{H}\widetilde{\mathbf{K}}(\mathbf{HBH}^T + \mathbf{R})\left(\mathbf{H}\widetilde{\mathbf{B}}\mathbf{H}^T + \widetilde{\mathbf{R}}\right)^{-1}\widetilde{\mathbf{R}} \\
&= \mathbf{H}\widetilde{\mathbf{A}}\mathbf{H}^T\widetilde{\mathbf{R}}^{-1}(\mathbf{HBH}^T + \mathbf{R})^{-1}\left(\mathbf{H}\widetilde{\mathbf{B}}\mathbf{H}^T + \widetilde{\mathbf{R}}\right)^{-1}\widetilde{\mathbf{R}} \\
&= \mathbf{HA}^e\mathbf{H}^T \approx \mathbf{HAH}^T
\end{aligned}$$

Innovation Statistics

Innovation Statistics

$$\langle \mathbf{d}^{o-b}(\mathbf{d}^{o-b})^T \rangle = \mathbf{HBH}^T + \mathbf{R}$$

$$\langle \mathbf{d}^{o-a}(\mathbf{d}^{o-b})^T \rangle = \widetilde{\mathbf{R}}\left(\mathbf{H}\widetilde{\mathbf{B}}\mathbf{H}^T + \widetilde{\mathbf{R}}\right)^{-1}(\mathbf{HBH}^T + \mathbf{R}) = \mathbf{R}^e$$

$$\langle \mathbf{d}^{a-b}(\mathbf{d}^{o-b})^T \rangle = \mathbf{H}\widetilde{\mathbf{B}}\mathbf{H}^T\left(\mathbf{H}\widetilde{\mathbf{B}}\mathbf{H}^T + \widetilde{\mathbf{R}}\right)^{-1}(\mathbf{HBH}^T + \mathbf{R}) = \mathbf{HB}^e\mathbf{H}^T$$

$$\langle \mathbf{d}^{a-b}(\mathbf{d}^{o-a})^T \rangle = \mathbf{HB}^e\mathbf{H}^T\left(\mathbf{H}\widetilde{\mathbf{B}}\mathbf{H}^T\right)^{-1}\mathbf{H}\widetilde{\mathbf{A}}\mathbf{H}^T = \mathbf{HA}^e\mathbf{H}^T$$

Their Relationship

$$\mathbf{R}^e + \mathbf{HB}^e\mathbf{H}^T = \mathbf{R} + \mathbf{HBH}^T$$

NOTE: We need to consider DA uses imperfect B & R in the real-world applications

$\mathbf{R}, \mathbf{B}, \mathbf{A}$: Truth

$\widetilde{\mathbf{R}}, \widetilde{\mathbf{B}}, \widetilde{\mathbf{A}}$: DA (maybe imperfect)

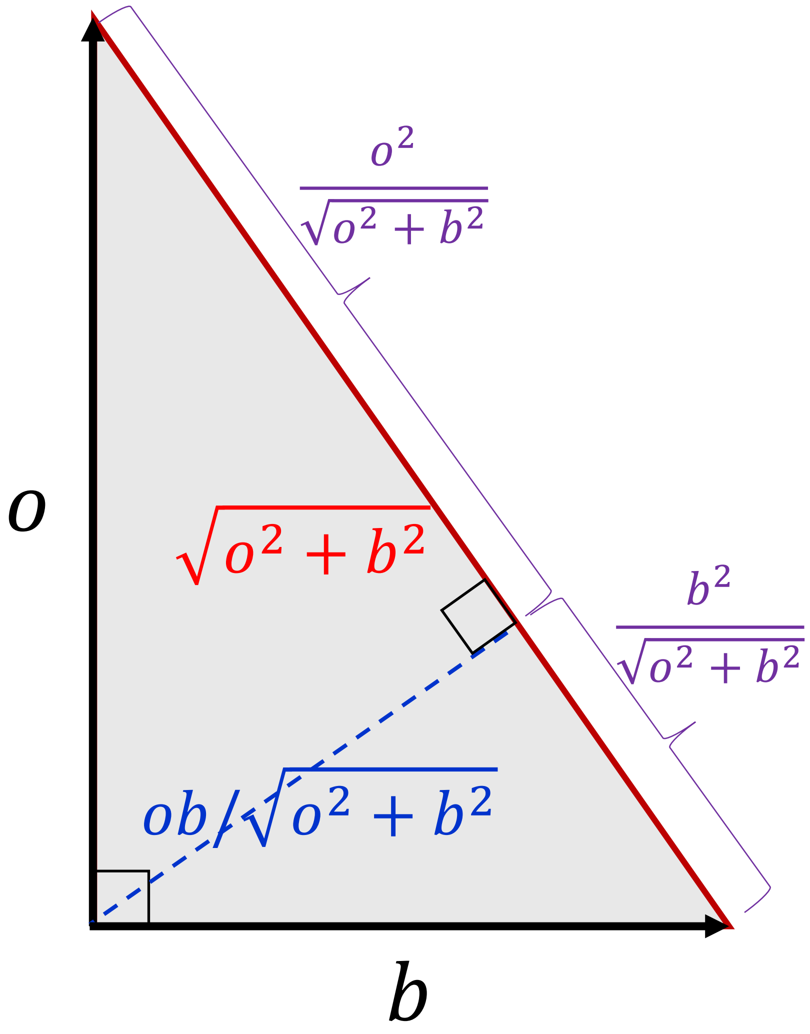
$\mathbf{R}^e, \mathbf{B}^e, \mathbf{A}^e$: Estimated

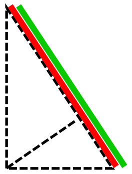
o, R: obs
b, B: background
a, A: analysis

Geometric Interpretations of Data Assimilation

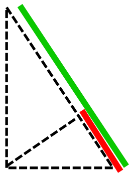
For simplicity, following discussion assumes a scalar problem

Pythagorean theorem

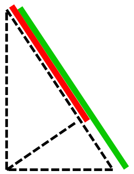




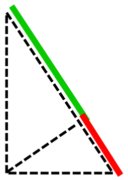
$$\sqrt{o^2+b^2}\sqrt{o^2+b^2} = o^2+b^2$$



$$\frac{b^2}{\sqrt{o^2+b^2}}\sqrt{o^2+b^2} = b^2$$

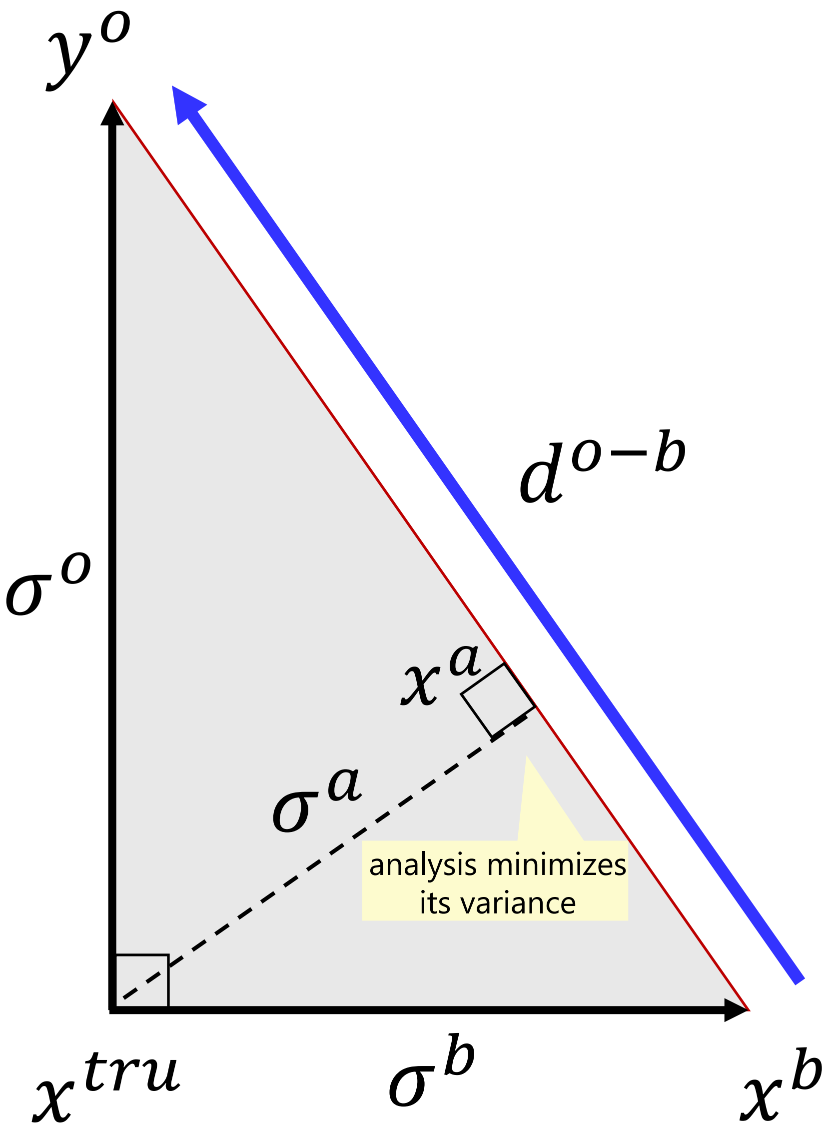


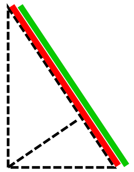
$$\frac{a^2}{\sqrt{o^2+b^2}}\sqrt{o^2+b^2} = o^2$$



$$\frac{b^2}{\sqrt{o^2+b^2}}\frac{o^2}{\sqrt{o^2+b^2}} = \frac{o^2b^2}{o^2+b^2}$$

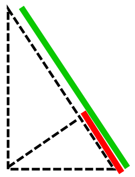
Innovation Statistics





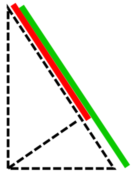
(1) *OMB-OMB Statistics* $\mathbf{HBH}^T + \mathbf{R}$

$$\langle d^{o-b} d^{o-b} \rangle = (\sigma^b)^2 + (\sigma^o)^2$$



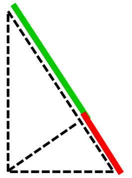
(2) *AMB-OMB Statistics* $\mathbf{HBH}^T$

$$\langle d^{a-b} d^{o-b} \rangle = (\sigma^b)^2$$



(3) *OMA-OMB Statistics* $\mathbf{R}$

$$\langle d^{o-a} d^{o-b} \rangle = (\sigma^o)^2$$



(4) *AMB-OMA Statistics* $\mathbf{HAH}^T$

$$\langle d^{a-b} d^{o-a} \rangle = (\sigma^a)^2$$

cross terms correspond to right angle: $\langle \mathbf{H}\boldsymbol{\varepsilon}^b (\boldsymbol{\varepsilon}^o)^T \rangle = \langle (\boldsymbol{\varepsilon}^o)^T \mathbf{H}\boldsymbol{\varepsilon}^b \rangle = 0$

Kalman Gain

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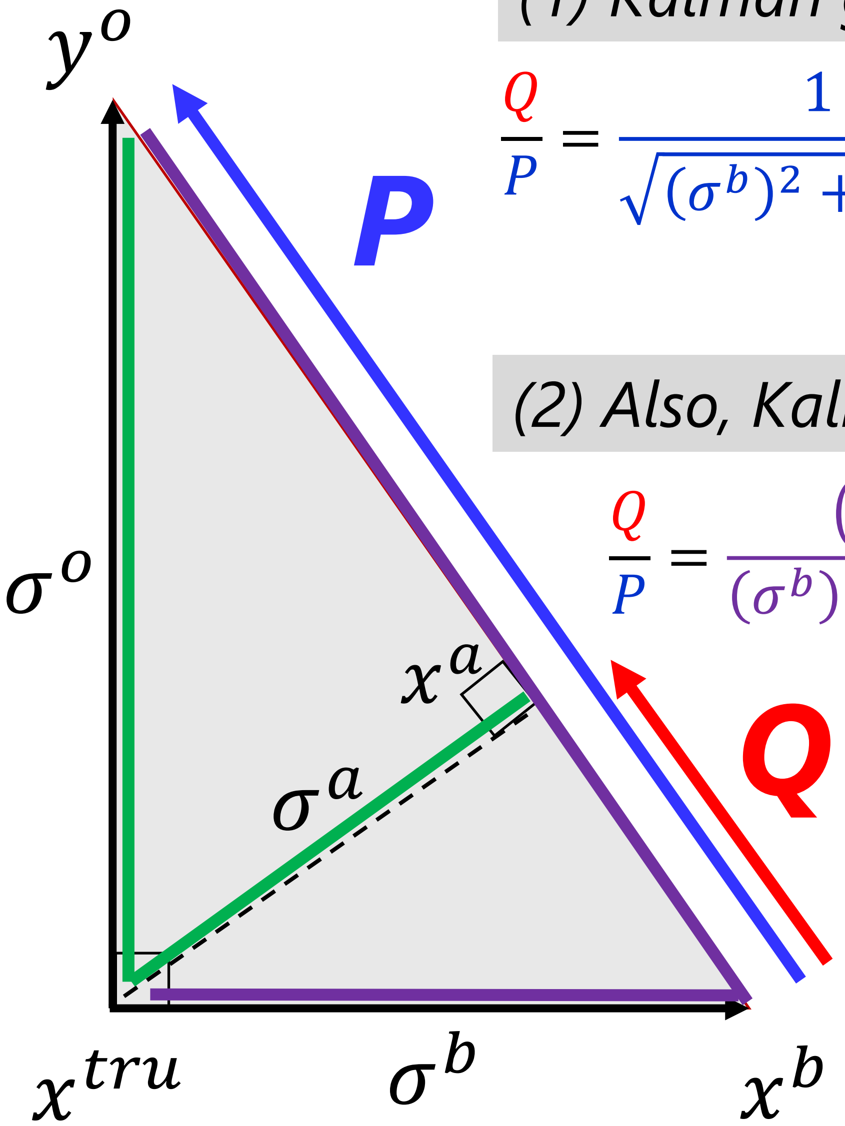


*(1) Kalman gain gives **weights***

$$\frac{Q}{P} = \frac{1}{\sqrt{(\sigma^b)^2 + (\sigma^o)^2}} \frac{(\sigma^b)^2}{\sqrt{(\sigma^b)^2 + (\sigma^o)^2}} = \frac{(\sigma^b)^2}{(\sigma^b)^2 + (\sigma^o)^2}$$

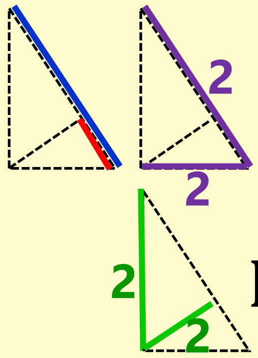
i.e., $\mathbf{K} = \mathbf{B}\mathbf{H}^T(\mathbf{R} + \mathbf{H}\mathbf{B}\mathbf{H}^T)^{-1}$

(2) Also, Kalman gain is

$$\frac{Q}{P} = \frac{(\sigma^b)^2}{(\sigma^b)^2 + (\sigma^o)^2} = \frac{(\sigma^a)^2}{(\sigma^o)^2}$$

i.e., $\mathbf{K} = \mathbf{A}\mathbf{H}^T\mathbf{R}^{-1}$

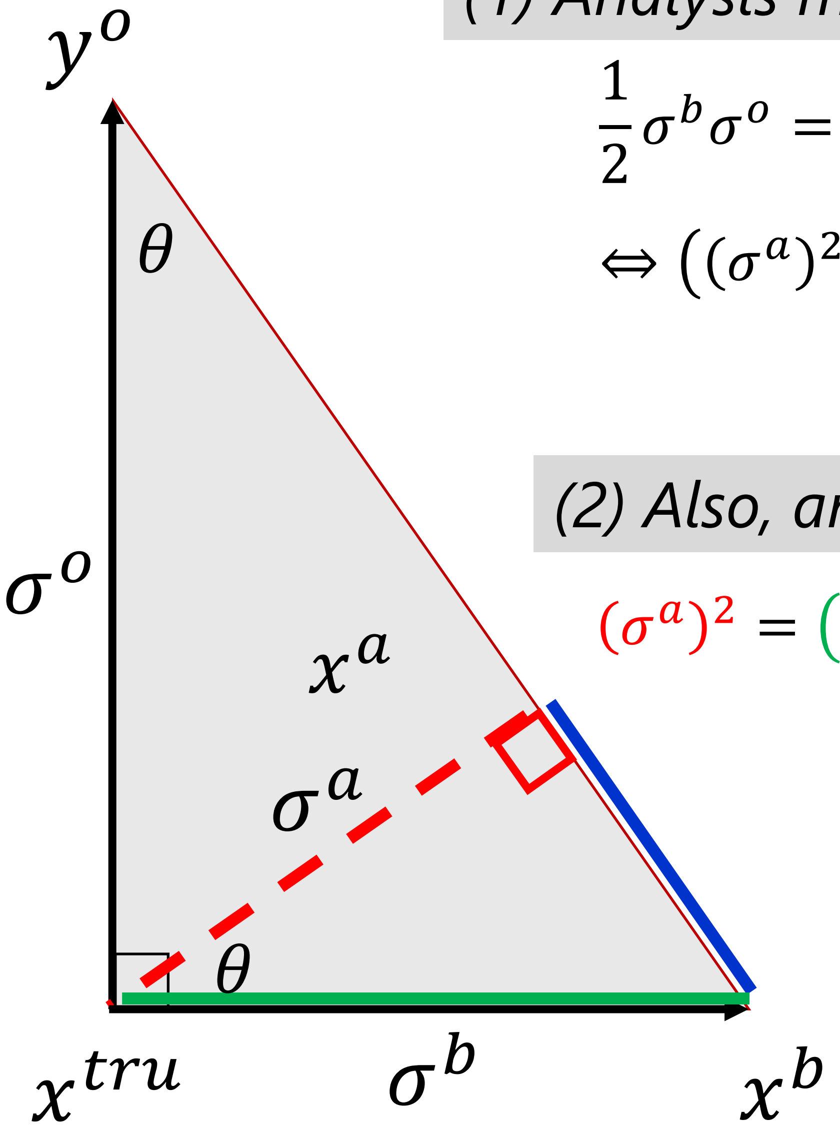
Namely, Kalman gain is uncertainty of posterior error cov. w.r.t. obs. error cov.



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

$\mathbf{K} = \mathbf{A}\mathbf{H}^T\mathbf{R}^{-1}$

Analysis Error Covariance



(1) Analysis minimizes variance of estimation

$$\frac{1}{2}\sigma^b\sigma^o = \frac{1}{2}\sigma^a\sqrt{(\sigma^b)^2 + (\sigma^o)^2}$$

→ vertical

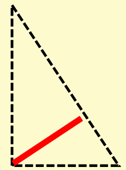
$$\Leftrightarrow \left((\sigma^a)^2\right)^{-1} = \left((\sigma^b)^2\right)^{-1} + \left((\sigma^o)^2\right)^{-1}$$

i.e., $\mathbf{A}^{-1} = \mathbf{B}^{-1} + \mathbf{H}^T\mathbf{R}^{-1}\mathbf{H}$

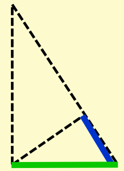
(2) Also, analysis is

$$(\sigma^a)^2 = (\sigma^b)^2 - \sin^2\theta\,(\sigma^b)^2$$

i.e., $\mathbf{A} = (\mathbf{I} - \mathbf{KH})\mathbf{B}$

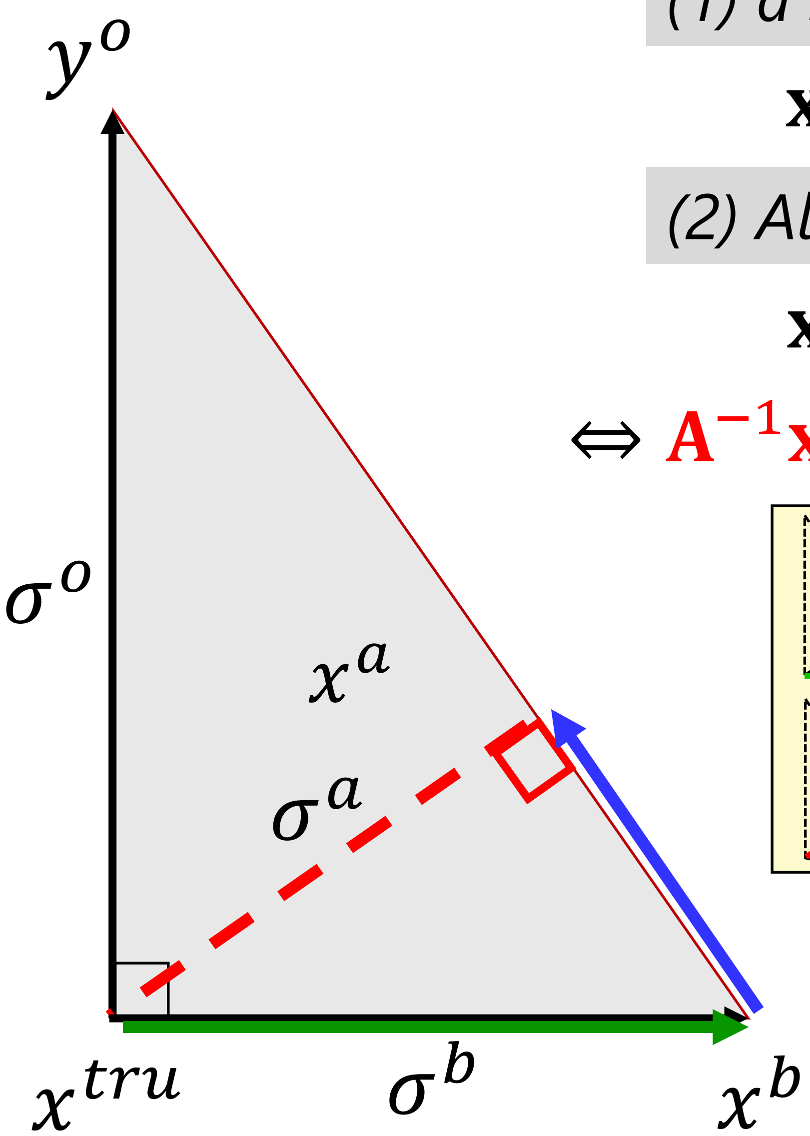


$\mathbf{A}^{-1} = \mathbf{B}^{-1} + \mathbf{H}^T\mathbf{R}^{-1}\mathbf{H}$



$\mathbf{A} = (\mathbf{I} - \mathbf{KH})\mathbf{B}$

Analysis State



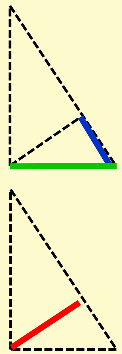
(1) a standard update equation

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

(2) Also, analysis is given by

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

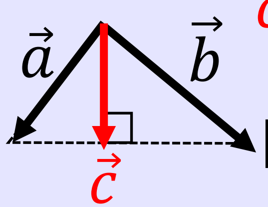
$$\Leftrightarrow \mathbf{A}^{-1}\mathbf{x}_t^a = \mathbf{B}^{-1}\mathbf{x}_t^b + \mathbf{H}^T\mathbf{R}^{-1}\mathbf{y}_t^o$$



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

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

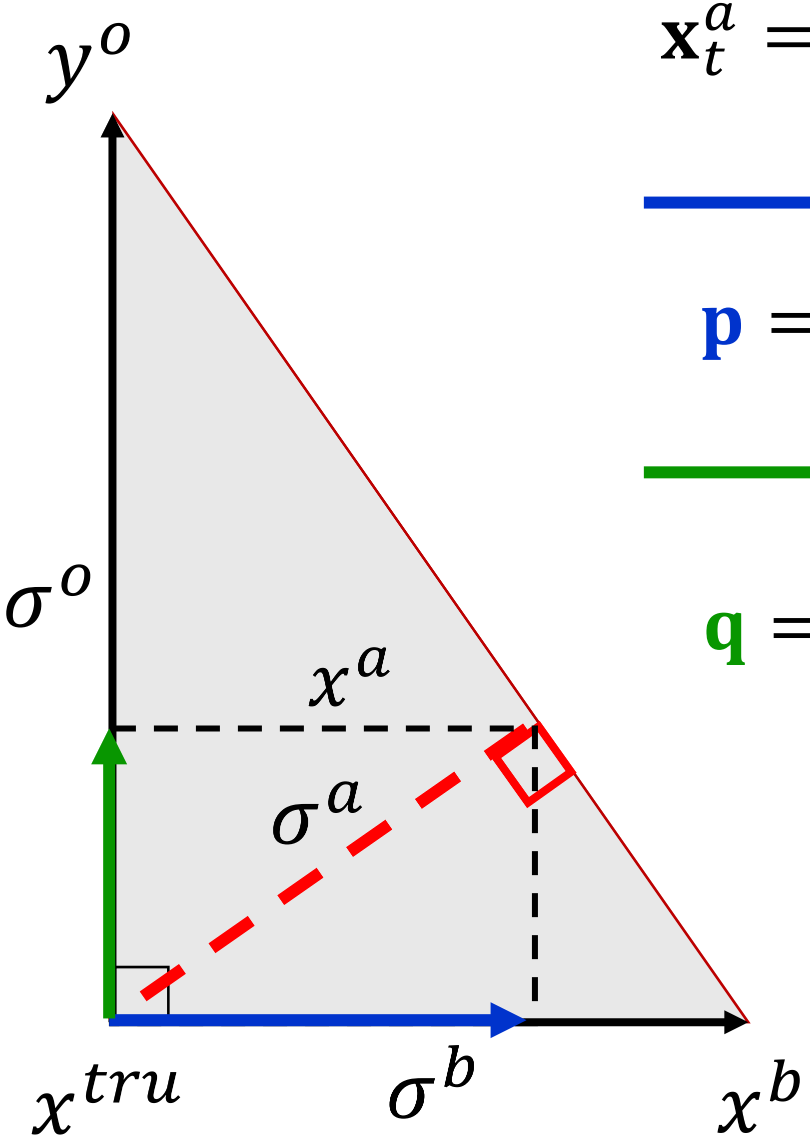
Review



$$\vec{c} = \frac{\beta^2\vec{a}+\alpha^2\vec{b}}{\alpha^2+\beta^2} \Leftrightarrow \frac{\vec{c}}{\gamma^2} = \frac{\vec{a}}{\alpha^2} + \frac{\vec{b}}{\beta^2}$$

$$|\vec{a}| = \alpha, \left|\vec{b}\right| = \beta, |\vec{c}| = \gamma = \frac{\alpha\beta}{\sqrt{\alpha^2+\beta^2}}$$

Analysis State (cont’d)

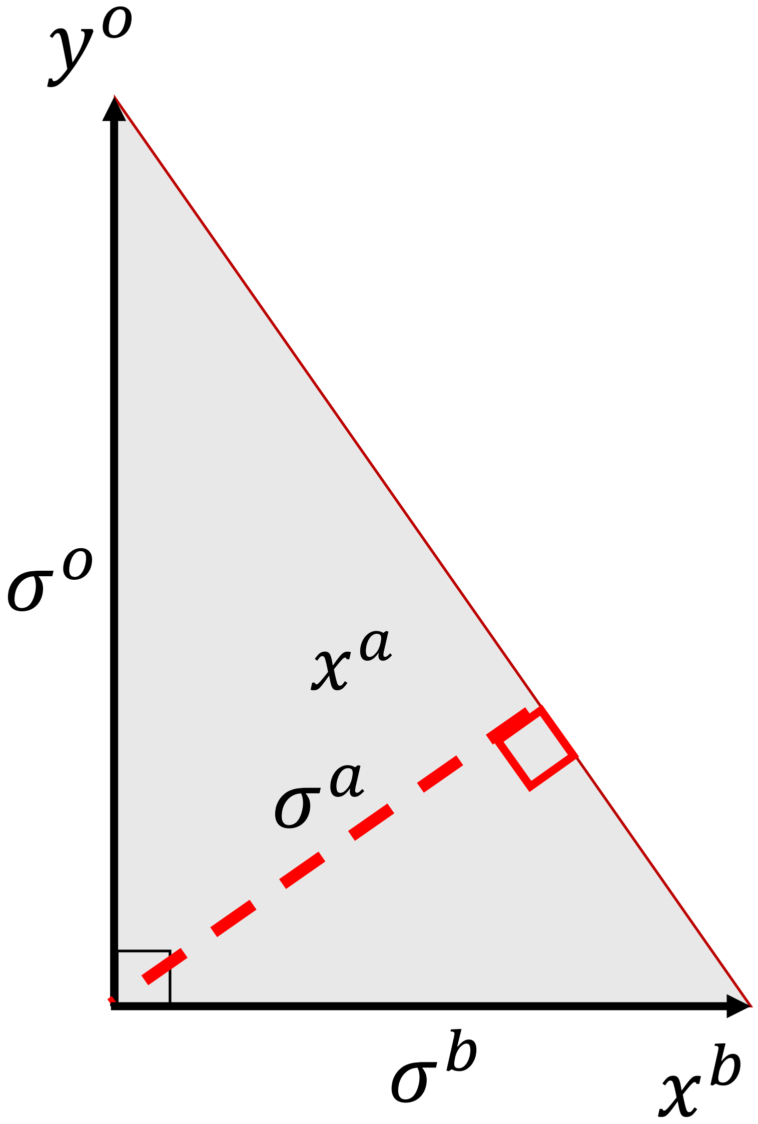


$$\mathbf{x}_t^a = \mathbf{A}\left[\mathbf{B}^{-1}\mathbf{x}_t^b + \mathbf{H}^T\mathbf{R}^{-1}\mathbf{y}_t^o\right]$$

$$\mathbf{p} = \mathbf{x}_t^b\left(\frac{(\sigma^o)^2}{(\sigma^b)^2 + (\sigma^o)^2}\right)$$

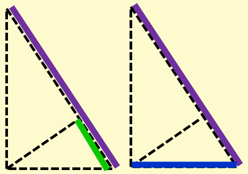
$$\mathbf{q} = \mathbf{y}_t^o\left(\frac{(\sigma^b)^2}{(\sigma^b)^2 + (\sigma^o)^2}\right)$$

Geometric Interpretations



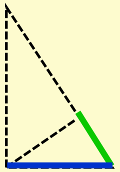
Focusing on the weights gives:

$$\mathbf{K}_t = \mathbf{BH}^T(\mathbf{R} + \mathbf{HBH}^T)^{-1}$$



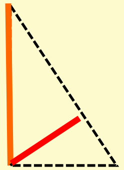
$$\mathbf{A} = \mathbf{B} - \mathbf{KHB}$$

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



Focusing on the AN cov. gives:

$$\mathbf{K} = \mathbf{AH}^T\mathbf{R}^{-1}$$



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

To understand DA via two ways

(1) Kalman gain gives the optimal weight

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

From the view point of <u>analysis states</u>

(2) Kalman gain is the analysis error cov. normalized by R

$$\mathbf{K} = \mathbf{A}\mathbf{H}^T\mathbf{R}^{-1}$$

From the view point of <u>analysis uncertainty</u>

To discuss information (or entropy), (2) is more important

For example, DFS (Degrees of Freedom for the Signal): $DFS = trace(\mathbf{S})$ where

$$\mathbf{S} = \frac{\partial \mathbf{y}^a}{\partial \mathbf{y}^o} = \frac{\partial}{\partial \mathbf{y}^o}(\mathbf{H}\mathbf{x}^a) = \frac{\partial}{\partial \mathbf{y}^o}\left(\mathbf{H}\mathbf{x}^b + \mathbf{H}\mathbf{K}\left(\mathbf{y}^o - \mathbf{H}\mathbf{x}^b\right)\right) = \mathbf{H}\mathbf{K}$$

$$= \mathbf{H}\mathbf{K} = \mathbf{H}\mathbf{A}\mathbf{H}^T\mathbf{R}^{-1}$$

i.e., DFS is obs-space **A** normalized by **R**

S: *influence matrix*

DFS (cont'd)

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Preparation: SVD to the observability matrix

$$\mathbf{G} = \mathbf{R}^{-1/2}\mathbf{H}\mathbf{B}^{1/2} = \mathbf{E}\boldsymbol{\Gamma}^{1/2}\mathbf{C}^T$$

DFS

$$DFS = trace(\mathbf{S}) = trace(\mathbf{R}^{-1/2}\mathbf{H}\mathbf{A}\mathbf{H}^T\mathbf{R}^{-1/2})$$

$$= trace(\mathbf{HK}) = trace(\mathbf{HBH}^T(\mathbf{R} + \mathbf{HBH}^T)^{-1})$$

$$= trace\left(\mathbf{R}^{-1/2}\mathbf{HBH}^T\mathbf{R}^{-1/2}\left(\mathbf{I} + \mathbf{R}^{-1/2}\mathbf{HBH}^T\mathbf{R}^{-1/2}\right)^{-1}\right)$$

$$= trace(\mathbf{E}\boldsymbol{\Gamma}\mathbf{E}^T(\mathbf{I} + \mathbf{E}\boldsymbol{\Gamma}\mathbf{E}^T)^{-1})$$

$$DFS = trace(\mathbf{S})$$

To discuss information (or entropy), (2) is more important

$$\mathbf{S} = \frac{\partial \mathbf{y}^a}{\partial \mathbf{y}^o} = \frac{\partial}{\partial \mathbf{y}^o}(\mathbf{H}\mathbf{x}^a) = \frac{\partial}{\partial \mathbf{y}^o}\left(\mathbf{H}\mathbf{x}^b + \mathbf{HK}\left(\mathbf{y}^o - \mathbf{H}\mathbf{x}^b\right)\right) = \mathbf{HK}$$

where

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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