

Fundamentals of Data Assimilation

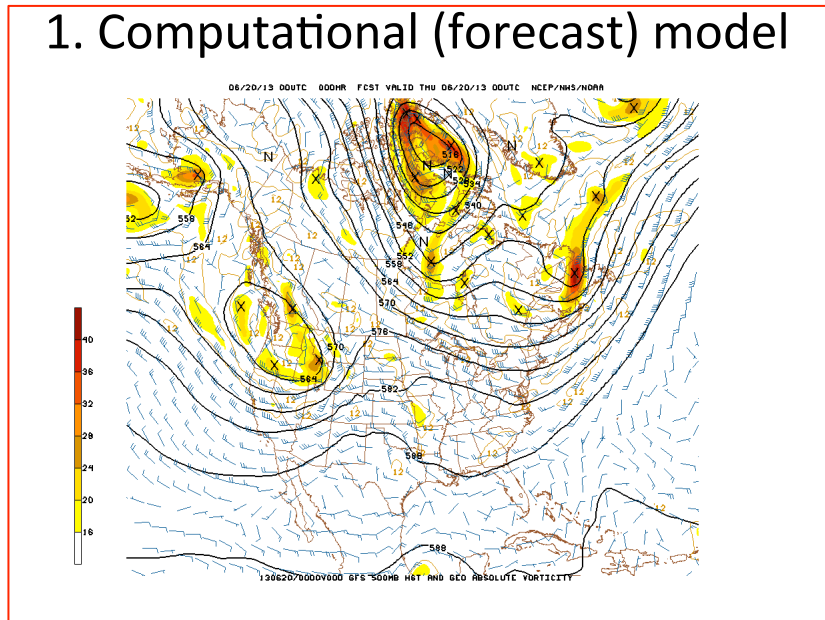
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2013 Joint DTC-EMC-JCSDA GSI Tutorial

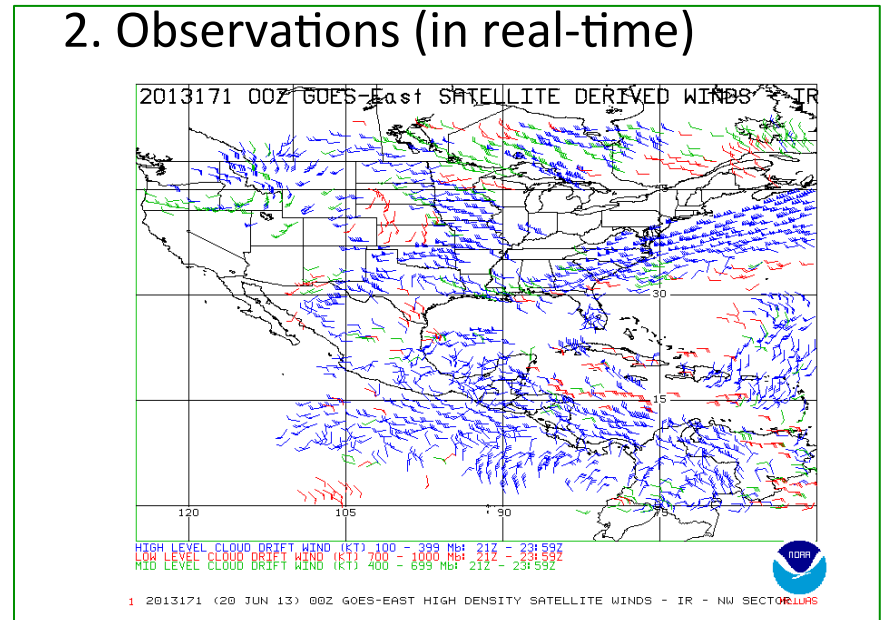
Objectives of Data Assimilation from NWP Viewpoint

- ◆ Primary objectives of data assimilation:
 - Estimation of the current state
 - Forecast of the future stateby periodically integrating information from

1. Computational (forecast) model



2. Observations (in real-time)



- ◆ DA is a growing area:
 - Many variants, extensions, applications etc exist & are being developed

Objectives of This Lecture

- ◆ Basic ideas of data assimilation
- ◆ Unifying perspectives of currently popular & practical approaches
- ◆ Understanding of the variational formulation
 - Cost function for minimization(=optimization)

$$J(\mathbf{x}) = J^b(\mathbf{x}) + J^o(\mathbf{x}) \quad [+ J^c(\mathbf{x})]$$

$$J^b(\mathbf{x}) = 1/2(\mathbf{x} - \mathbf{x}^b)^T \mathbf{B}^{-1}(\mathbf{x} - \mathbf{x}^b) \quad : \text{*b*ackground cost function}$$

$$J^o(\mathbf{x}) = 1/2(\mathbf{y}^o - \mathbf{h}(\mathbf{x}))^T \mathbf{R}^{-1}(\mathbf{y}^o - \mathbf{h}(\mathbf{x})) \quad : \text{*o*bservation cost function}$$

$$J^c(\mathbf{x}) \quad : \text{*c*onstraint cost function}$$

Where (\mathbf{x}, \mathbf{B}) : model state vector & background error covariance matrix

(\mathbf{y}, \mathbf{R}) : observation vector & observation error covariance matrix

$\mathbf{y} = \mathbf{h}(\mathbf{x})$: forward model / observation operator

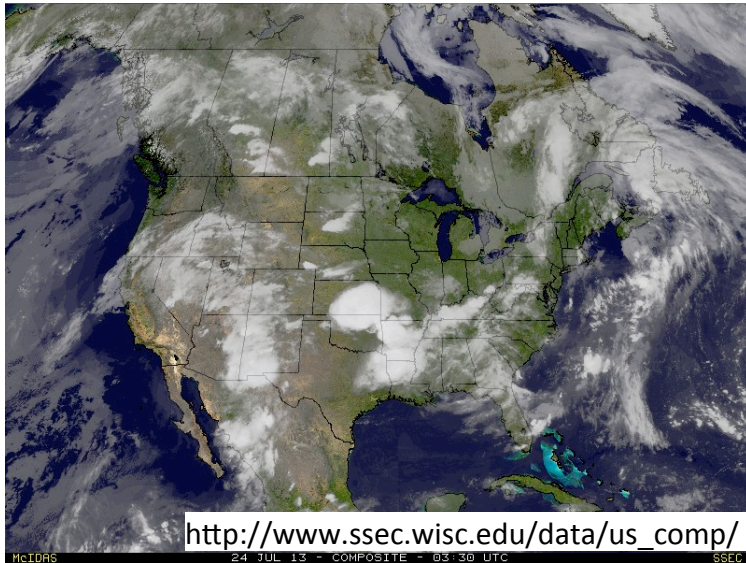
- With emphasis on
 - Role of \mathbf{B}
 - Flexibility of variational approach

Outline

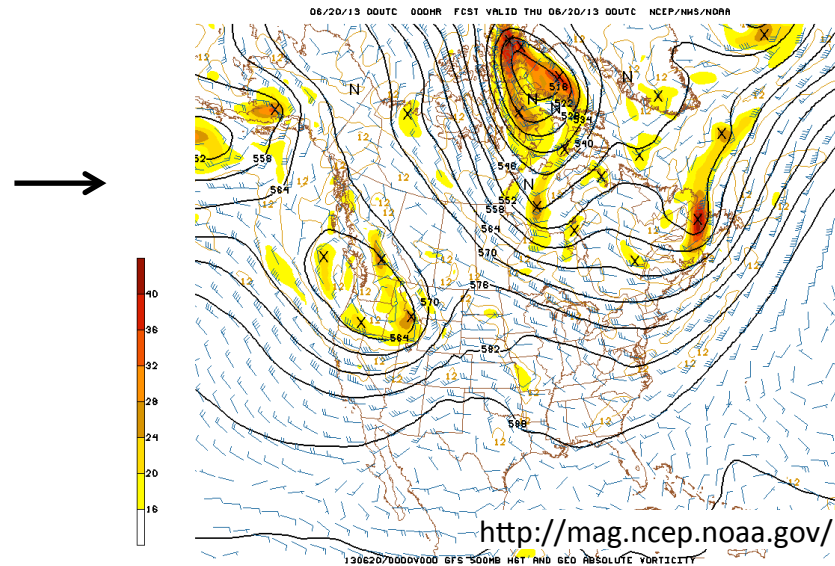
- ◆ Objectives
- ◆ Background
 - State \mathbf{x} & Observation \mathbf{y} - also $\mathbf{m}(\mathbf{x})$ & $\mathbf{h}(\mathbf{x})$
 - Probability $p(\mathbf{x})$ - also $p(\mathbf{x}|\mathbf{y})$ & $p(\mathbf{y}|\mathbf{x})$
 - Data assimilation perspectives
- ◆ 3D Method - 3 dimensions in space
 - OI = Optimal Interpolation
 - 3DVar = Variational
- ◆ 3D to 4D - 4th dimension is time
 - EKF/EnKF= Extended/Ensemble Kalman filter
 - FGAT = First Guess at Appropriate Time
 - 4DVar
 - Hybrid = between Var and EnKF - Current operational system
- ◆ Concluding remarks

State \mathbf{x} and \mathbf{x}^t ?

◆ Real atmosphere



◆ Atmospheric modeling



“true state” \mathbf{x}_k^t :
target of data assimilation
[= consistent projection of real state
onto \mathbf{x}]
→ representation of \mathbf{x}^t has uncertainty
→ Probability $p(\mathbf{x})$

Computational model (from time t_{k-1} to t_k)

$$\mathbf{x}_k = \mathbf{m}_{k,k-1}(\mathbf{x}_{k-1})$$

\mathbf{m} : model

\mathbf{x} : N -dim spatially discretized
vector of atmospheric variables
($N \sim 10^7$)

Computational Model: $\mathbf{x}_k = \mathbf{m}_{k,k-1}(\mathbf{x}_{k-1})$

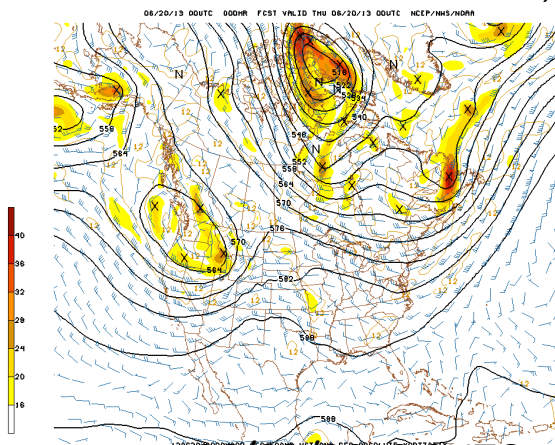
- ◆ Variables: \mathbf{x} is high-dimensional state vector $N \sim O(10^{6-7})$

Ex: GFS

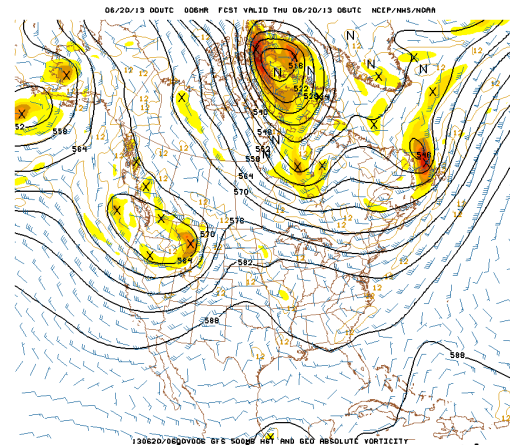
$$\mathbf{x} = \begin{pmatrix} T \\ \mathbf{q} \\ \mathbf{D} \\ \zeta \\ p_s \\ \vdots \end{pmatrix} = \begin{pmatrix} \text{Temperature} \\ \text{moisture} \\ \text{divergence} \\ \text{vorticity} \\ \text{surface pressure} \\ \vdots \end{pmatrix} \quad \text{All grid points}$$

- ◆ Forecast model:

- Model $\mathbf{m}_{k,k-1}$: flow dependent, complex, and nonlinear
- Initial condition(IC) \mathbf{x}_{k-1} : accurate representation of the current condition
- Skill: $\mathbf{m}_{k,k-1}$, \mathbf{x}_{k-1} , and underlying system itself



GFS \mathbf{x}_{k-1} at =06/23/2013 00UTC



$\mathbf{x}_k = \mathbf{m}_{k,k-1}(\mathbf{x}_{k-1})$ at $t_k = t_{k-1} + 6\text{hr}$

Observation & Forward Model : $\mathbf{y}=\mathbf{h}(\mathbf{x})$

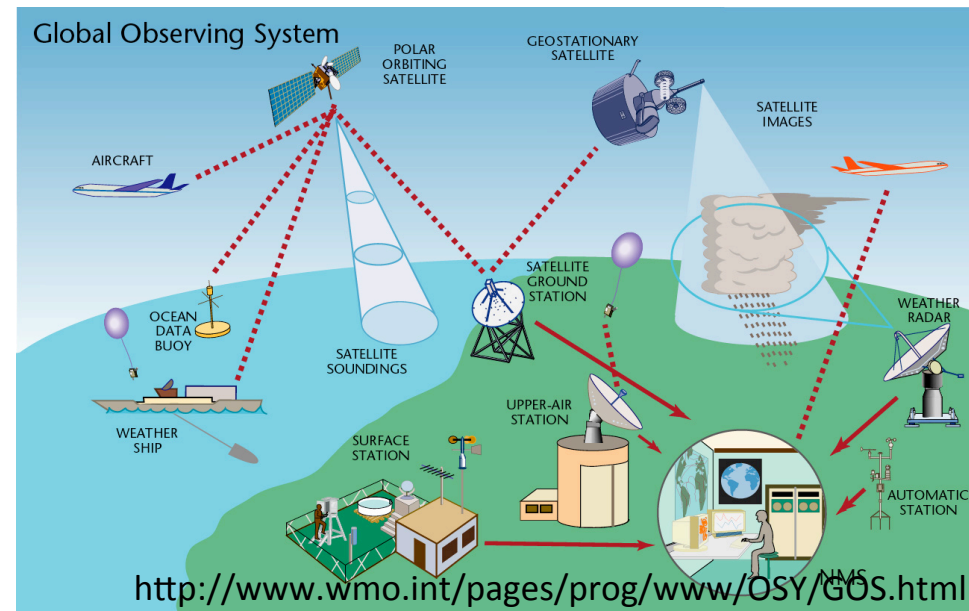
- ◆ Observation vector \mathbf{y} : Sampling of (real) atmospheric state

- Ex: GSI

$$\mathbf{y} = \begin{pmatrix} \mathbf{y}_T \\ \mathbf{y}_q \\ \mathbf{y}_{\text{wind}} \\ \mathbf{y}_{ps} \\ \vdots \end{pmatrix} = \begin{pmatrix} \text{Temperature} \\ \text{moisture} \\ \text{wind field} \\ \text{surface pressure} \\ \vdots \end{pmatrix}$$

- Platforms

- In situ
- Remote sensing



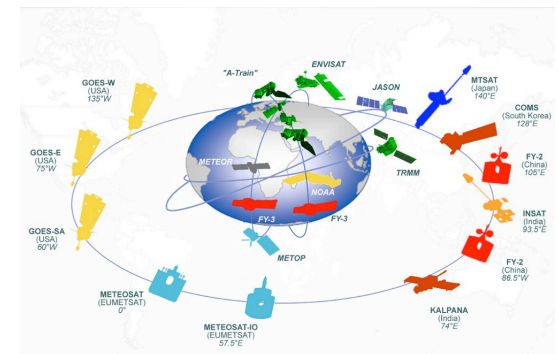
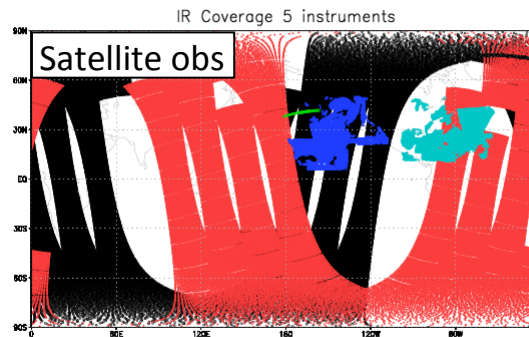
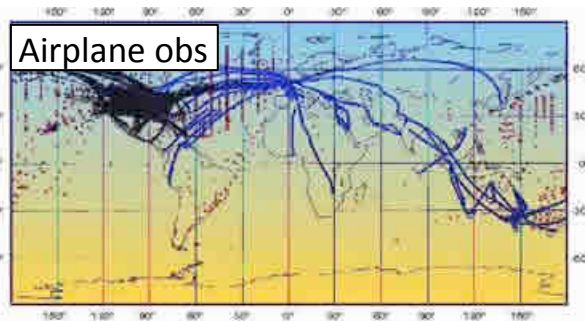
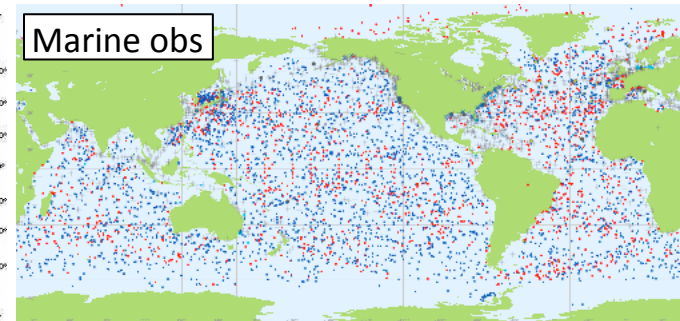
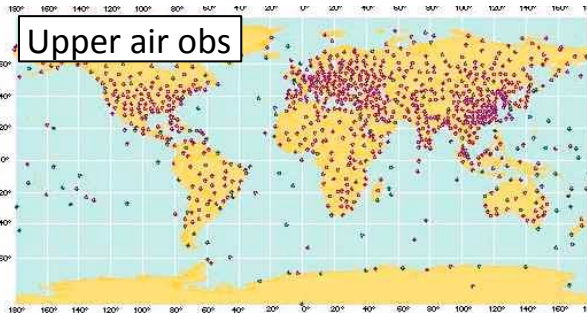
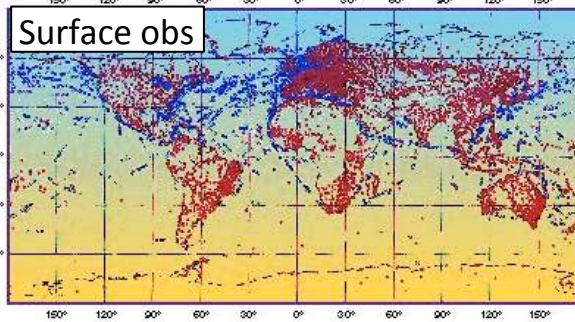
- ◆ Forward model $\mathbf{h}(\mathbf{x})$: Relationship between \mathbf{x} and \mathbf{y}

- Can be simple or complex

Uncertainty in Observations

◆ Characteristics of \mathbf{y}^0

- Heterogeneous, asynchronous, & noisy sampling of the evolving state \mathbf{x}^t
→ Uncertainty in the representation $\mathbf{y}=\mathbf{h}(\mathbf{x})$ [$\mathbf{y}^t=\mathbf{h}(\mathbf{x}^t)$?]
→ Modeling of observation likelihood: $p(\mathbf{y}|\mathbf{x})$



<http://www.wmo.int/pages/prog/www/OSY/GOS.html>

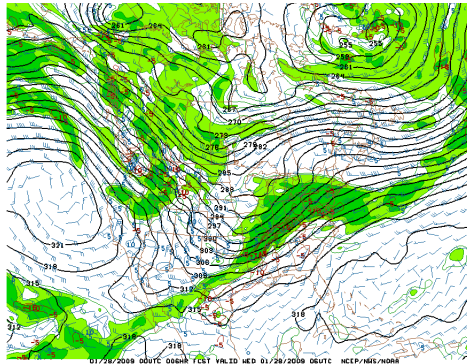
Schematic of Data Assimilation: Assimilation Window

- ◆ Data assimilation is a **method** that iterates the cycle over a window:

6hr for Operational System

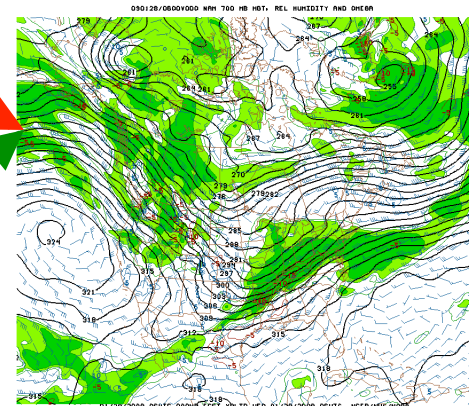
- **Model forecast: \mathbf{x}^b**

6h forecast (700mb) for 1.28.09 06UTC



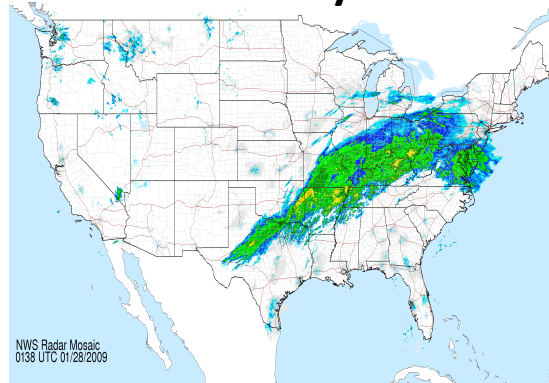
$p(\mathbf{x})$
[prior]

- **Analyzed model state: \mathbf{x}^a**



$p(\mathbf{x}|\mathbf{y})$
[posterior]

- **Observations: \mathbf{y}^o**

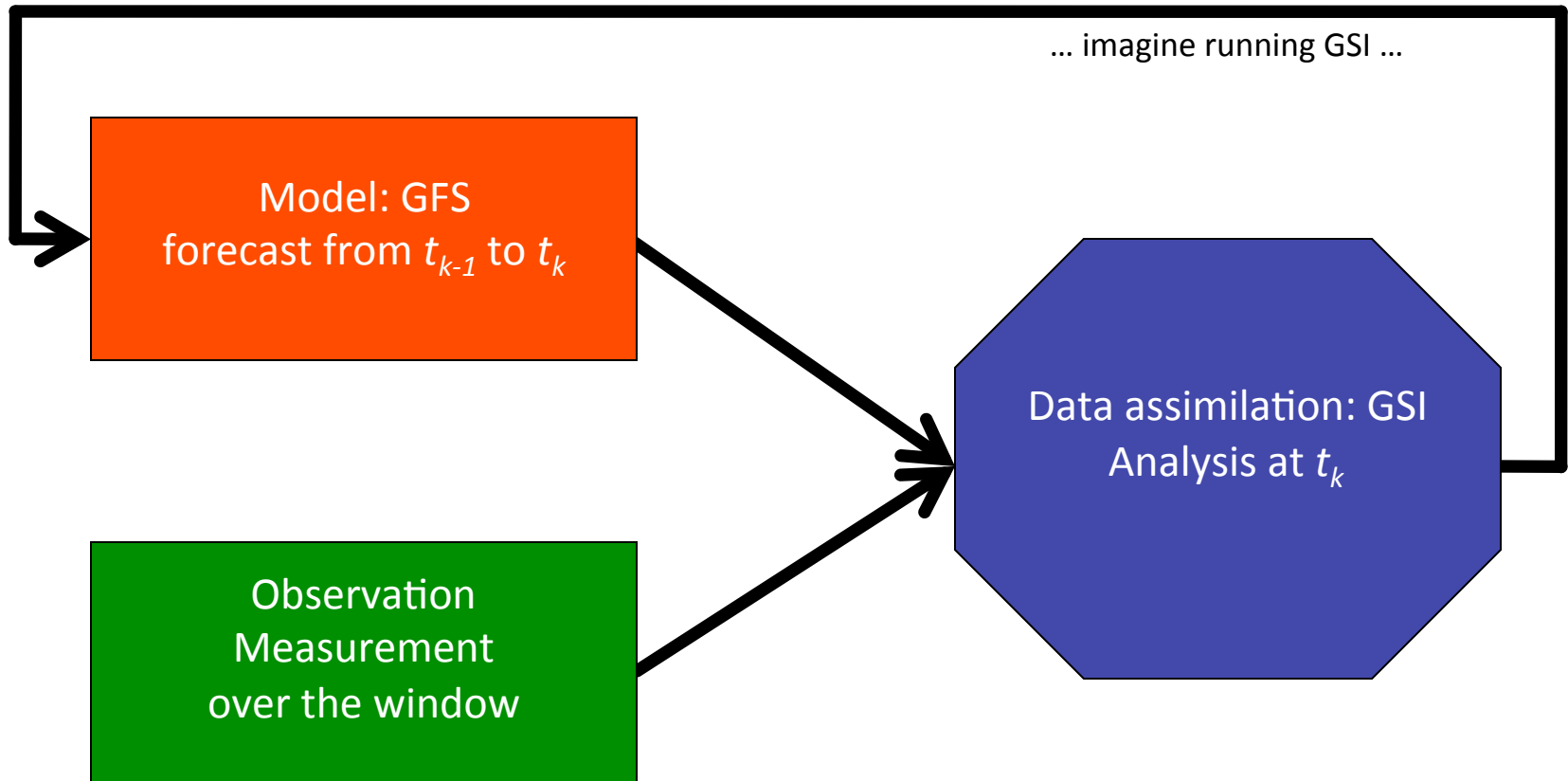


$p(\mathbf{y}|\mathbf{x})$
[obs likelihood]

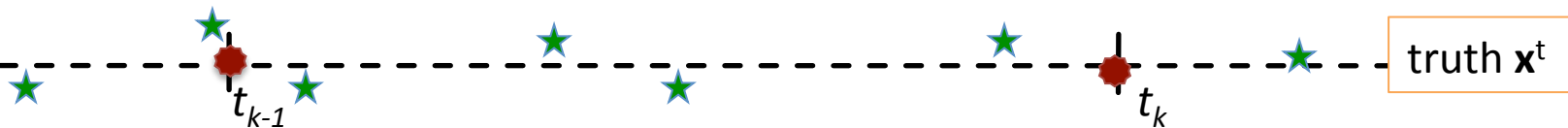
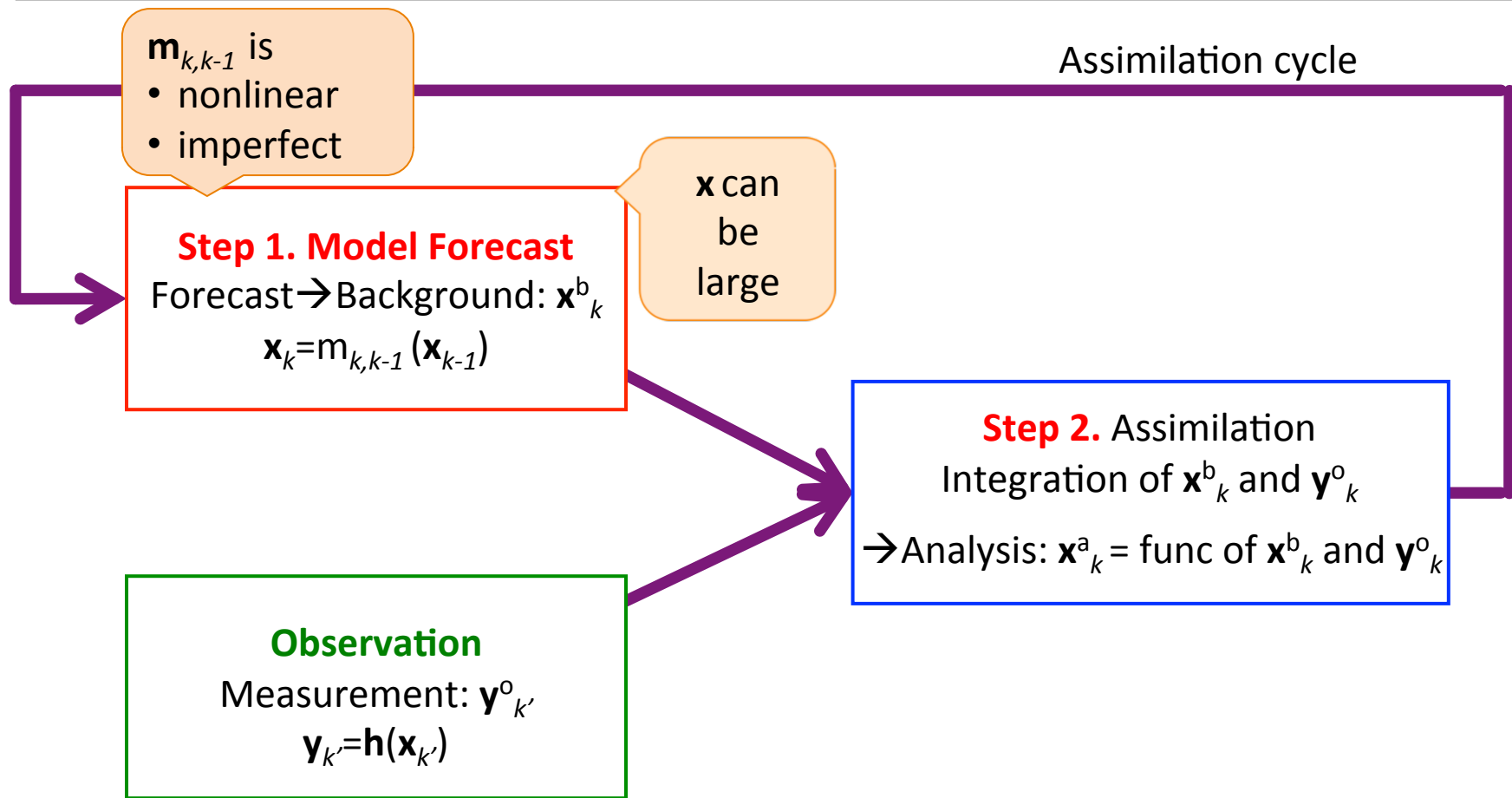
Elements of Data Assimilation

6hr Assimilation Window

... imagine running GSI ...



Challenges of Data Assimilation: Model



Challenges of Data Assimilation: Observation

Assimilation cycle

Step 1. Model Forecast

Forecast \rightarrow Background: \mathbf{x}_k^b

$$\mathbf{x}_k = m_{k,k-1}(\mathbf{x}_{k-1})$$

$h_{k'}$ is/may be

- nonlinear
- imperfect

Observation

Measurement: $\mathbf{y}_{k'}^o$

$$\mathbf{y}_{k'} = h(\mathbf{x}_{k'})$$

\mathbf{y} may be large or too small

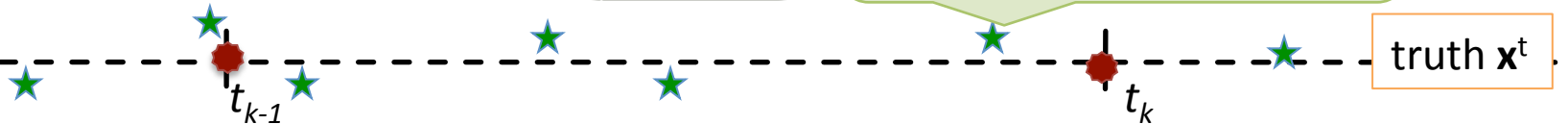
$\mathbf{y}_{k'}$ is/may be

- insufficient to determine \mathbf{x}_k
- not exactly at t_k

Step 2. Assimilation

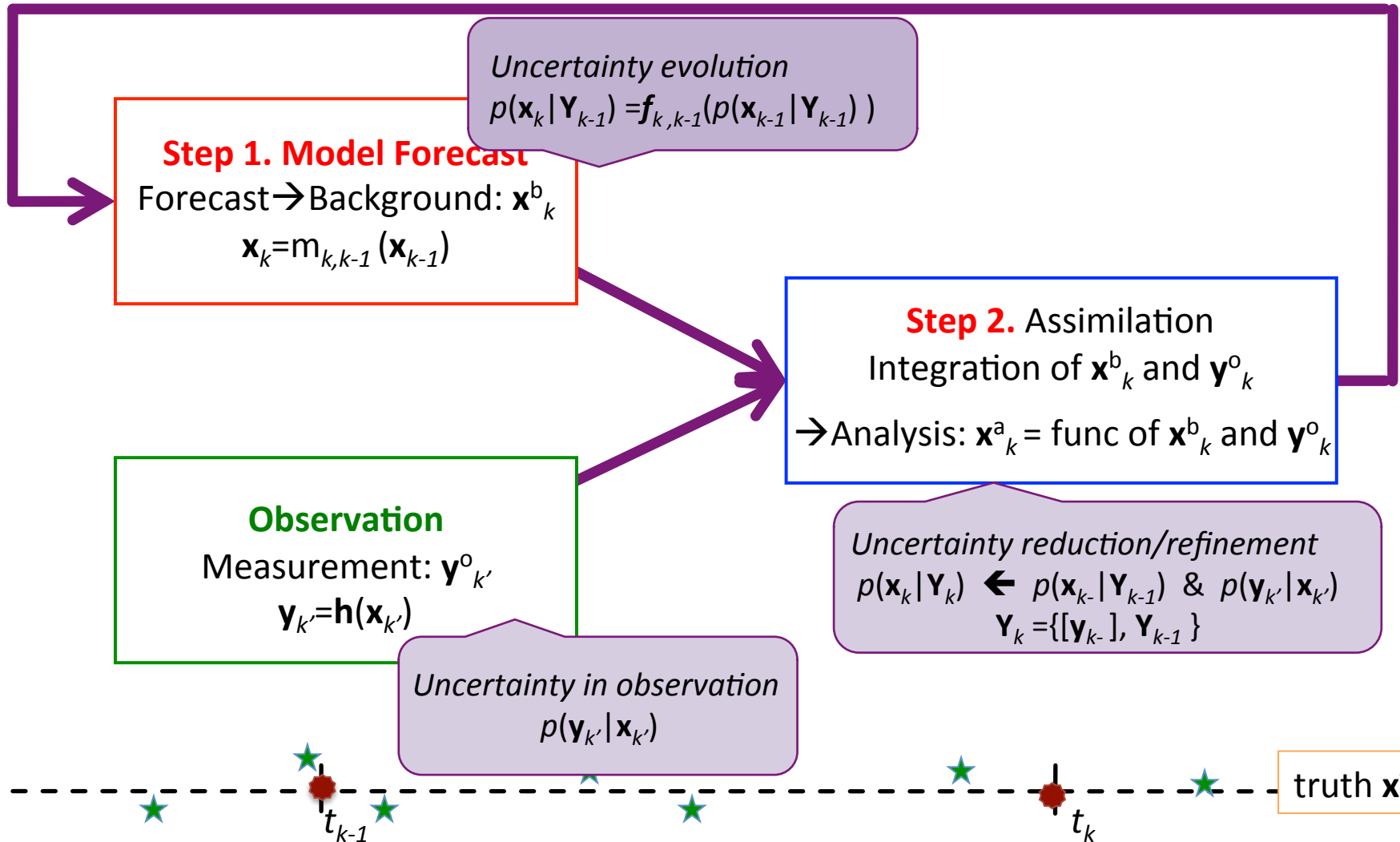
Integration of \mathbf{x}_k^b and \mathbf{y}_k^o

\rightarrow Analysis: $\mathbf{x}_k^a = \text{func of } \mathbf{x}_k^b \text{ and } \mathbf{y}_k^o$



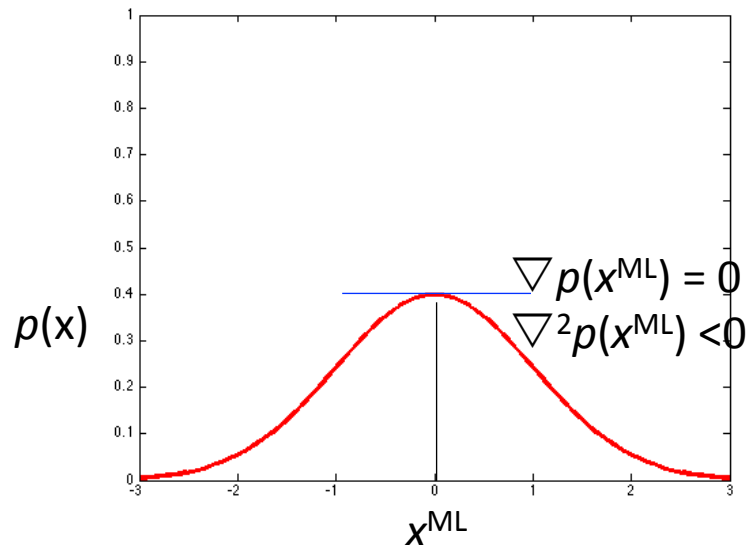
Data Assimilation Cycle With Probabilistic View

Assimilation cycle



Probability $p(\mathbf{x})$ & Data Assimilation Perspective I

- ◆ Probability $p(\mathbf{x}) \sim$ Likelihood (between 0 and 1) that value being \mathbf{x}
- ◆ Perspective: How to choose a “good” \mathbf{x} given $p(\mathbf{x})$
 - Maximum Likelihood (ML): \mathbf{x}^{ML} that is most likely
 - Conditions at $\mathbf{x}=\mathbf{x}^{\text{ML}}$ that maximizes $p(\mathbf{x})$
 - Extreme (=gradient $\mathbf{0}$): $\nabla p(\mathbf{x}) = \mathbf{0}$
 - Maximum (\sim convex) : $\nabla^2 p(\mathbf{x}) = (\text{semi-})\text{negative definite}$



Basic axioms

- $p(\mathbf{x}) > 0$ for all \mathbf{x}
- $\int p(\mathbf{x}) d\mathbf{x} = 1$

Expectation Based on Probability $p(\mathbf{x})$

◆ Expectation: $E[f(\mathbf{x})] = \int f(\mathbf{x})p(\mathbf{x})d\mathbf{x}$

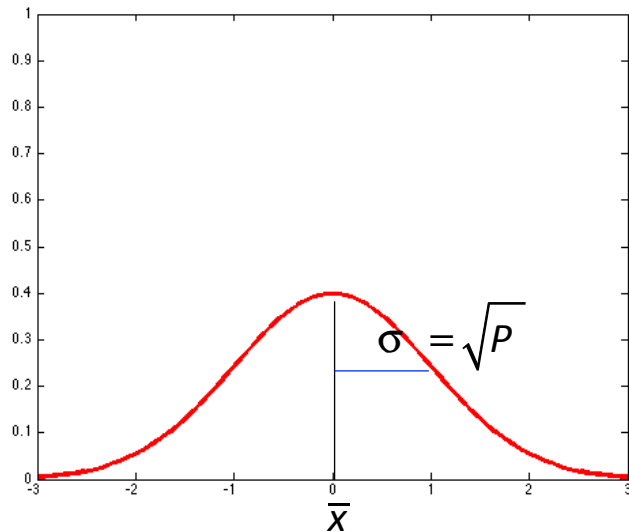
■ Mean $\bar{\mathbf{x}}$ = expected value of \mathbf{x}

$$\bar{x}_n = E[x_n] = \int x_n p(\mathbf{x}) d\mathbf{x}$$

■ Variance = (standard deviation)²
= Uncertainty around $\bar{\mathbf{x}}$

$$P_{nn} = E[(x_n - \bar{x}_n)^2] = \int (x_n - \bar{x}_n)^2 p(\mathbf{x}) d\mathbf{x}$$

$$\sigma_n = \sqrt{P_{nn}}$$



$$\bar{\mathbf{x}} = E[\mathbf{x}] = \int \mathbf{x} p(\mathbf{x}) d\mathbf{x} = \begin{pmatrix} \bar{x}_1 \\ \vdots \\ \bar{x}_N \end{pmatrix}$$

Cross-variable:

• Covariance

$$P_{in} = P_{ni} = E[(x_i - \bar{x}_i)(x_n - \bar{x}_n)] \\ = \int (x_i - \bar{x}_i)(x_n - \bar{x}_n) p(\mathbf{x}) d\mathbf{x}$$

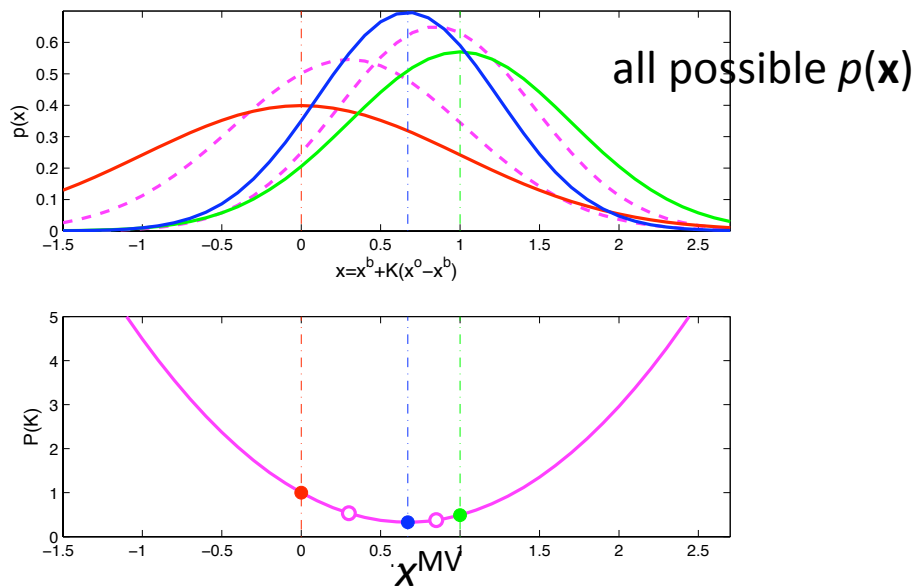
• Covariance matrix

$$\mathbf{P} = E[(\mathbf{x} - \bar{\mathbf{x}})(\mathbf{x} - \bar{\mathbf{x}})^T] = \int (\mathbf{x} - \bar{\mathbf{x}})(\mathbf{x} - \bar{\mathbf{x}})^T p(\mathbf{x}) d\mathbf{x}$$

$$= \begin{pmatrix} P_{11} & \dots & P_{1N} \\ & \ddots & \\ & & P_{ni} & \vdots \\ \vdots & P_{in} & \dots & P_{nn} & \vdots \\ & & & & \ddots \\ P_{N1} & \dots & & & P_{NN} \end{pmatrix}$$

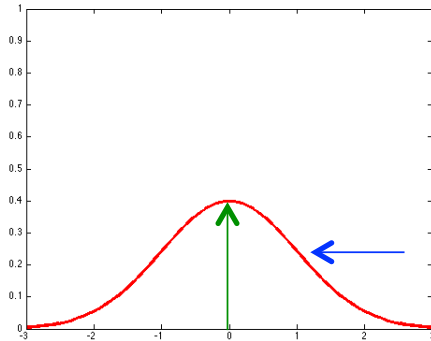
Probability $p(\mathbf{x})$ & Data Assimilation Perspective II

- ◆ Total uncertainty \sim total variance associated with $p(\mathbf{x})$: $\sum_{n=1}^N P_{nn} = \text{tr}\mathbf{P} = \sigma^2$
- ◆ Perspective: How to choose a “good” \mathbf{x}
 - Minimum Variance (MV): \mathbf{x}^{MV} with the least the risk
 - Conditions
 - Corresponding $p^{\text{MV}}(\mathbf{x})$ has the minimum variance among all $p(\mathbf{x})$
 - \mathbf{x}^{MV} is the expectation (mean) associated with $p^{\text{MV}}(\mathbf{x})$



Maximum Likelihood, Minimum Variance, and Data Assimilation

◆ Relationship between \mathbf{x}^{ML} and \mathbf{x}^{MV}



$$\int p(\mathbf{x}) d\mathbf{x} = 1$$
$$p_G(\mathbf{x}) = \frac{1}{(2\pi)^{N/2} |\mathbf{P}|^{1/2}} \exp\{-J_G(\mathbf{x})\}$$
$$J_G(\mathbf{x}) = \frac{1}{2}(\mathbf{x} - \bar{\mathbf{x}})^T \mathbf{P}^{-1}(\mathbf{x} - \bar{\mathbf{x}})$$

If probability density function (pdf) is Gaussian $p_G(\mathbf{x})$ & obs is linear, then $\mathbf{x}^{\text{ML}} = \mathbf{x}^{\text{MV}}$

◆ Practical data assimilation

- Estimation of $\bar{\mathbf{x}}$ and \mathbf{P}

- For large N , not easy to completely estimate \mathbf{P}

- Statistical:

3D methods

- Dynamical

- Tangent linear model:

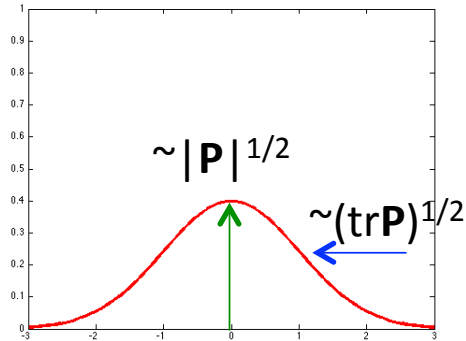
Extended Kalman filter / 4DVar

- Monte Carlo:

Ensemble Kalman Filter

Gaussian $p_G(\mathbf{x})$; 1D and 2D

◆ 1D

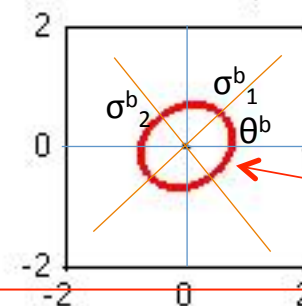
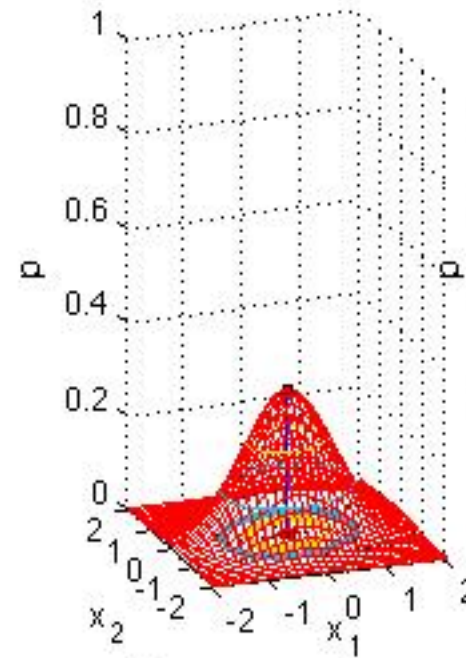


$$p_G(\mathbf{x}) = \frac{1}{(2\pi)^{N/2} |\mathbf{P}|^{1/2}} \exp\{-J_G(\Delta\mathbf{x})\}$$

$$\mathbf{x} = \bar{\mathbf{x}} + \Delta\mathbf{x}$$

$$J_G(\Delta\mathbf{x}) = \frac{1}{2} (\Delta\mathbf{x})^T \mathbf{P}^{-1} (\Delta\mathbf{x})$$

◆ 2D



$$(\Delta\mathbf{x})^T \mathbf{P}^{-1} (\Delta\mathbf{x}) = 1$$

P gives size of uncertainty as “ellipsoid”

Ensemble Approach to Represent $p(\mathbf{x})$

◆ Ensemble

- Members $\mathbf{x} = \{\mathbf{x}^{(m)}\} = \{\mathbf{x}^{(1)}, \dots, \mathbf{x}^{(M)}\}$
- Spread $\Delta\mathbf{X} = \{\mathbf{x}^{(m)} - \bar{\mathbf{x}}\} = \{\mathbf{x}^{(1)} - \bar{\mathbf{x}}, \dots, \mathbf{x}^{(M)} - \bar{\mathbf{x}}\}$

■ Mean

$$\bar{x}_n = \frac{1}{M} \sum_{m=1}^M x_n^{(m)}$$

$$\bar{\mathbf{x}} = \frac{1}{M} \sum_{m=1}^M \mathbf{x}^{(m)}$$

■ Covariance

$$P_{nn} = \frac{1}{M-1} \sum_{m=1}^M (x_n^{(m)} - \bar{x}_n)^2$$

$$P_{in} = P_{ni} = \frac{1}{M-1} \sum_{m=1}^M (x_i^{(m)} - \bar{x}_i)(x_n^{(m)} - \bar{x}_n)$$

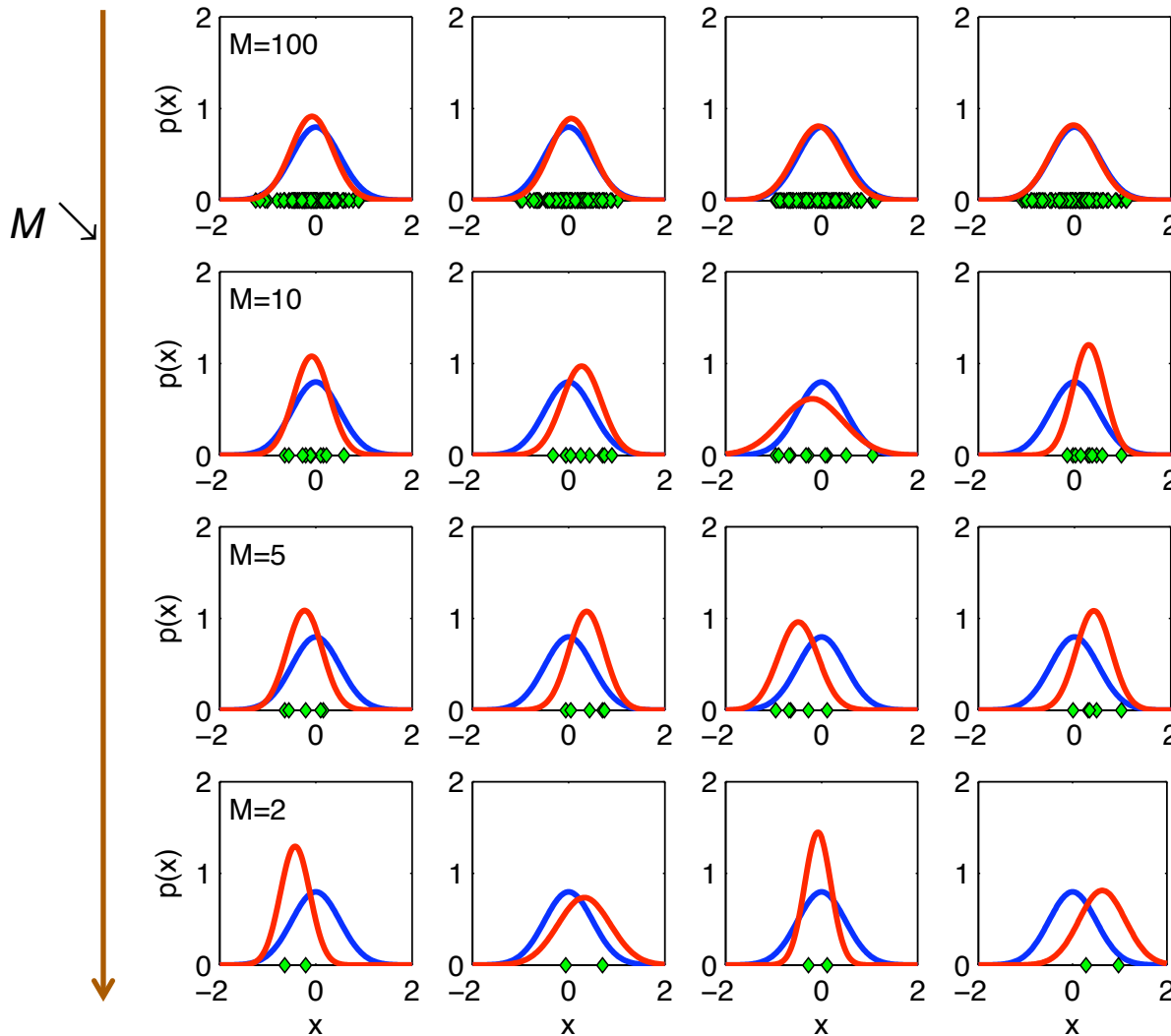
$$\mathbf{P} = \frac{1}{M-1} (\Delta\mathbf{X})(\Delta\mathbf{X})^T$$

◆ Issues

- Sampling of by ensemble can be lousy, especially for
 - Small M
 - Small P_{in}
- Rank of \mathbf{P} is at most $M-1$
- There infinitely many $\Delta\mathbf{X}$ that have the same $\mathbf{P} = (1/M-1)\Delta\mathbf{X}(\Delta\mathbf{X})^T$

$p(x)$ Sampling & Reconstruction by Ensemble: 1D

different realizations



Assuming Gaussian pdfs

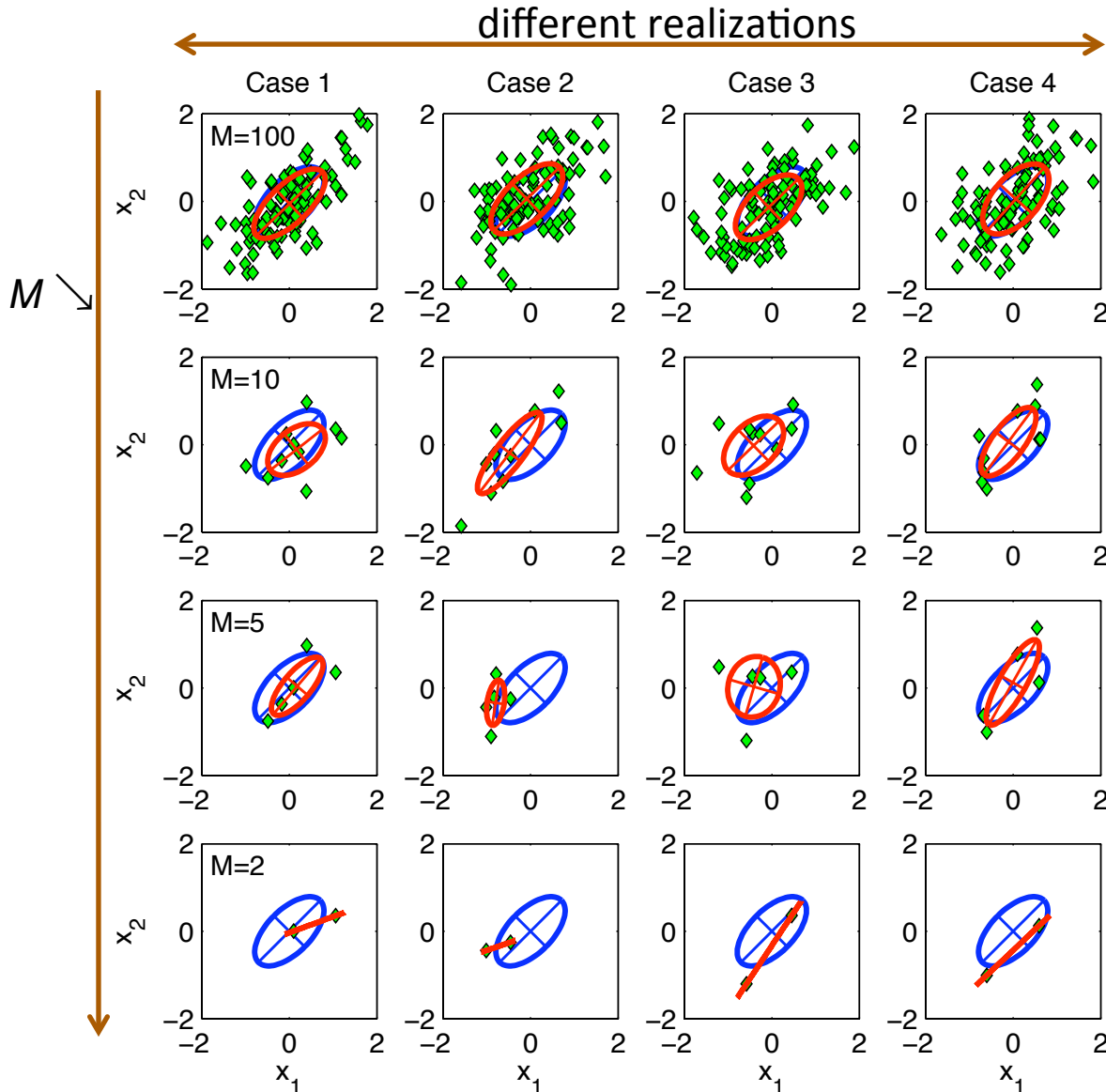
$$p(x) = \frac{1}{(2\pi)^{1/2} P^{1/2}} \exp\left(-\frac{1}{2} \frac{(x - \bar{x})^2}{P}\right)$$

$$p(\mathbf{x}) \Rightarrow \{\mathbf{x}_m\}$$

- orig. $p(x)$ by $(\bar{x}, P) = (0, 0.5)$
 - ◆ M sample* from $p(x)$
 - Reconstructed $p^*(x)$ by (\bar{x}^*, P^*)
- $$\{\mathbf{x}_m\} \Rightarrow p^*(\mathbf{x})$$

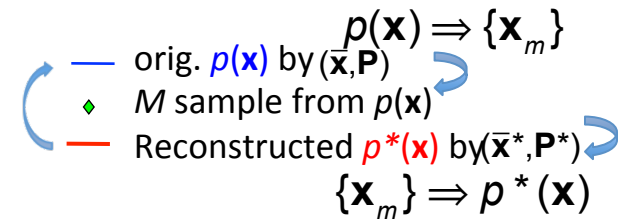
- If sampling is well-done, then $p^*(x) \sim p(x)$.
- 'Fitness' of $p^*(x)$ to $p(x)$ vary case by case particularly for small M .
- All cases, $N < M$.

$p(\mathbf{x})$ Sampling & Reconstruction by Ensemble: 2D



Assuming Gaussian pdfs

$$p(\mathbf{x}) = \frac{1}{(2\pi)^{N/2} |\mathbf{P}|^{1/2}} \exp\left(-\frac{1}{2}(\mathbf{x} - \bar{\mathbf{x}})^T \mathbf{P}^{-1}(\mathbf{x} - \bar{\mathbf{x}})\right)$$

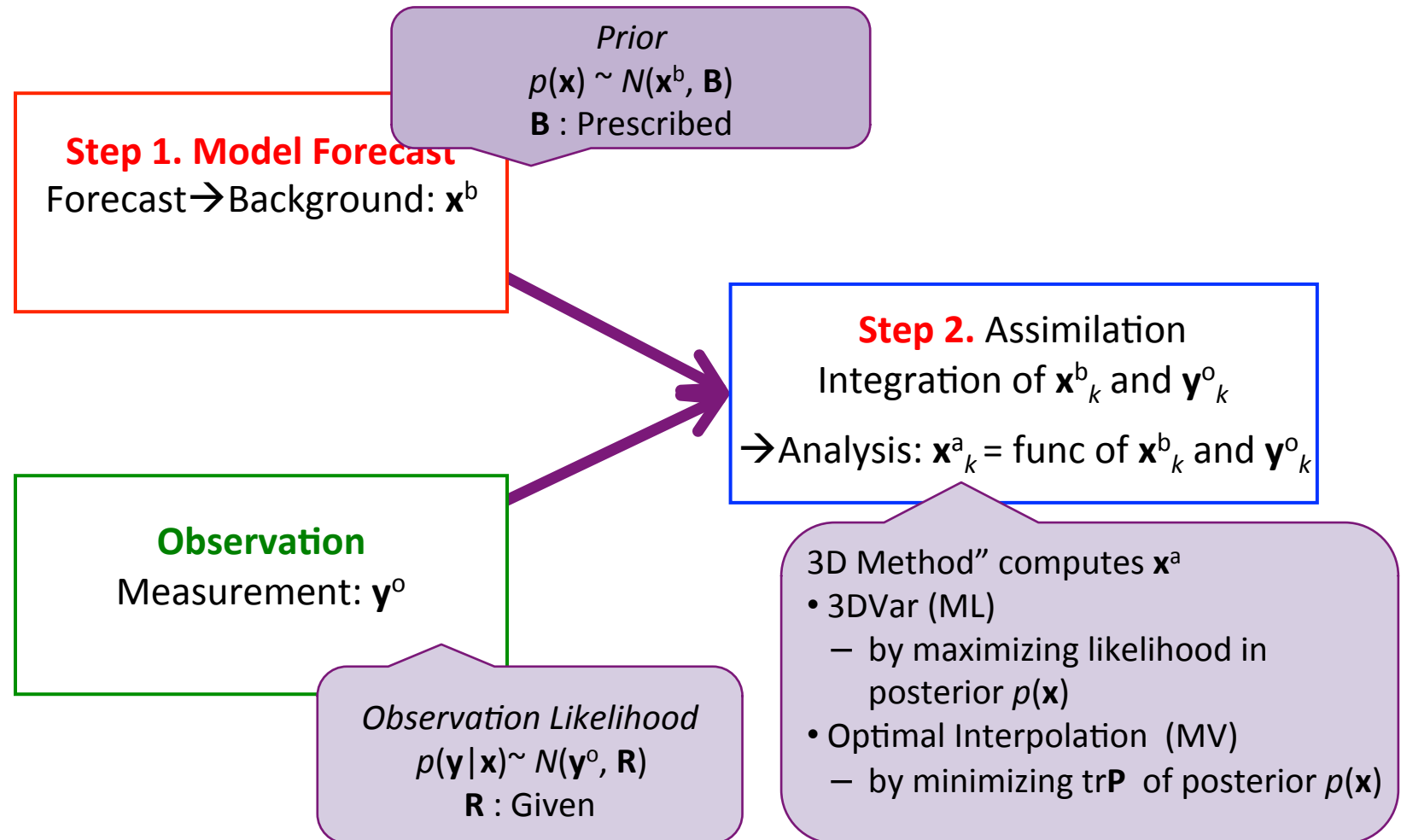


- If sampling is well-done, then $p^*(\mathbf{x}) \sim p(\mathbf{x})$.
- 'Fitness' of $p^*(\mathbf{x})$ to $p(\mathbf{x})$ vary case by case particularly for small M .
- All cases, $N \leq M$.

Outline

- ◆ Objectives
- ◆ Background
 - State \mathbf{x} & Observation \mathbf{y} - also $\mathbf{m}(\mathbf{x})$ & $\mathbf{h}(\mathbf{x})$
 - Probability $p(\mathbf{x})$ - also $p(\mathbf{x}|\mathbf{y})$ & $p(\mathbf{y}|\mathbf{x})$
 - Data assimilation perspectives
- ◆ 3D Method - 3 dimensions in space
 - OI = Optimal Interpolation
 - 3DVar = Variational
- ◆ 3D to 4D - 4th dimension is time
 - EKF/EnKF= Extended/Ensemble Kalman filter
 - FGAT = First Guess at Appropriate Time
 - 4DVar
 - Hybrid = between Var and EnKF - Current operational system
- ◆ Concluding remarks

Data Assimilation With Probabilistic View in 3D



Perspectives of Data Assimilation

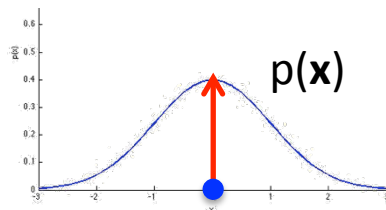
- ◆ Two main perspectives of practical data assimilation & hybrid approach

Variational Approach:

Least square estimation

[maximum likelihood]

- 3D-Var (3 dim in space)
- 4D-Var (4th dim is time)

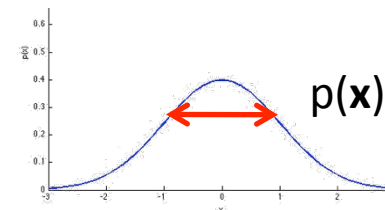


Sequential (KF) Approach:

Minimum Variance estimate

[least uncertainty]

- Optimal Interpolation (OI)
- (Extended / Ensemble) Kalman Filter



Hybrid

- ◆ Data assimilation is fast growing domain
 - Advanced methods are being developed as interdisciplinary science
 - A variety of extension & applications exist and are under development

OI

◆ Approach: MV using Best Linear Unbiased Estimation (BLUE)

- Idea: Determine \mathbf{x} as linear combination of the two information

$$\mathbf{x} = \mathbf{G} \mathbf{x}^b + \mathbf{K} \mathbf{y}^o = \mathbf{x}^t + \boldsymbol{\varepsilon} \quad \text{with } \boldsymbol{\varepsilon} \sim (0, \mathbf{P}) \quad \text{or } \mathbf{P} = E[\boldsymbol{\varepsilon}(\boldsymbol{\varepsilon})^T]$$

such that resulting \mathbf{x}^{OI} has

- Minimum variance (least risk) min: $tr\mathbf{P} = \sum_n^N P_{nn}$
- No bias: $E[\boldsymbol{\varepsilon}] = \mathbf{0}$
- Mathematical problem: Determine \mathbf{G} and \mathbf{K} as such.
- Statistical property: $\mathbf{x}^a = \mathbf{x}^{OI}$ has less risk (=is better) than \mathbf{x}^b or \mathbf{y}^o

◆ Solution

- Analytical:

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

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

Although not required

$$\mathbf{P}^a = \mathbf{P}^{OI} = (\mathbf{I} - \mathbf{K}^{OI} \mathbf{H})\mathbf{B}$$

- Computational:

$$\mathbf{x}^a = \mathbf{x}^{OI} = \mathbf{x}^b + \mathbf{B}\mathbf{H}^T \mathbf{z}$$

where \mathbf{z} is solution to $(\mathbf{H}\mathbf{B}\mathbf{H}^T + \mathbf{R})^{-1} \mathbf{z} = \mathbf{d}$

$$\mathbf{d} = \mathbf{y}^o - \mathbf{h}(\mathbf{x}^b)$$

OI: 1D Example

◆ Background (x^b, B)

◆ Observation (x^o, R) with $y=x$

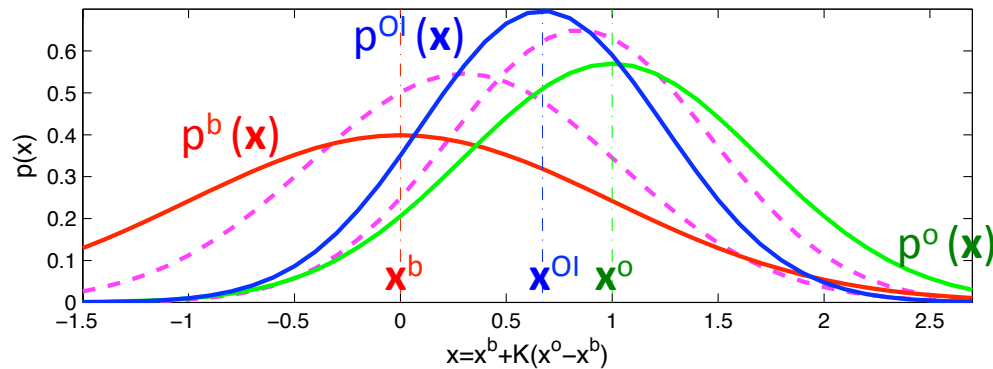
→ Analysis

$$x^a = x^{OI} = (1-K^{OI})x^b + K^{OI}x^o$$

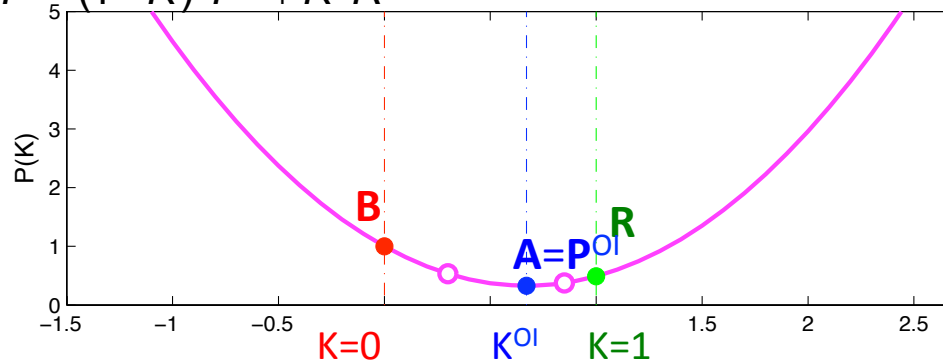
$$trP^{OI} = (1-K^{OI})B = R/(B+R)$$

$$K^{OI} = \frac{B}{R+B}$$

$$= \frac{(B/R)}{1+(B/R)} \rightarrow \begin{cases} 0 & \text{as } B/R \rightarrow 0 \\ 1 & \text{as } B/R \rightarrow \infty \end{cases}$$



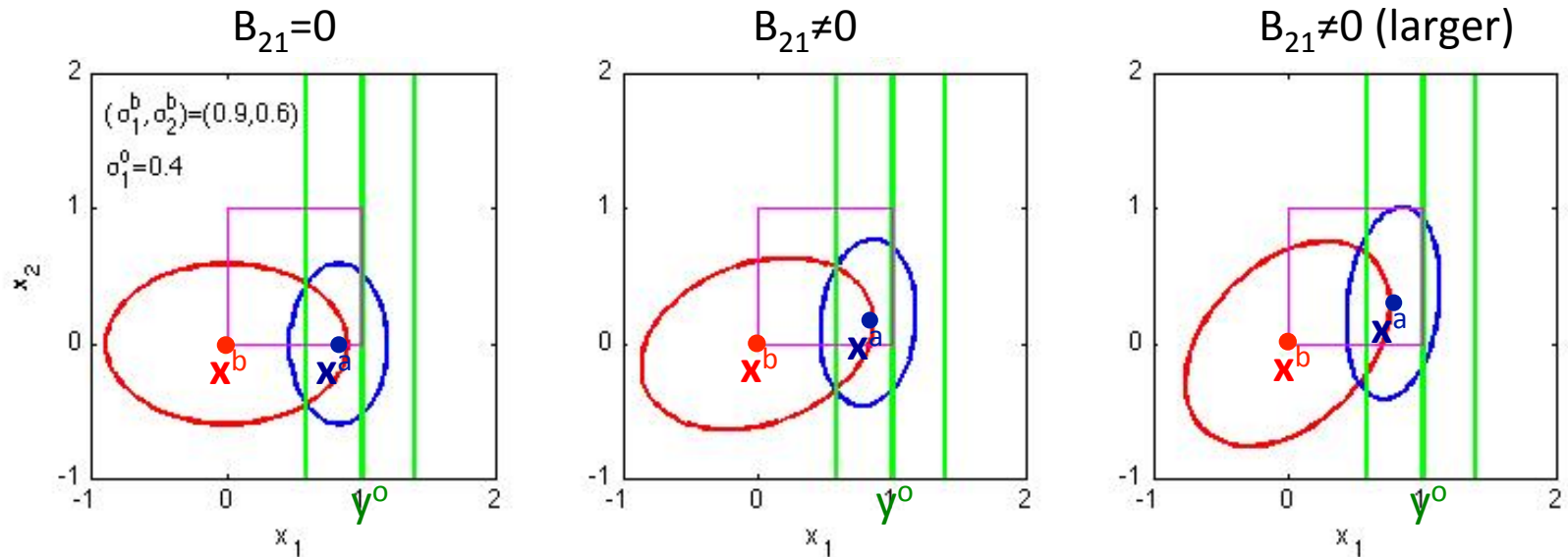
$$P = (1-K)^2 P^b + K^2 R^o$$



OI: 2D Example with Effect of Correlation B_{21}

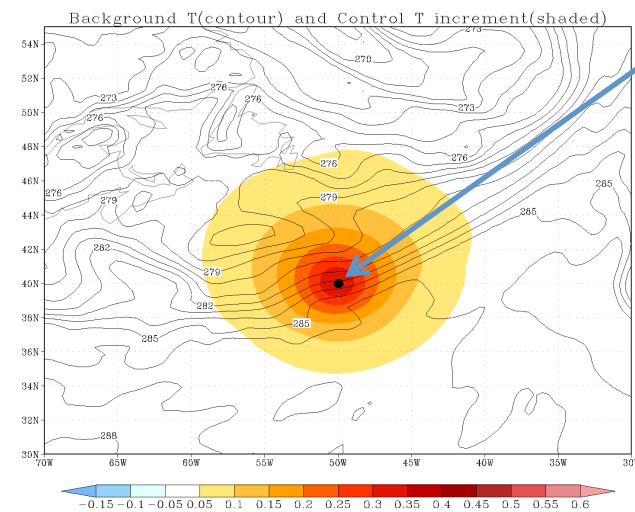
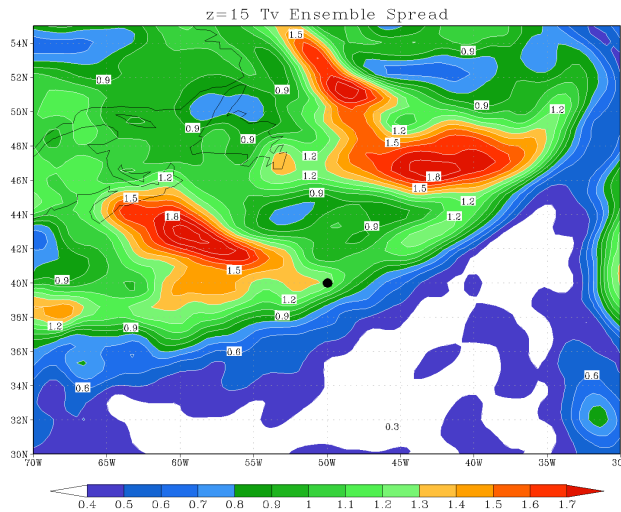
- ◆ Background $\mathbf{x}^b = \begin{pmatrix} x_1^b \\ x_2^b \end{pmatrix}$, $\mathbf{B} = \begin{pmatrix} B_{11} & B_{12} \\ B_{21} & B_{22} \end{pmatrix}$
- ◆ Observation $y^o = x_1^o$, R with $\mathbf{H}\mathbf{x} = [1, 0]\mathbf{x}$
- Analysis $\mathbf{x}^{OI} = \mathbf{x}^b + \Delta\mathbf{x}^{OI}$ $\Delta\mathbf{x}^{OI} = \begin{pmatrix} \Delta x_1^{OI} \\ \Delta x_2^{OI} \end{pmatrix} = \frac{1}{B_{11} + R} \begin{pmatrix} B_{11} \\ B_{21} \end{pmatrix} (x_1^o - x_1^b)$

$\Delta\mathbf{x}^{OI}$ and $\mathbf{B}\mathbf{H}^T$ has the same form



Optimal Interpolation (OI): GSI Example

- ◆ Effect of correlation: $\mathbf{B} \rightarrow \Delta x_n^{OI}$ (single obs for x_i) with GSI



x_i position

3DVar
[=OI]

$$\begin{pmatrix} \Delta x_1^{OI} \\ \vdots \\ \Delta x_i^{OI} \\ \vdots \\ \Delta x_N^{OI} \end{pmatrix} = \frac{1}{R + B_{ii}} \begin{pmatrix} B_{1i} \\ \vdots \\ B_{ii} \\ \vdots \\ B_{Ni} \end{pmatrix} (y^o - x^b)$$

\mathbf{B} determines the quality of Δx^{OI}

Single 850mb Tv observation (1K O-F, 1K error) – Courtesy of D. Kleist

Perspectives of Data Assimilation

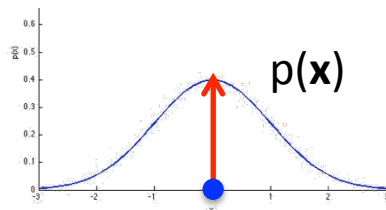
- ◆ Two main perspectives of practical data assimilation & hybrid approach

Variational Approach:

Least square estimation

[maximum likelihood]

- 3D-Var (3 dim in space)
- 4D-Var (4th dim is time)

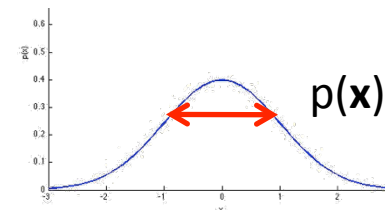


Sequential (KF) Approach:

Minimum Variance estimate

[least uncertainty]

- Optimal Interpolation (OI)
- (Extended / Ensemble) Kalman Filter



Hybrid

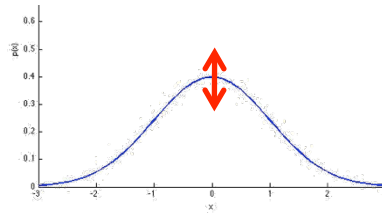
- ◆ Data assimilation is fast growing domain
 - Advanced methods are being developed as interdisciplinary science
 - A variety of extension & applications exist and are under development

3DVar: Setting

Baye's theorem for Maximum Likelihood (ML / MLL)

$$p(\mathbf{x}|\mathbf{y}) = \frac{p(\mathbf{y}|\mathbf{x})p(\mathbf{x})}{p(\mathbf{y})} \quad \leftarrow p(\mathbf{x},\mathbf{y})=p(\mathbf{x}|\mathbf{y})p(\mathbf{y})=p(\mathbf{y}|\mathbf{x})p(\mathbf{x})$$

- ◆ Goal: find \mathbf{x} that maximizes $p(\mathbf{x}|\mathbf{y})$ obtained by maximum (log)likelihood.



- ◆ Base PDFs in RHS.

- Background (prior \mathbf{x}): $\boldsymbol{\varepsilon}^b = \mathbf{x}^b - \mathbf{x}^t$ is Gaussian

$$p(\mathbf{x}) = \frac{1}{(2\pi)^{N/2} |\mathbf{B}|^{1/2}} \exp\{-J^b(\mathbf{x})\} \quad J^b(\mathbf{x}) = \frac{1}{2}(\mathbf{x} - \mathbf{x}^b)^T \mathbf{B}^{-1}(\mathbf{x} - \mathbf{x}^b)$$

- Observation (conditional \mathbf{y}): $\boldsymbol{\varepsilon}^o = \mathbf{y}^o - \mathbf{y}^t$ is Gaussian

$$p(\mathbf{y}|\mathbf{x}) = \frac{1}{(2\pi)^{L/2} |\mathbf{R}|^{1/2}} \exp\{-J^o(\mathbf{x})\} \quad J^o(\mathbf{x}) = \frac{1}{2}(\mathbf{y}^o - \mathbf{h}(\mathbf{x}))^T \mathbf{R}^{-1}(\mathbf{y}^o - \mathbf{h}(\mathbf{x}))$$

3DVar: Formulation

- ◆ Maximum Likelihood (ML) by Bayes' theorem

$$p(\mathbf{x}|\mathbf{y}) = \frac{\exp\{-J(\mathbf{x})\}}{(2\pi)^{(N+L)/2} |\mathbf{R}|^{1/2} |\mathbf{B}|^{1/2} p(\mathbf{y})}$$

= Minimum of the Cost function

$$J(\mathbf{x}) = J^b(\mathbf{x}) + J^o(\mathbf{x})$$

$$J^b(\mathbf{x}) = (1/2) (\mathbf{x}-\mathbf{x}^b)^T \mathbf{B}^{-1}(\mathbf{x}-\mathbf{x}^b)$$

$$J^o(\mathbf{x}) = (1/2) (\mathbf{y}^o-\mathbf{h}(\mathbf{x}))^T \mathbf{R}^{-1}(\mathbf{y}^o-\mathbf{h}(\mathbf{x}))$$

Conditions

- $\nabla J(\mathbf{x}) = 0$
- $\nabla^2 J(\mathbf{x}) = \text{semi-positive definite}$

- ◆ For linear observation $\mathbf{y}=\mathbf{H}\mathbf{x}$, analytical solution

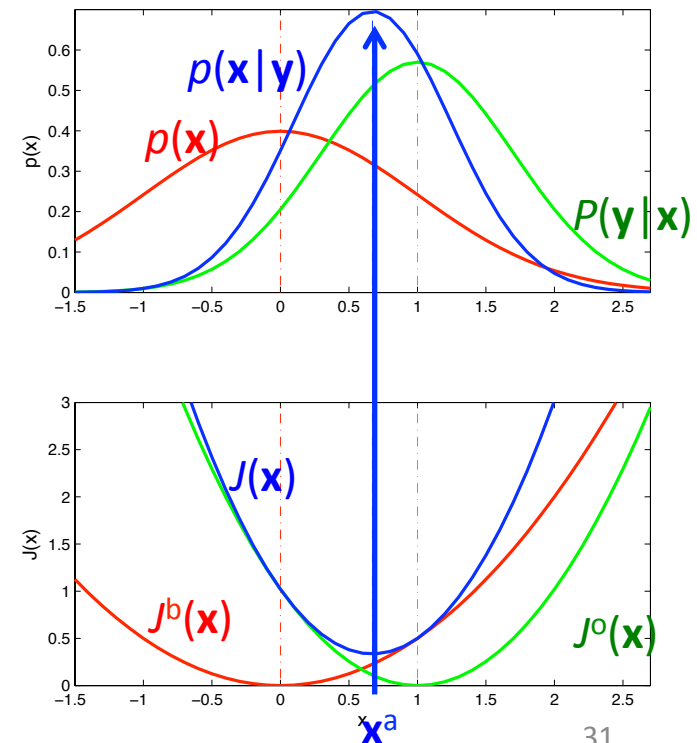
$$\mathbf{x}^a = \mathbf{x}^{OI} = \mathbf{x}^{3DVar}$$

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

1D schematics

ML at \mathbf{x}^a

$(\mathbf{x}^b, \mathbf{P}^b) = (0, 1)$ & $(\mathbf{x}^o, \mathbf{P}^o) = (1, 0.49) \rightarrow (\mathbf{x}^a, \mathbf{P}^a) = (0.67114, 0.32886)$



3DVar: Computational Approach

◆ Computational algorithm: Given

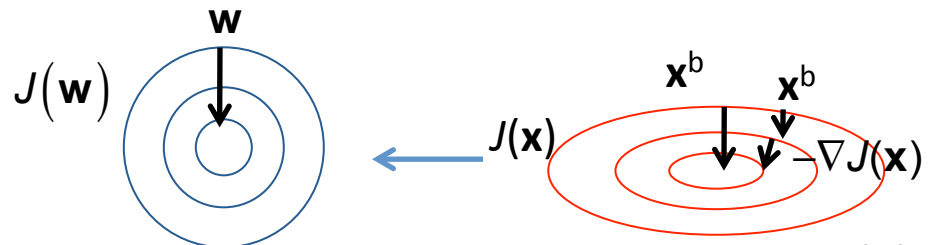
- Cost function $J(\mathbf{x})$
- Gradient function $\nabla J(\mathbf{x})$
- Initial “guess” \mathbf{x}^b

Using algorithms such as

- Conjugate gradient
- Quasi-Newton method

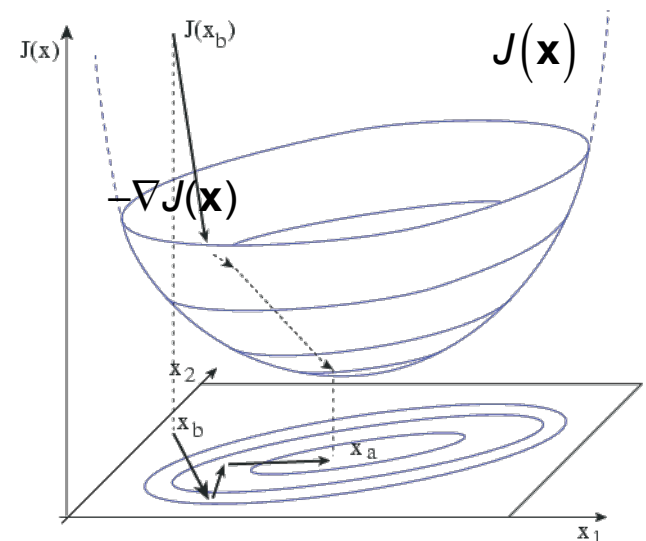
◆ Efficiency

- Pre-conditioning
 - Change of coordinate \mathbf{x} to \mathbf{w}



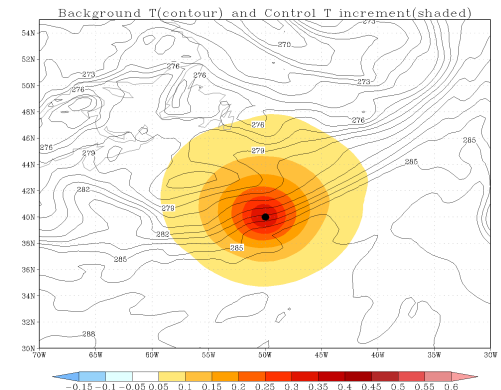
- (In)homogeneity around the minimum: Controlled by the Hessian of $J(\mathbf{x})$
- For nonlinear forward model for observation,
 - Inner loop by incremental 3DVar (linearization of nonlinear model)
 - Occasional outer loop with full nonlinear forward model

ECMWF Technical Note



3DVar: Additional Topics

- ◆ Flexibility of $J(\mathbf{x})$ $= J^b(\mathbf{x}) + J^o(\mathbf{x})$
 - Quadratic, under the Gaussian assumption for the error distribution but can be other functional form
 - Variational quality control for observations
 - Can add constraint : $J(\mathbf{x}) = J^b(\mathbf{x}) + J^o(\mathbf{x}) + J^c(\mathbf{x})$
 - Reduction of unwanted fast gravity waves
 - Can use variable transformation (weak constraint)
 - Improved use of observations & preservation of dynamic balance
- ◆ Challenges: Modeling of static \mathbf{B} (same for OI)
 - Cross-variable correlations
 - ← Variable transformation for better representation
 - Mostly homogenous
(can add some flow dependence but not much)



Outline

- ◆ Objectives
- ◆ Background
 - State \mathbf{x} & Observation \mathbf{y} - also $\mathbf{m}(\mathbf{x})$ & $\mathbf{h}(\mathbf{x})$
 - Probability $p(\mathbf{x})$ - also $p(\mathbf{x}|\mathbf{y})$ & $p(\mathbf{y}|\mathbf{x})$
 - Data assimilation perspectives
- ◆ 3D Method - 3 dimensions in space
 - OI = Optimal Interpolation
 - 3DVar = Variational
- ◆ 3D to 4D - 4th dimension is time
 - EKF/EnKF= Extended/Ensemble Kalman filter -- Dynamics
 - FGAT = First Guess at Appropriate Time -- Obs
 - 4DVar
 - Hybrid = between Var and EnKF - Current operational system
- ◆ Concluding remarks

Kalman Filters: Extension to Sequential Methods

- ◆ By explicitly targeting \mathbf{P} , the analytical form of \mathbf{P}^{OI} ($=\mathbf{A}$) is also available.
- ◆ OI itself doesn't require the computation of \mathbf{P}^{OI} .

$$\mathbf{x}_k^{\text{b}} \rightarrow \mathbf{x}_k^{\text{a}} \quad [\mathbf{B} \text{ is static, no need for } \mathbf{A}]$$

- ◆ Extended/Ensemble Kalman filter makes use of \mathbf{A} ,

$$(\mathbf{x}_k^{\text{b}}, \mathbf{B}_k) \rightarrow (\mathbf{x}_k^{\text{a}}, \mathbf{A}_k) \quad [\mathbf{A}_k \text{ is obtained along with } \mathbf{x}_k^{\text{a}}]$$

to estimate \mathbf{B}_{k+1} in the next assimilation cycle

$$(\mathbf{x}_k^{\text{a}}, \mathbf{A}_k) \rightarrow (\mathbf{x}_{k+1}^{\text{b}}, \mathbf{B}_{k+1}) \quad [\text{Model needs to forecast } \mathbf{A}_k \text{ to } \mathbf{B}_{k+1}]$$

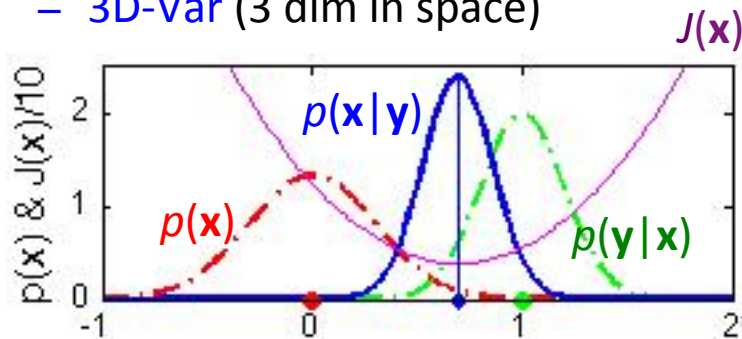
“4D”ness in Dynamic Forecast: Extended Kalman Filter

Variational Approach:

Least square estimation

[maximum likelihood]

- 3D-Var (3 dim in space)



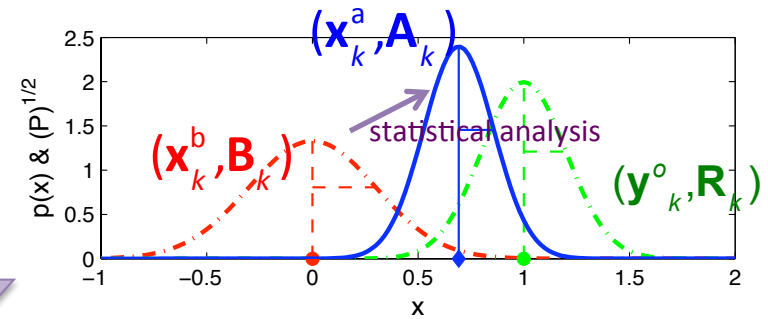
- 4D-Var (4th dim is time)

“Sequential” Approach:

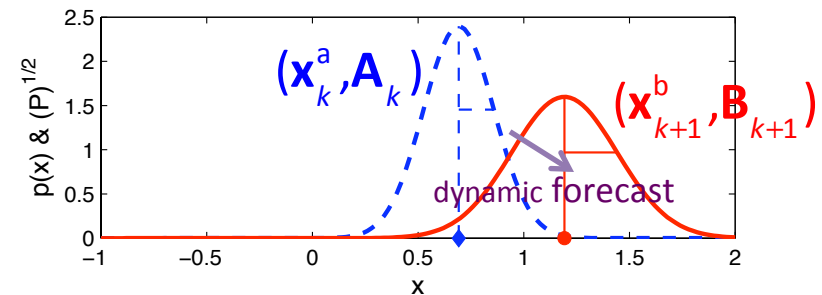
Minimum Variance estimate

[least uncertainty]

- Optimal Interpolation (OI)



- Extended Kalman Filter



x forecast: Nonlinear model

A->**B** forecast: Tangent linear model (TLM)

Sequential Approach: Extended Kalman Filter

- ◆ Basic concept for dynamic estimation of \mathbf{A}_{k-1} to \mathbf{B}_k by perturbation growth
- ◆ Extended Kalman Filter (EKF)
 - Error covariance $\mathbf{P}_k = E[\boldsymbol{\varepsilon}_k (\boldsymbol{\varepsilon}_k)^T]$ evolution using Tangent Linear Model (TLM)

$$\mathbf{P}_k = \mathbf{M}_{k,k-1} \mathbf{P}_{k-1} (\mathbf{M}_{k,k-1})^T$$

$$[\boldsymbol{\varepsilon}_k = \mathbf{M}_{k,k-1} \boldsymbol{\varepsilon}_{k-1}]$$

- Formulation

Step 1. Forecast

$$\mathbf{x}_k^b = \mathbf{m}_{k,k-1} (\mathbf{x}_{k-1}^a)$$

$$\mathbf{B}_k = \mathbf{M}_{k,k-1} \mathbf{A}_k \mathbf{M}_{k,k-1}^T \quad [+ \mathbf{Q}_k]$$

Step 2. Analysis

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

$$\mathbf{A}_k = (\mathbf{I} - \mathbf{K}_k \mathbf{H}_k) \mathbf{B}_k$$

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

Extended Kalman Filter

Step 1. Forecast ($\mathbf{x}_k^b, \mathbf{B}_k$)

Obtained by integrating

$$\mathbf{x}_k^b = \mathbf{m}_{k,k-1}(\mathbf{x}_{k-1}^a)$$

$$\mathbf{B}_k = \mathbf{M}_{k,k-1} \mathbf{A}_k \mathbf{M}_{k,k-1}^T [+ \mathbf{Q}_k]$$

starting from ($\mathbf{x}_{k-1}^a, \mathbf{A}_{k-1}$) over $[t_{k-1}, t_k]$

Model

Forecast: \mathbf{x}^b, \mathbf{B}

$$\mathbf{x}_k = \mathbf{m}_{k,k-1}(\mathbf{x}_{k-1}) : \quad \mathbf{x} \in \mathbb{R}^N$$

Observation

Measurement: \mathbf{y}^o

$$\mathbf{y}_k = \mathbf{h}_k(\mathbf{x}_k) : \quad \mathbf{y} \in \mathbb{R}^L$$

$(\mathbf{y}^o, \mathbf{R})$

\mathbf{R} : prescribed

EKF

Analysis: \mathbf{x}^a, \mathbf{A}

$$(\mathbf{x}_k^a, \mathbf{A}_k) = \text{fnc. of } (\mathbf{x}_k^b, \mathbf{B}_k; \mathbf{y}_k^o, \mathbf{R}_k)$$

Step 2. Analysis ($\mathbf{x}_k^a, \mathbf{A}_k$)

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

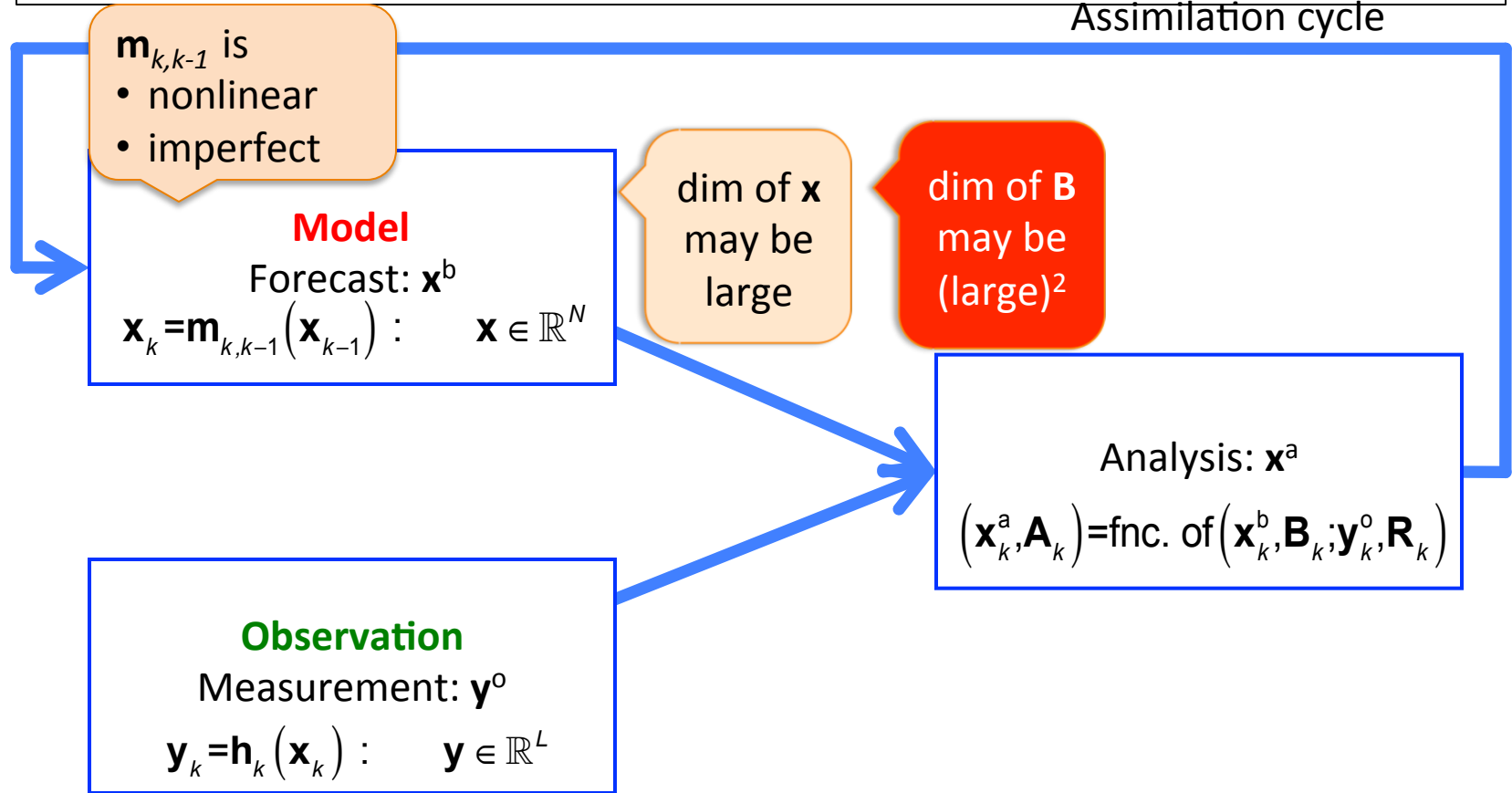
$$\mathbf{A}_k = (\mathbf{I} - \mathbf{K}_k \mathbf{H}_k) \mathbf{B}_k$$

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

time 

Extended Kalman Filter: Challenges

Assimilation cycle



\mathbf{x}_{k-1}

\mathbf{x}_k

Assimilation window
time

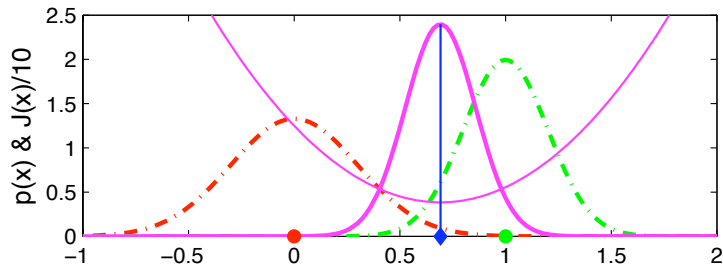
“4D”ness in Dynamic Forecast: Ensemble Kalman Filter (EnKF)

Variational Approach:

Least square estimation

[maximum likelihood]

– 3D-Var (3 dim in space)



– 4D-Var (4th dim is time)

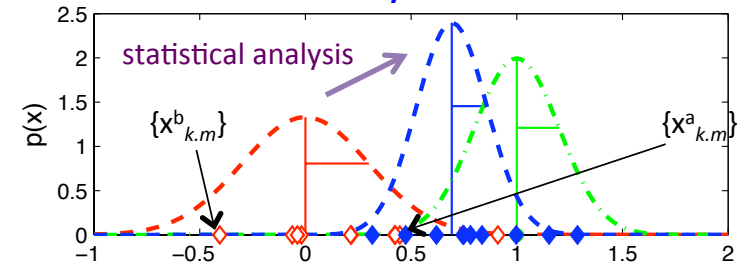
“Ensemble Kalman Filter (EnKF)”

Approach :

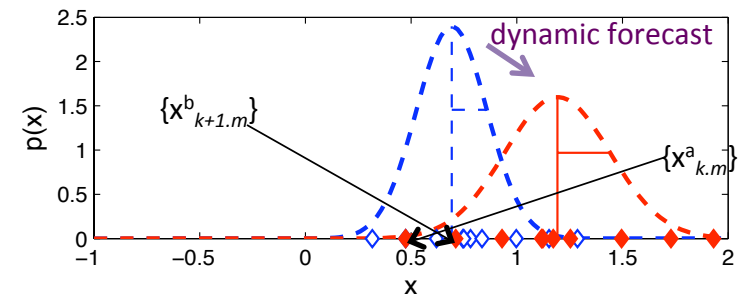
Minimum Variance estimate

use $\{\mathbf{x}_{k,m}\}$ to infer/approx. $p(\mathbf{x}, t_k)$

– Ensemble analysis



– Ensemble forecast



$$\{\mathbf{x}_{k,m}\} = (\mathbf{x}_{k,1}, \dots, \mathbf{x}_{k,M}) \in \mathbb{R}^{N \times M}$$

k : time t_k M : ensemble size

Ensemble Kalman Filter

Step 1. Forecast $\{\mathbf{x}^{b(m)}_k\}$
 Obtained by integrating

$$\mathbf{x}_k^{b(m)} = \mathbf{m}_{k,k-1}(\mathbf{x}_{k-1}^{a(m)})$$

starting from $\mathbf{x}_{k-1}^{a(m)}$ over $[t_k, t_k]$

Model

Forecast: \mathbf{x}^b

$$\mathbf{x}_k = \mathbf{m}_{k,k-1}(\mathbf{x}_{k-1}) : \quad \mathbf{x} \in \mathbb{R}^N$$

Observation

Measurement: \mathbf{y}^o

$$\mathbf{y}_k = \mathbf{h}_k(\mathbf{x}_k) : \quad \mathbf{y} \in \mathbb{R}^L$$

$(\mathbf{y}^o, \mathbf{R})$
 \mathbf{R} : prescribed

EnKF

Analysis: \mathbf{x}^a

$$(\mathbf{x}_k^a, \mathbf{A}_k) = \text{fnc. of } (\mathbf{x}_k^b, \mathbf{B}_k; \mathbf{y}_k^o, \mathbf{R}_k)$$

Step 2. Analysis $\{\mathbf{x}^{a(m)}_k\}$ that achieves

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

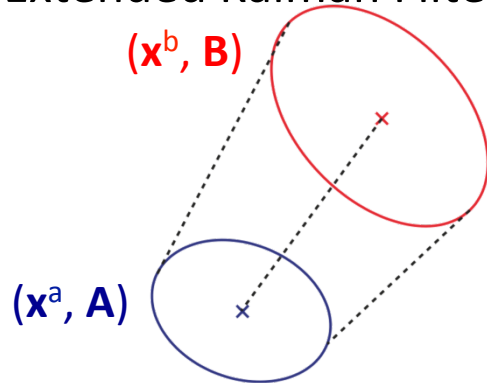
$$\mathbf{A}_k = (\mathbf{I} - \mathbf{K}_k \mathbf{H}_k) \mathbf{B}_k$$

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

time

Two Main Branches of EnKF: Analysis Processes at a Fixed t_k

◆ Extended Kalman Filter



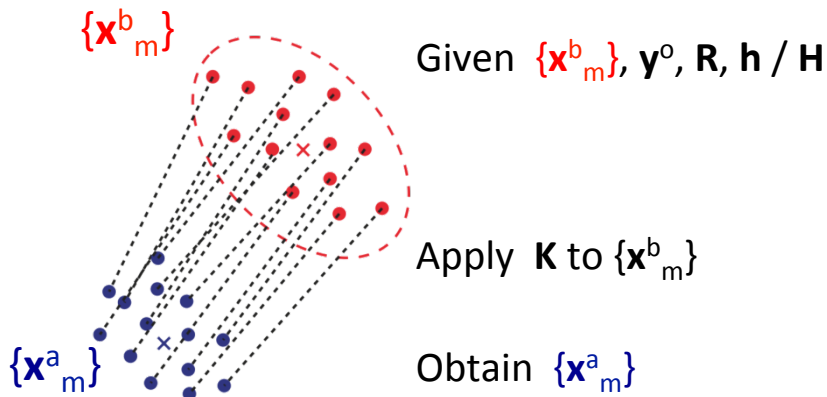
Given $\mathbf{x}^b, \mathbf{B}, \mathbf{y}^o, \mathbf{R}, \mathbf{h} / \mathbf{H}$

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

Obtain $\mathbf{x}^a = \mathbf{x}^b + \Delta\mathbf{x}^a$; $\Delta\mathbf{x}^a = \mathbf{K}(\mathbf{y}^o - \mathbf{h}(\mathbf{x}^b))$
& $\mathbf{A} = (\mathbf{I} - \mathbf{K}\mathbf{H})\mathbf{B}$

◆ Stochastic EnKF approach

- Perturbed Observation (PO)
(Houtekamer & Mitchell, MWR, 1998)
(Burgers et al, MWR, 1998)



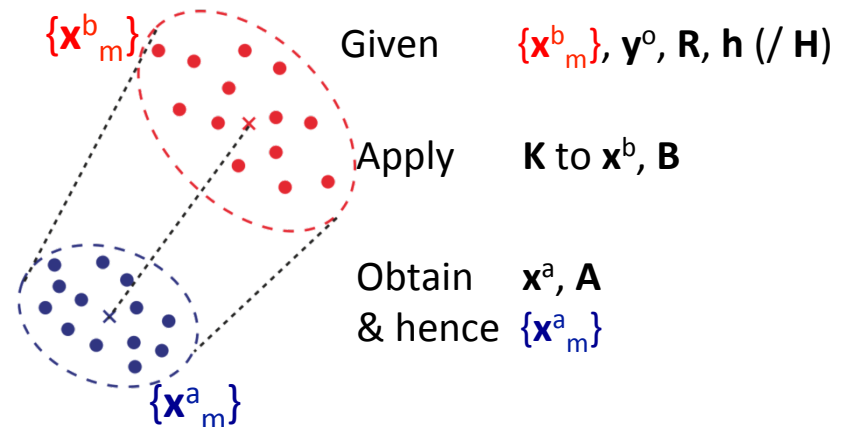
Given $\{\mathbf{x}_m^b\}, \mathbf{y}^o, \mathbf{R}, \mathbf{h} / \mathbf{H}$

Apply \mathbf{K} to $\{\mathbf{x}_m^b\}$

Obtain $\{\mathbf{x}_m^a\}$

◆ Square-Root EnKF approach

- Serial Ensemble Square Root Filter (EnSRF)
(Whitaker & Hamill, MWR, 2002)
- [Local] ensemble transform KF ([L]ETKF)
(Hunt et al, Physica D, 2007)



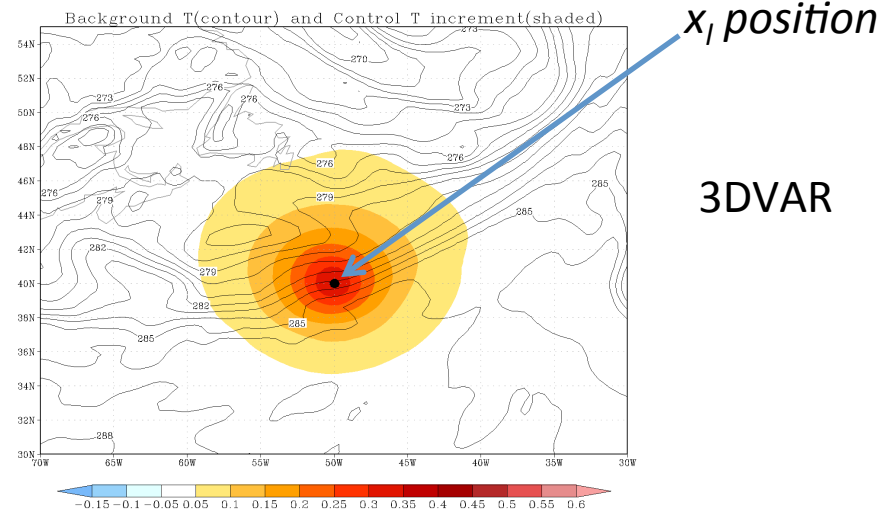
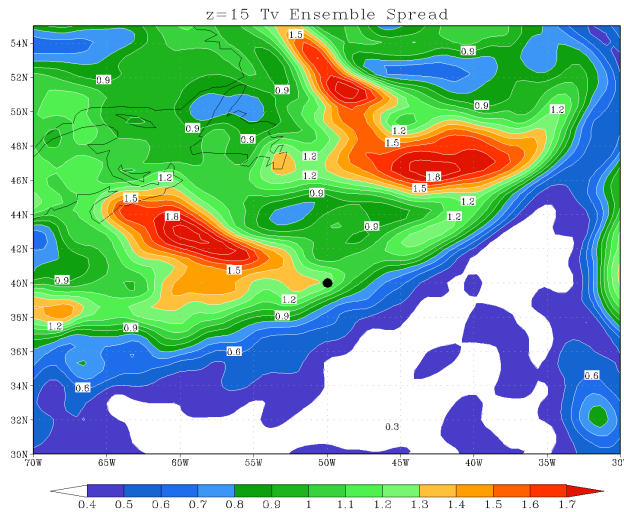
Given $\{\mathbf{x}_m^b\}, \mathbf{y}^o, \mathbf{R}, \mathbf{h} (/ \mathbf{H})$

Apply \mathbf{K} to \mathbf{x}^b, \mathbf{B}

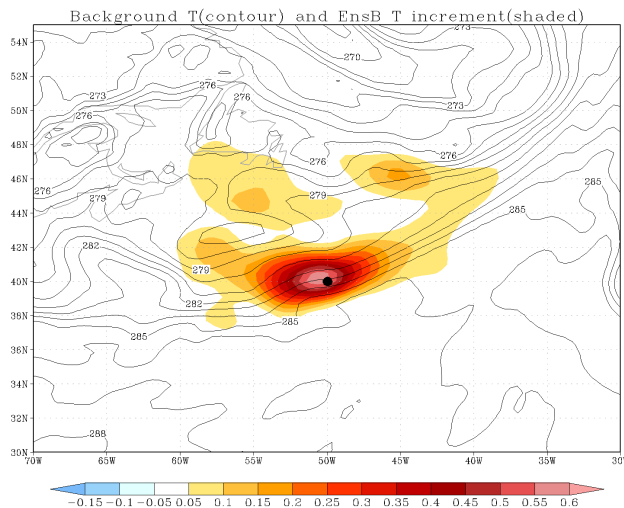
Obtain \mathbf{x}^a, \mathbf{A}
& hence $\{\mathbf{x}_m^a\}$

3DVar/OI vs EnKF: GSI Example

- ◆ Effect of correlation: $\mathbf{B} \Rightarrow \Delta x_n$ (single obs for x_i) with GSI



EnKF



$$\begin{pmatrix} \Delta x_1^a \\ \vdots \\ \Delta x_i^a \\ \vdots \\ \Delta x_N^a \end{pmatrix} = \frac{1}{R + B_{ii}} \begin{pmatrix} B_{1i} \\ \vdots \\ B_{ii} \\ \vdots \\ B_{Ni} \end{pmatrix} (y^o - x^b)$$

\mathbf{B} determines the quality of Δx^a

Single 850mb Tv observation (1K O-F, 1K error) – Courtesy of D. Kleist

Var Representation of EnKF: \mathbf{L} and ρ

◆ 3DVAR: Static \mathbf{B}_{3DVAR}

$$J_{3DVAR}(\Delta \mathbf{x}) = J_{3DVAR}^b(\Delta \mathbf{x}) + J^o(\Delta \mathbf{x}); \quad \Delta \mathbf{x} = \mathbf{x} - \mathbf{x}^b \quad \& \quad \mathbf{d} = \mathbf{y}^o - \mathbf{h}(\mathbf{x}^b)$$

$$J_{3DVAR}^b(\Delta \mathbf{x}) = \frac{1}{2}(\Delta \mathbf{x})^T (\mathbf{B}_{3DVAR})^{-1}(\Delta \mathbf{x});$$

$$J^o(\Delta \mathbf{x}) = \frac{1}{2}(\mathbf{d}^o - \mathbf{H}\Delta \mathbf{x})^T (\mathbf{R}^o)^{-1}(\mathbf{d}^o - \mathbf{H}\Delta \mathbf{x})$$

◆ EnKF flow evolving covariance estimation

$$J_{EnKF}(\alpha) = J_{EnKF}^b(\alpha) + J_{EnKF}^o(\alpha);$$

$$J_{EnKF}^b(\alpha) = \frac{1}{2\rho}(\alpha)^T (\mathbf{L})^{-1}(\alpha); \quad J_{EnKF}^o(\alpha) = J^o(\Delta \mathbf{x})$$

$$\Delta \mathbf{x} = \sum_{m=1}^M \alpha^{(m)} \circ \Delta \mathbf{x}^{(m)}$$

$\alpha^{(m)}$: ~local weight of individual members, scaled by $(M-1)^{1/2}$

\mathbf{L} : Localization matrix on extended control

ρ : inflation of background covariance matrix

$\Delta \mathbf{x}^{(m)}$: ensemble perturbations

Full 4D Data Assimilation: Problem Setting

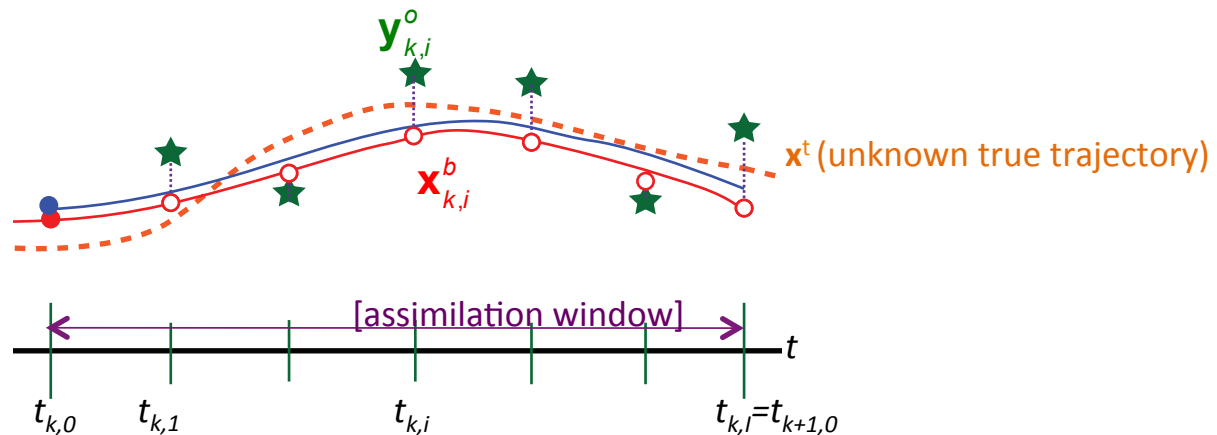
- ◆ Goal: Over a window $[t_{k-1}, t_k]=[t_{k,0}, t_{k,l}]$,
Obtain the 'best possible' estimate of the unknown true state \mathbf{x}_{k-1}^t (\mathbb{R}^N) from two information resources

1. Background by model forecast $\mathbf{x}_{k,i}^b$ (\mathbb{R}^N)

$$\mathbf{x}_{k,i} = \mathbf{m}_k(\mathbf{x}_{k,0})$$

2. Asynchronous Observations $\mathbf{y}_{k,i}^o$ (\mathbb{R}^L)

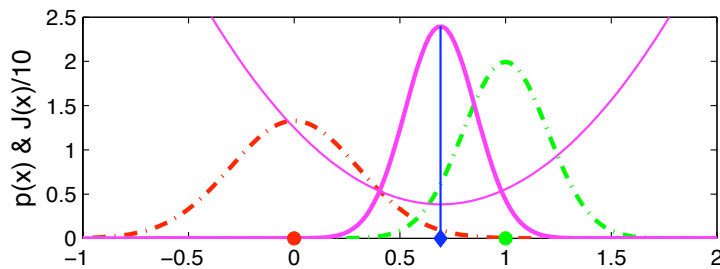
$$\mathbf{y}_{k,i} = \mathbf{h}_{k,i}(\mathbf{x}_{k,i})$$



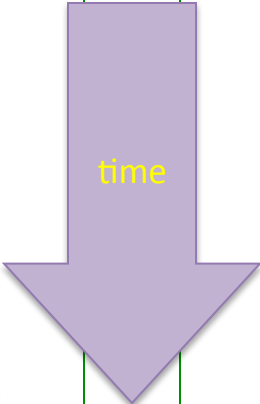
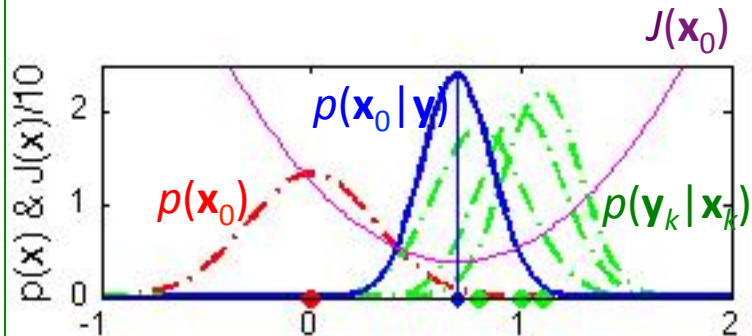
“4D”ness

Variational Approach:

- Least square estimation
- [maximum likelihood]
- 3D-Var (3 dim in space)



- 4D-Var (4th dim is time)

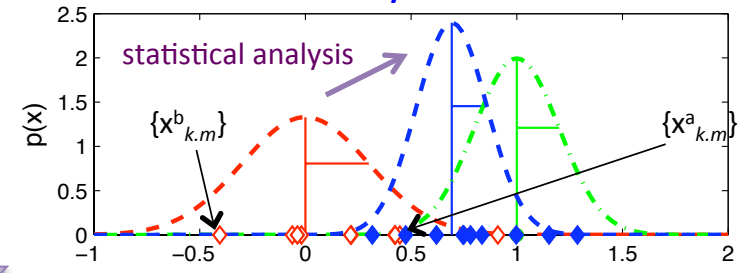


“Ensemble Kalman Filter (EnKF)”

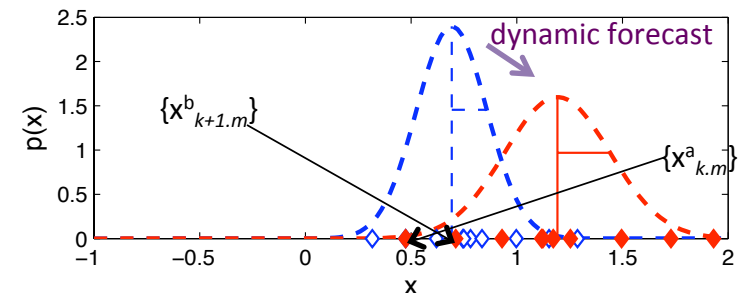
Approach :

- Minimum Variance estimate
- use $\{\mathbf{x}_{k,m}\}$ to infer/approx. $p(\mathbf{x}, t_k)$

– Ensemble analysis



– Ensemble forecast



$$\{\mathbf{x}_{k,m}\} = (\mathbf{x}_{k,1}, \dots, \mathbf{x}_{k,M}) \in \mathbb{R}^{N \times M}$$

k : time t_k M : ensemble size

3DVar Approach to 4D (Asynchronous) Observation: FGAT

- FGAT (First Guess at Appropriate Time)

- Basic idea: Incorporate the time distribution of $\mathbf{y}^o_{k,i}$ of incremental 3D-Var while keeping the control variable $\Delta\mathbf{x}_k$ at t_l

$$J_{3DFGAT}(\Delta\mathbf{x}) = J_{3DVAR}^b(\Delta\mathbf{x}) + J_{FGAT}^o(\Delta\mathbf{x}); \quad \Delta\mathbf{x} = \mathbf{x} - \mathbf{x}^b \quad \& \quad \mathbf{d} = \mathbf{y}_{k,i}^o - \mathbf{h}(\mathbf{x}_{k,i}^b)$$

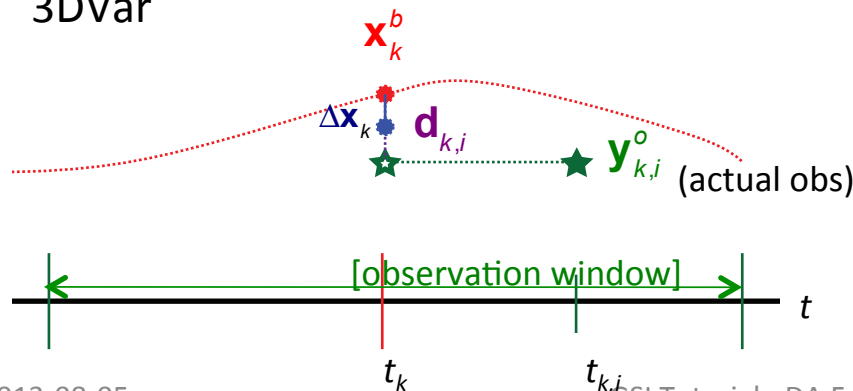
$$J_{3DVAR}^b(\Delta\mathbf{x}) = \frac{1}{2}(\Delta\mathbf{x})^T \mathbf{B}^{-1}(\Delta\mathbf{x});$$

$$J_{FGAT}^o(\Delta\mathbf{x}) = \frac{1}{2} \sum_{i=1}^l (\mathbf{d}_{k,i} - \mathbf{H}_{k,i} \Delta\mathbf{x})^T \mathbf{R}_{k,i}^{-1} (\mathbf{d}_{k,i} - \mathbf{H}_{k,i} \Delta\mathbf{x})$$

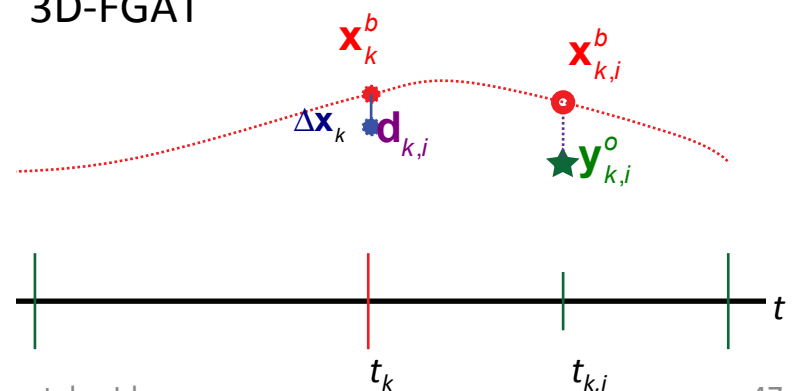
$$\mathbf{d}_{i,k}^{ob} = \mathbf{y}_{i,k}^o - \mathbf{h}_{i,k}(\mathbf{x}_{i,k}^b)$$

If $\mathbf{x}_{i,k}^b$ is available (stored)

3DVar

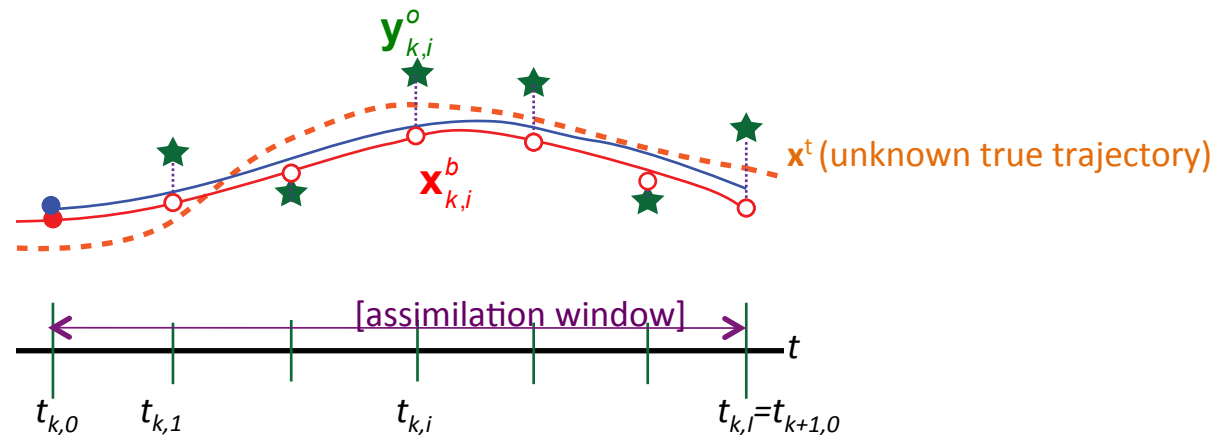


3D-FGAT



Variational Approach to “4D”ness in Dynamics: 4DVar

- Addressing “4D”- ness
 - 4D-Var is the extension of 3D-Var to the time domain and forward model takes into the account the dynamical evolution the model state
 - Two obvious and related advantages of 4D-Var over 3D-Var are:
 - Better representation of the temporal distribution of the observations, like FGAT
 - Time evolution of the model state



- In the 4D-Var, the observation window and the forecast window (in the simplest form) coincide, which we call the assimilation cycle.
 - One assimilation cycle at a time → drop the window index k , use only i .

4DVar: Formulation

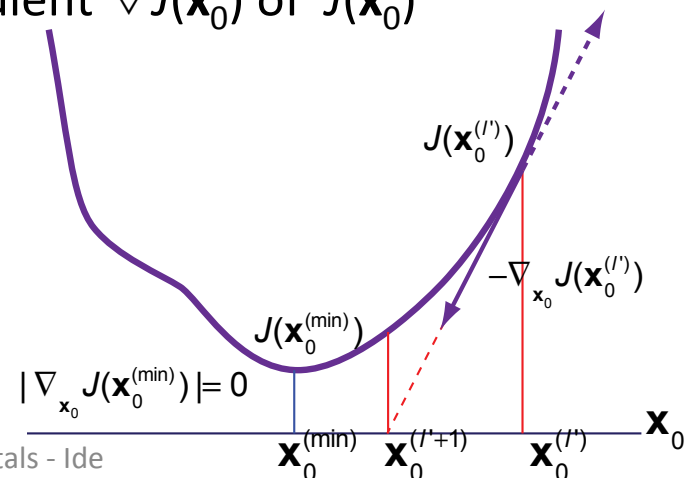
◆ Standard 4D-Var:

■ Cost function

$$\begin{aligned}
 J(\mathbf{x}_0) &= \frac{1}{2}(\mathbf{x}_0 - \mathbf{x}_0^b)^T \mathbf{B}^{-1}(\mathbf{x}_0 - \mathbf{x}_0^b) + \sum_{i=1}^I \frac{1}{2}(\mathbf{y}_i^o - \mathbf{h}_i(\mathbf{x}_i))^T (\mathbf{R}_i)^{-1}(\mathbf{y}_i^o - \mathbf{h}_i(\mathbf{x}_i)) \\
 &= \frac{1}{2}(\mathbf{x}_0 - \mathbf{x}_0^b)^T \mathbf{B}^{-1}(\mathbf{x}_0 - \mathbf{x}_0^b) + \sum_{i=1}^I \frac{1}{2}(\mathbf{y}_i^o - \mathbf{h}_i(\mathbf{m}_{i,0}(\mathbf{x}_0)))^T (\mathbf{R}_i)^{-1}(\mathbf{y}_i^o - \mathbf{h}_i(\mathbf{m}_{i,0}(\mathbf{x}_0))) \\
 &= J^b(\mathbf{x}_0) + J^o(\mathbf{x}_0) \\
 &= J^b(\mathbf{x}_0) + \sum_{i=1}^I J_i^o(\mathbf{x}_0) \\
 \nabla J(\mathbf{x}_0) &= \nabla J^b(\mathbf{x}_0) + \sum_{i=1}^I \nabla J_i^o(\mathbf{x}_0) \\
 \nabla J_i^o(\mathbf{x}_0) &= -(\mathbf{H}_i \mathbf{M}_{i,0})^T (\mathbf{R}_i)^{-1}(\mathbf{y}_i^o - \mathbf{h}_i(\mathbf{m}_{i,0}(\mathbf{x}_0)))
 \end{aligned}$$

■ Minimization algorithms require the gradient $\nabla J(\mathbf{x}_0)$ of $J(\mathbf{x}_0)$

→ Adjoint $\mathbf{M}_{i,0}$ of nonlinear model $\mathbf{m}_{i,0}$



4DVar: Additional Topics

- ◆ Flexibility of $J(\mathbf{x})$ $= J^b(\mathbf{x}) + J^o(\mathbf{x})$ [+ $J^c(\mathbf{x})$]
 - Similar to 3DVar, once minimization of $J(\mathbf{x})$ is in place.
 - Variational quality control
 - Constraints
 - Preconditioning
 - Outer loop (for nonlinearity in both dynamic and forward models)

- ◆ Challenges: Modeling of static \mathbf{B} (similar to 3DVar)
 - 4DVar is not a sequential method: \mathbf{B} is still static though evolves over the assimilation window, effectively just like EKF, i.e., $\mathbf{B}_{i,0} = \mathbf{M}_{i,0} \mathbf{B} \mathbf{M}_{i,0}^T$
 - Computationally intensive: in particular TLM $\mathbf{M}_{i,0}$ and its adjoint $\mathbf{M}_{i,0}^T$

Integrated Approach: Hybrid

- ◆ Incremental 4DVar with Static \mathbf{B}_f

$$J(\Delta \mathbf{x}_0) = \frac{1}{2} (\Delta \mathbf{x}_0)^T \mathbf{B}^{-1} (\Delta \mathbf{x}_0) + \sum_{i=1}^I \frac{1}{2} (\mathbf{d}_i^o - \mathbf{H}_i \Delta \mathbf{x}_i)^T (\mathbf{R}_i)^{-1} (\mathbf{d}_i^o - \mathbf{H}_i \Delta \mathbf{x}_i)$$

- ◆ EnKF in Var formulation with dynamic \mathbf{B}_e

$$J_{\text{EnKF}}(\boldsymbol{\alpha}) = \frac{1}{2\rho} \boldsymbol{\alpha}^T \mathbf{L}^{-1} \boldsymbol{\alpha} + \sum_{i=1}^I \frac{1}{2} (\mathbf{d}_i^o - \mathbf{H}_i \Delta \mathbf{x}_i)^T (\mathbf{R}_i)^{-1} (\mathbf{d}_i^o - \mathbf{H}_i \Delta \mathbf{x}_i);$$

$$\Delta \mathbf{x}_i = \sum_{m=1}^M \boldsymbol{\alpha}^{(m)} \circ \Delta \mathbf{x}_i^{(m)}$$

- ◆ Hybrid: with $\mathbf{P}^b = \beta_f \mathbf{B}_f + \beta_e \mathbf{B}_e$

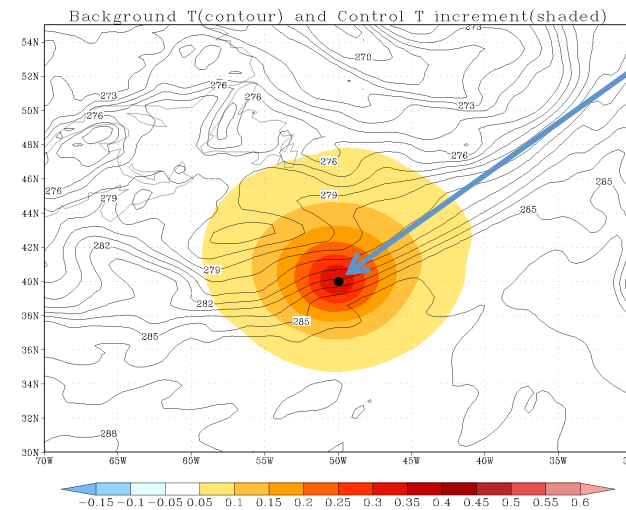
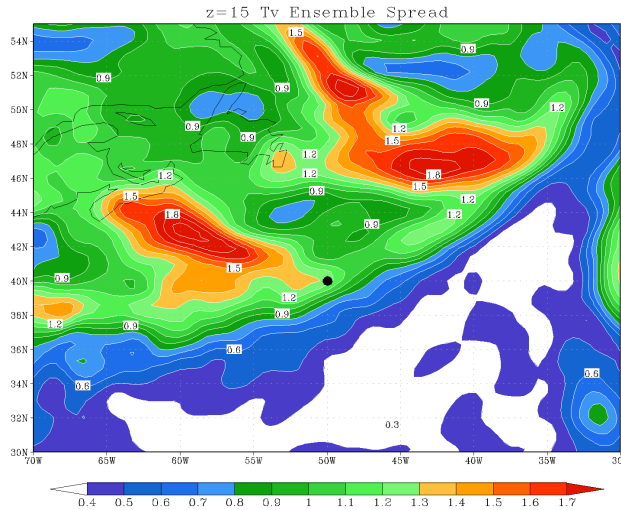
$$J_{\text{hybrid}}(\Delta \mathbf{x}_f, \boldsymbol{\alpha}) = \beta_f \frac{1}{2} (\Delta \mathbf{x}_0)^T \mathbf{B}^{-1} (\Delta \mathbf{x}_0) + \beta_e \frac{1}{2\rho} \boldsymbol{\alpha}^T \mathbf{L}^{-1} \boldsymbol{\alpha} \\ + \sum_{i=1}^I \frac{1}{2} (\mathbf{d}_i^o - \mathbf{H}_i \Delta \mathbf{x}_i)^T (\mathbf{R}_i)^{-1} (\mathbf{d}_i^o - \mathbf{H}_i \Delta \mathbf{x}_i)$$

$$1/\beta_f + 1/\beta_e = 1$$

$$\Delta \mathbf{x}_i = \Delta \mathbf{x}_f + \sum_{m=1}^M \boldsymbol{\alpha}^{(m)} \circ \Delta \mathbf{x}_i^{(m)}$$

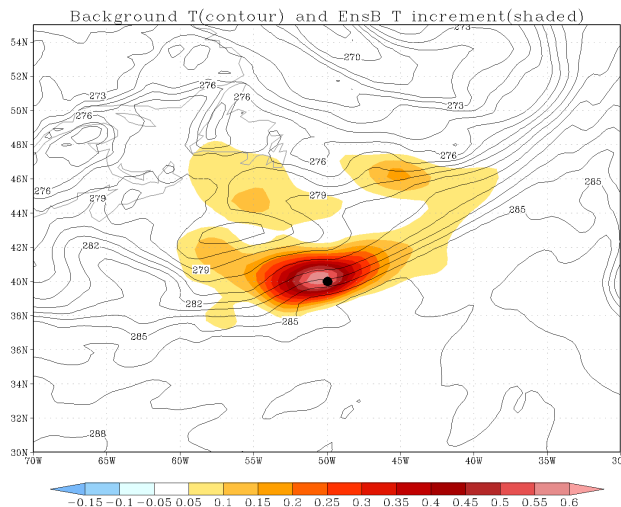
Hybrid: GSI Example

- ◆ Effect of correlation: $\mathbf{P}^b \Rightarrow \Delta \mathbf{x}_n$ (single obs for x_i) with GSI



3DVAR
 $\beta_e=0$
 $\beta_f=1$

EnKF
 $\beta_e=1$
 $\beta_f=0$



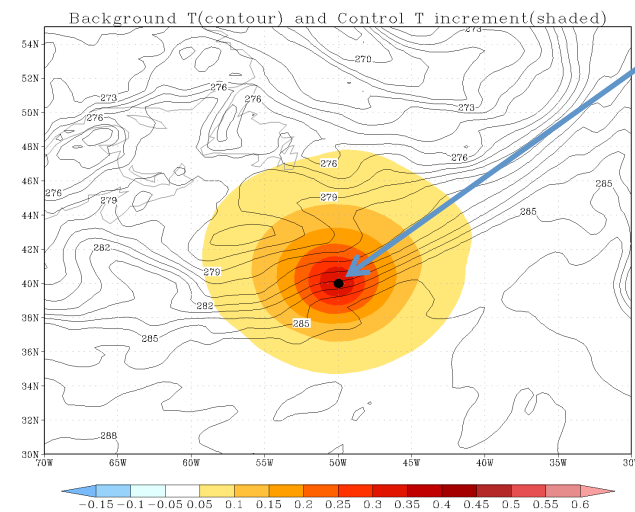
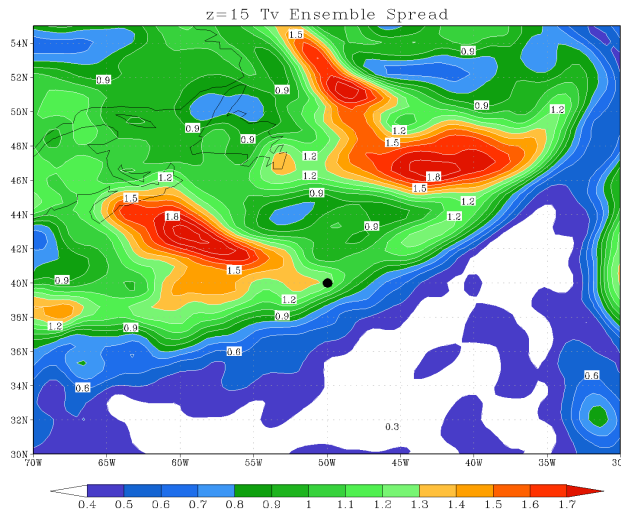
$$\Delta \mathbf{x}^a = \begin{pmatrix} P_{1l}^b / P_{ll}^b \\ \vdots \\ P_{ll}^b / P_{ll}^b \\ \vdots \\ P_{nl}^b / P_{ll}^b \end{pmatrix} \frac{P_{ll}^b}{P_{ll}^b + R_{ll}} (y_l^o - x_l^b)$$

$$\mathbf{P}^b = \beta_f \mathbf{B}_f + \beta_e \mathbf{B}_e \quad : \text{ hybrid}$$

Single 850mb Tv observation (1K O-F, 1K error) – Courtesy of D. Kleist

Hybrid: GSI Example

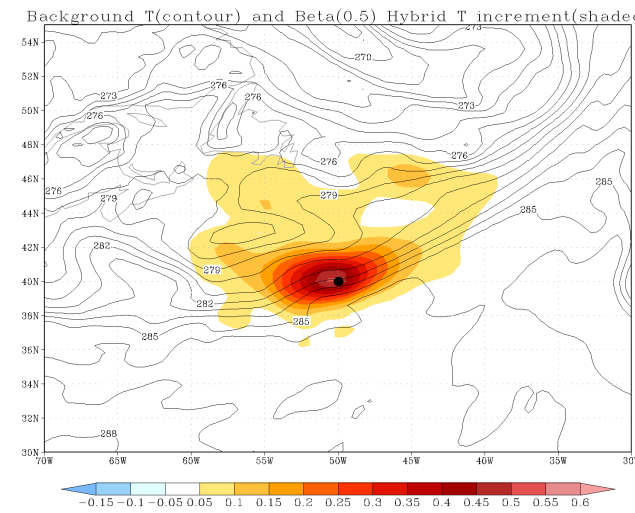
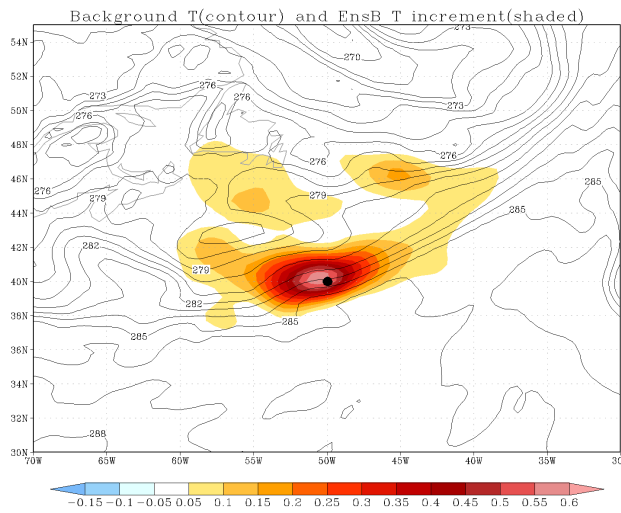
- ◆ Effect of correlation: $\mathbf{P}^b \Rightarrow \Delta \mathbf{x}_n$ (single obs for x_i) with GSI



x_i position

3DVAR
 $\beta_e=0$
 $\beta_f=1$

EnKF
 $\beta_e=1$
 $\beta_f=0$



Hybrid
 $\beta_e=1/2$
 $\beta_f=1/2$

Single 850mb Tv observation (1K O-F, 1K error) – Courtesy of D. Kleist

Summary

- ◆ Background ideas of data assimilation
- ◆ Unifying perspectives of the current approaches
- ◆ Understanding of the variational formulation

- Cost function

$$J(\mathbf{x}) = J^b(\mathbf{x}) + J^o(\mathbf{x}) \quad [+ J^c(\mathbf{x})]$$

$$J^b(\mathbf{x}) = 1/2(\mathbf{x} - \mathbf{x}^b)^T \mathbf{B}^{-1}(\mathbf{x} - \mathbf{x}^b) \quad : \text{*b*ackground cost function}$$

$$J^o(\mathbf{x}) = 1/2(\mathbf{y}^o - \mathbf{h}(\mathbf{x}))^T \mathbf{R}^{-1}(\mathbf{y}^o - \mathbf{h}(\mathbf{x})) \quad : \text{*o*bservation cost function}$$

$$J^c(\mathbf{x}) \quad : \text{*c*onstraint cost function}$$

Where (\mathbf{x}, \mathbf{B}) : model state vector & background error covariance matrix

(\mathbf{y}, \mathbf{R}) : observation vector & observation error covariance matrix

$\mathbf{y} = \mathbf{h}(\mathbf{x})$: forward model / observation operator

- With emphasis on
 - Role of \mathbf{B}
 - Flexibility of variational approach