Basics of Data Assimilation

Zhiquan (Jake) Liu

Prediction, Assimilation, and Risk Communication Section
Mesoscale & Microscale Meteorology Laboratory
National Center for Atmospheric Research

NCAR

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Outline

- Scalar case
- Case with two state variables
- General n-dimensional case

What is data assimilation?

- A probabilistic method to obtain the best estimate of state variables
- In the atmospheric sciences, DA typically involves combining model forecast (Prior) and observations, along with their respective errors characterization, to produce an *analysis (Posterior)* that can initialize a numerical weather prediction model (e.g., WRF)

Scalar Case

- State variable to estimate "x", e.g., consider today's temperature in Taoyuan at 06 UTC.

- Now we have a "background" (or "prior") information x_b of x, which is from a 6-h GFS or MPAS forecast initiated from 00 UTC analysis.

- We also have an observation y of x at a surface station in Taoyuan

- What is the best estimate (analysis) x_a of x?

Scalar Case

- We can simply average them: $x_a = \frac{1}{2}(x_b + y)$
  - This actually means we trust equally the background and observation, giving them equal weight

- But if their accuracy is different and we have some estimation of their errors
  - e.g., for background, we have statistics (e.g., mean and variance) of $x_b - y$ from the past
  - For observation, we have instrument error information from manufacturer

Scalar Case

- Then we can do a weighted mean: $x_a = ax_b + by$ in a least square sense, i.e.,

Minimize $$J(x) = \frac{1}{2}\frac{(x-x_b)^2}{\sigma_b^2} + \frac{1}{2}\frac{(x-y)^2}{\sigma_o^2}$$

Requires $$\frac{dJ(x)}{dx} = \frac{(x-x_b)}{\sigma_b^2} + \frac{(x-y)}{\sigma_o^2} = 0$$

Then we can easily get $$x_a = \frac{\sigma_o^2}{\sigma_b^2+\sigma_o^2}x_b + \frac{\sigma_b^2}{\sigma_b^2+\sigma_o^2}y = \frac{1}{1+\sigma_b^2/\sigma_o^2}x_b + \frac{1}{1+\sigma_o^2/\sigma_b^2}y$$

Or we can write in the form of analysis increment

$$x_a - x_b = \frac{\sigma_b^2}{\sigma_b^2+\sigma_o^2}(y - x_b) = \frac{1}{1+\sigma_o^2/\sigma_b^2}(y - x_b)$$

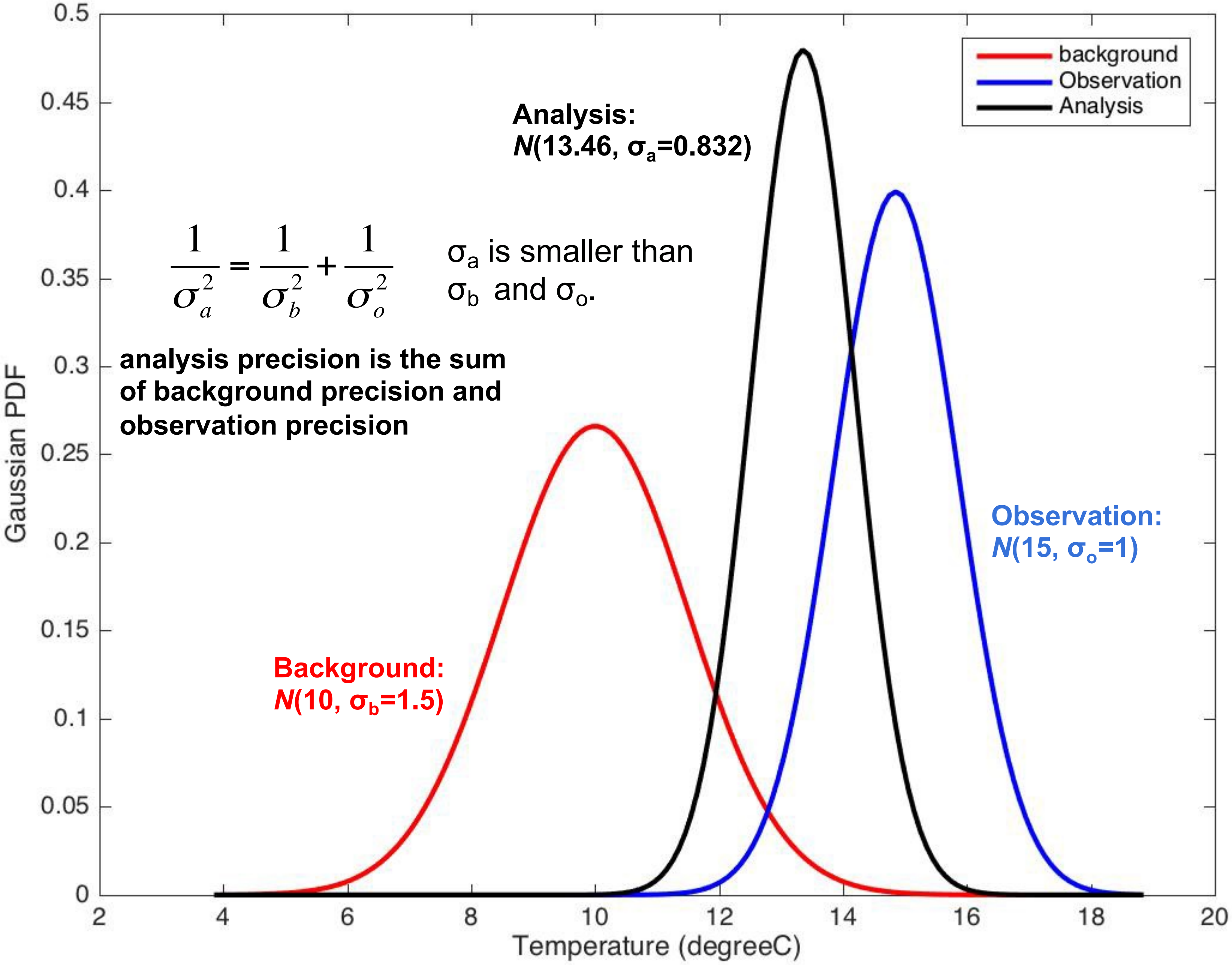
Scalar Case

Minimize $$J(x)=\frac{1}{2}\frac{(x-x_b)^2}{\sigma_b^2}+\frac{1}{2}\frac{(x-y)^2}{\sigma_o^2}$$

is actually equivalent to maximize a Gaussian Probability Distribution Function (PDF)

$$ce^{-J(x)}$$

Assume errors of X_b and y are unbiased



background
Observation
Analysis
Analysis:
N(13.46, σa=0.832)
1/σa² = 1/σb² + 1/σo²
σa is smaller than σb and σo.
analysis precision is the sum of background precision and observation precision
Background:
N(10, σb=1.5)
Observation:
N(15, σo=1)
Gaussian PDF
Temperature (degreeC)
0
0.05
0.1
0.15
0.2
0.25
0.3
0.35
0.4
0.45
0.5
2
4
6
8
10
12
14
16
18
20

Two state variables case

- Consider two state variables to estimate: Taoyuan and Taipei's temperatures x_1 and x_2 at 06 UTC today.

- Background from 6-h forecast: x_1^b and x_2^b and their error covariance with correlation c

$$\mathbf{B} = \begin{bmatrix} \sigma_1^2 & c\sigma_1\sigma_2 \\ c\sigma_1\sigma_2 & \sigma_2^2 \end{bmatrix} = \begin{bmatrix} \sigma_1 & 0 \\ 0 & \sigma_2 \end{bmatrix} \begin{bmatrix} 1 & c \\ c & 1 \end{bmatrix} \begin{bmatrix} \sigma_1 & 0 \\ 0 & \sigma_2 \end{bmatrix}$$

- We only have an observation y_1 at a Taoyuan station and its error variance σ_o^2

Analysis increment for two variables

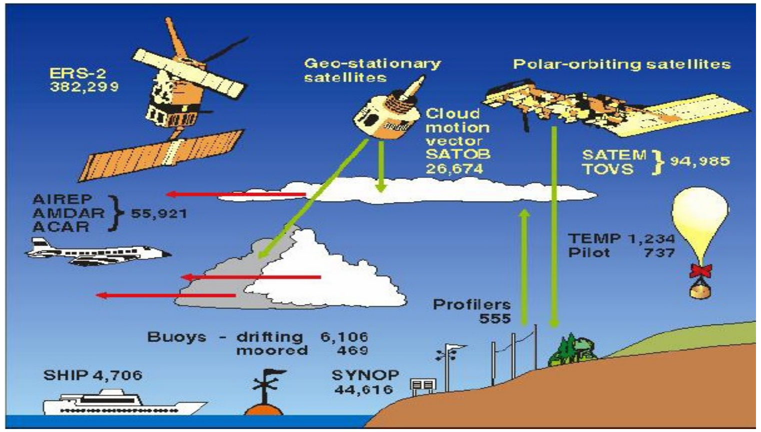
$$x_1^a - x_1^b = \frac{\sigma_1^2}{\sigma_1^2 + \sigma_o^2}(y_1 - x_1^b) \longleftarrow \text{Taoyuan}$$

$$x_2^a - x_2^b = \frac{c\sigma_1\sigma_2}{\sigma_1^2 + \sigma_o^2}(y_1 - x_1^b) \longleftarrow \text{Taipei}$$

Unobserved variable x_2 gets updated through the error correlation *c* in the background error covariance.

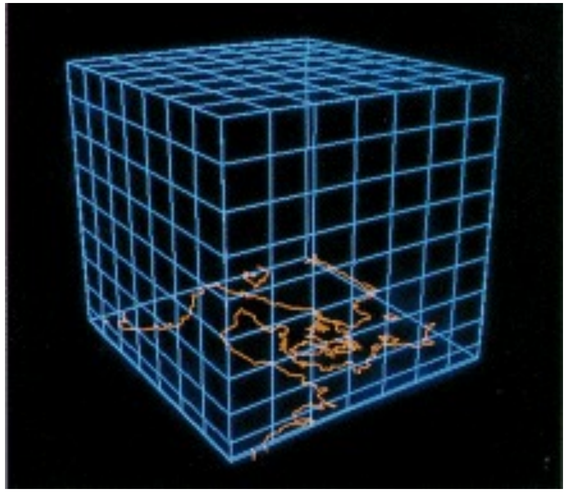
In general, this correlation can be correlation between two locations (spatial), two variables (multivariate), or two times (temporal).

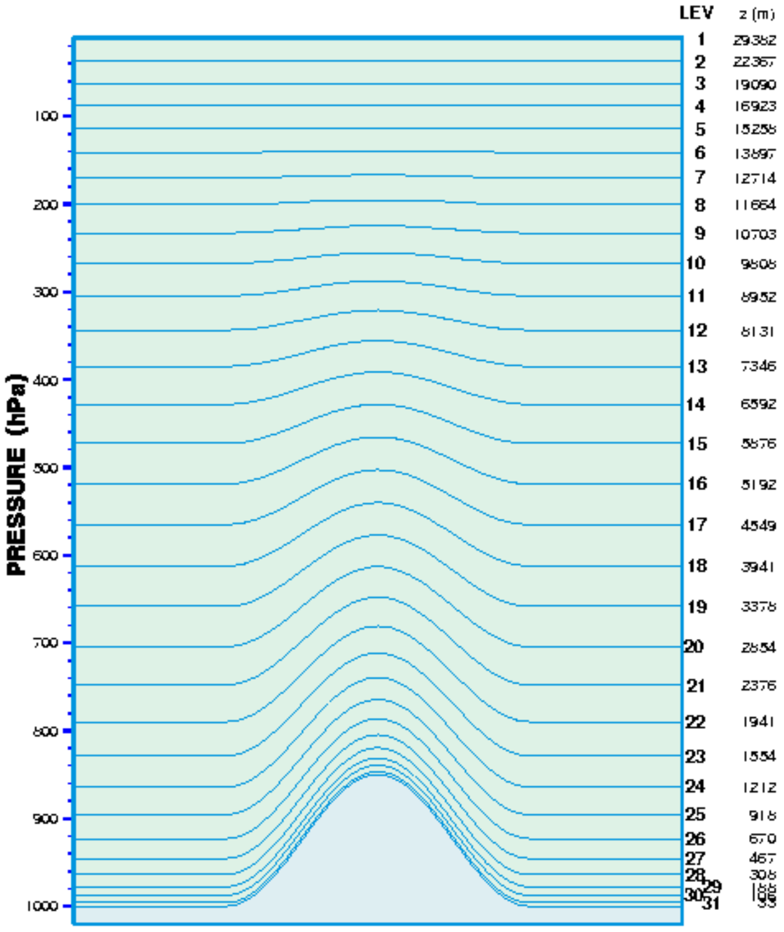
General Case



Observations
y^o, ~10^5-10^6

Model state
x, ~10^7





Vertical resolution of the DMI-HIRLAM system

General Case: vector and matrix notation

state vector

$$x = \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_m \end{bmatrix}$$

observation vector

$$y = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{bmatrix}$$

background error covariance

$$\mathbf{B} = \begin{bmatrix} \sigma_1^2 & c_{12}\sigma_1\sigma_2 & \cdots & \cdots \\ c_{12}\sigma_1\sigma_2 & \sigma_2^2 & \cdots & \cdots \\ \cdots & \cdots & \ddots & \cdots \\ \cdots & \cdots & \cdots & \sigma_m^2 \end{bmatrix} = \sigma\ \mathrm{C}\ \sigma$$

m x m

Correlation matrix

Observation error covariance

$$\mathbf{R} = \begin{bmatrix} \sigma_{o1}^2 & 0 & \cdots & 0 \\ 0 & \sigma_{o2}^2 & \cdots & 0 \\ \vdots & \cdots & \ddots & \vdots \\ 0 & \cdots & \cdots & \sigma_{on}^2 \end{bmatrix}$$

n x n

General Case: cost function

1 x 1 1 x m m x m m x 1 1 x n n x n n x 1

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

H maps x to y space, e. g., interpolation.
Terminology in DA: observation operator

Minimize J(x) is equivalent to maximize a multi-dimensional Gaussian PDF

Constant * $e^{-J(x)}$

General Case: analytical solution

Again, minimize J requires its gradient (a vector) with respect to x equal to zero:

$$\nabla J_{\mathbf{x}}(\mathbf{x}) = \mathbf{B}^{-1}(\mathbf{x} - \mathbf{x}_{\mathrm{b}}) - \mathbf{H}^{\mathrm{T}}\mathbf{R}^{-1}[\mathbf{y} - \mathbf{H}\mathbf{x}] = 0$$

m x 1

This leads to analytical solution for the analysis increment:

$$x^a - x^b = \underbrace{\boxed{\mathbf{BH}^{\mathrm{T}}(\mathbf{HBH}^{\mathrm{T}} + \mathbf{R})^{-1}}}_{\text{Kalman gain matrix}}\underbrace{\boxed{[y - \mathbf{H}x^b]}}_{\text{Innovation or OMB}}$$

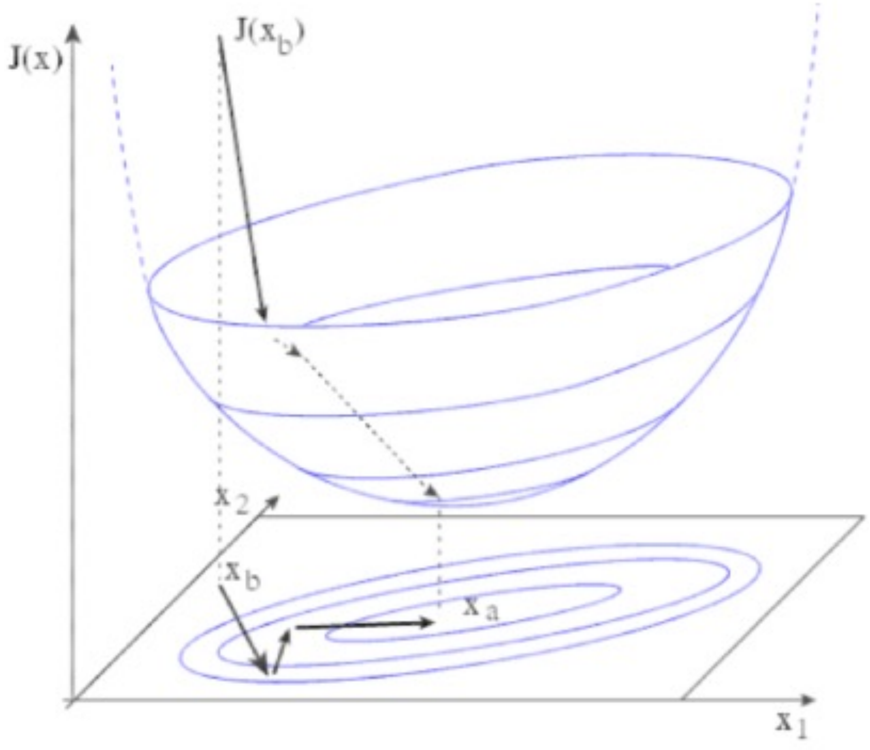
HBH^{T} : background error covariance projected into observation space

BH^{T} : background error covariance projected into cross background-observation space

Iterative algorithm to find minimum of cost function

- **Descending algorithms**
  - **Descending direction: γ_n (N-dimensional vector)**
  - **Descending step: μ_n**

$$\boxed{x_{n+1} = x_n + \mu_n \gamma_n}$$



from Bouttier and Courtier 1999

Precision of Analysis with optimal B and R

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

Generalization of scalar case $\dfrac{1}{\sigma_a^2} = \dfrac{1}{\sigma_b^2} + \dfrac{1}{\sigma_o^2}$

Or in another form: $\mathbf{A} = (\mathbf{I} - \mathbf{K}\mathbf{H})\mathbf{B}$

With

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

called Kalman gain matrix

Precision of analysis: more general formulation

$$\mathbf{A} = (\mathbf{I} - \mathbf{KH})\mathbf{B}_t(\mathbf{I} - \mathbf{KH})^{\mathrm{T}} + \mathbf{KR}_t\mathbf{K}^{\mathrm{T}}$$

where B_t and R_t are "true" background and observation error covariances.

This formulation is valid for any given gain matrix K, which could be suboptimal (e.g., due to incorrect estimation/specification of B and R).

Analysis increment with a single humidity observation

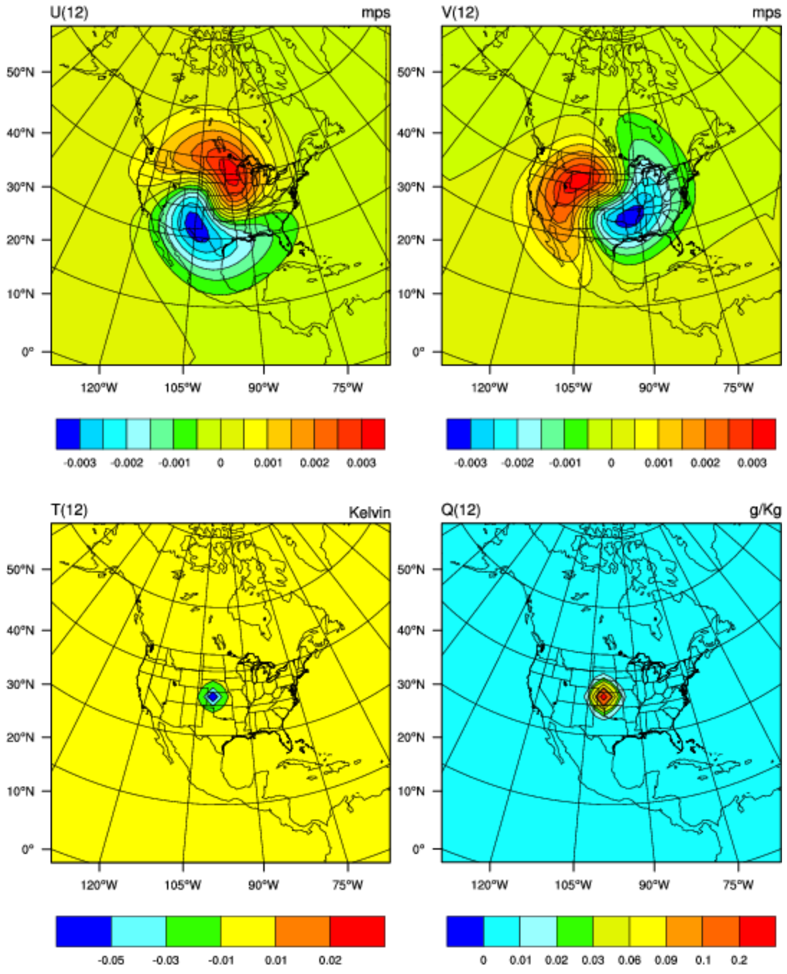
$$x^a - x^b = \mathbf{BH}^{\mathrm{T}}(\mathbf{HBH}^{\mathrm{T}} + \mathbf{R})^{-1}[y - \mathbf{H}x^b]$$

$$x_l^a - x_l^b = \frac{c_{lk}\sigma_l\sigma_k}{\sigma_k^2 + \sigma_{ok}^2}(y_k - x_k^b)$$

It is generalization of previous two variables case:

$$x_1^a - x_1^b = \frac{\sigma_1^2}{\sigma_1^2 + \sigma_o^2}(y_1 - x_1^b)$$

$$x_2^a - x_2^b = \frac{c\sigma_1\sigma_2}{\sigma_1^2 + \sigma_o^2}(y_1 - x_1^b)$$

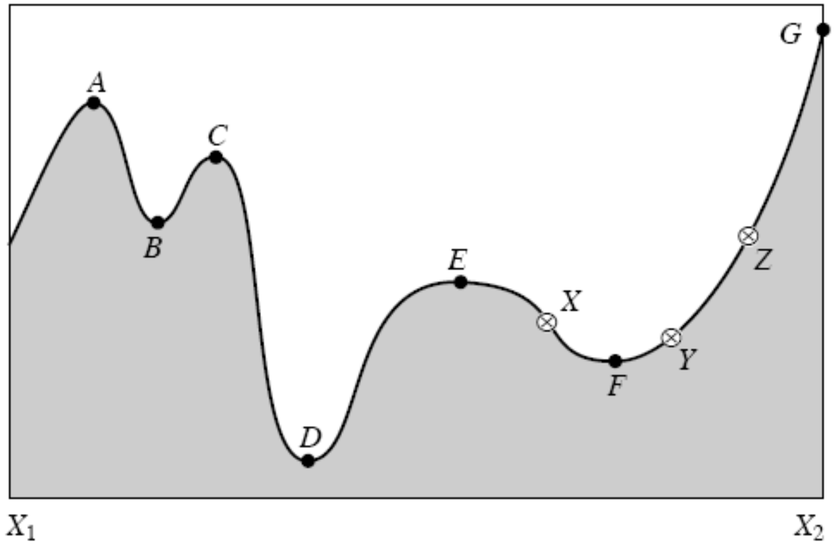


cv_options=6 in WRFDA

Other Remarks

- Observation operator can be non-linear and thus analysis error PDF is not necessarily Gaussian

- J(x) can have multiple local minima. Final solution of least square depends on starting point of iteration, e.g., choose the background x_b as the first guess.



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Other Remarks

- **B** matrix is of very large dimension, explicit inverse of **B** is impossible, substantial efforts in data assimilation were given to the estimation and modeling of **B**.
- **B** shall be spatially-varied and time-evolving according to weather regime.
- Analysis can be sub-optimal if using inaccurate estimate of **B** and **R**.
- Could use non-Gaussian PDF
  - Thus not a least square cost function
  - Difficult (usually slow) to solve; could transform into Gaussian problem via variable transform

Further reading