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Spring Colloquium on
'Regional Weather Predictability and Modeling'
April 11 - 22, 2005

1) Workshop **on Design and Use of Regional Weather Prediction Models,** *April 11 - 19*

2) Conference on **Current Efforts Toward Advancing the Skill of Regional Weather Prediction. Challenges and Outlook,** *April 20 - 22*

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The Maximum Likelihood Ensemble Filter (MLEF): An ensemble assimilation/prediction system based on control theory

M. Zupanski
Cooperative Institute for Research in the Atmosphere, CSU, Ft. Collins
USA

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The Maximum Likelihood Ensemble Filter (MLEF): An ensemble assimilation/prediction system based on Control Theory

Milija Zupanski

Cooperative Institute for Research in the Atmosphere
Colorado State University
Fort Collins, CO 80523-1375
ZupanskiM@CIRA.colostate.edu

In collaboration with:

Colorado State University: D. Zupanski, S. Fletcher, D. Randall, R. Heikes
Florida State University: I.M. Navon, B. Uzunoglu
Portland State University: D. Daescu

Outline

- MLEF algorithm
- Error covariance
- Parameter and model error estimation
- Non-Gaussian MLEF framework
- Future research directions

Maximum Likelihood Ensemble Filter (MLEF)

- Estimate of the *conditional mode* of the posterior PDF

- Ensembles used to estimate the *uncertainty* of the conditional mode

- *Non-derivative* minimization with Hessian preconditioning:
  (Generalized conjugate-gradient and BFGS quasi-Newton algorithms)

- *Non-Gaussian* errors allowed (minimization of non-Gaussian cost-function)

- Augmented control variable: *initial conditions*, *model bias*, *empirical parameters*, *boundary conditions*

- Related to: (*i*) variational data assimilation, (*ii*) Iterative Kalman filters, and (*iii*) Ensemble Transform Kalman Filter – ETKF

MLEF Mathematical Framework

Forecast (prior) error covariance

$$\boldsymbol{P}_f^{1/2} = [\boldsymbol{p}_1^f \quad \boldsymbol{p}_2^f \quad \cdots \quad \boldsymbol{p}_{N_E}^f]$$

$$\boldsymbol{p}_i^f = \mathcal{M}(\boldsymbol{x} + \boldsymbol{p}_i^a) - \mathcal{M}(\boldsymbol{x})$$

Minimize cost function in subspace spanned by ensemble perturbations $\boldsymbol{p}_i^f$

$$J = \frac{1}{2}[\boldsymbol{x} - \boldsymbol{x}^b]^T \boldsymbol{P}_f^{-1} [\boldsymbol{x} - \boldsymbol{x}^b] + \frac{1}{2}[\boldsymbol{y}_{obs} - \mathcal{H}(\boldsymbol{x})]^T \boldsymbol{R}^{-1} [\boldsymbol{y}_{obs} - \mathcal{H}(\boldsymbol{x})]$$

Non-derivative iterative minimization with preconditioning

- No differentiability assumption: works for all bounded operators
- Use with Conjugate gradient, LBFGS quasi-Newton algorithms
- Define generalized gradient, generalized Hessian

Employ Taylor formula for variations:

First variation = generalized gradient

Second variation = generalized Hessian

$$\Delta J = J(\boldsymbol{x} + \delta\boldsymbol{x}) - J(\boldsymbol{x}) = \delta J + \frac{1}{2}\delta^2 J + \frac{1}{3!}\delta^3 J + \cdots$$

MLEF Mathematical Framework

Generalized **inverse Hessian**

$$\left(\nabla_G^2 J\right)^{-1} = \boldsymbol{P}_f^{1/2}\left[\boldsymbol{I} + \left(\boldsymbol{Z}^b\right)^T \boldsymbol{Z}^b\right]^{-1} \boldsymbol{P}_f^{T/2}$$

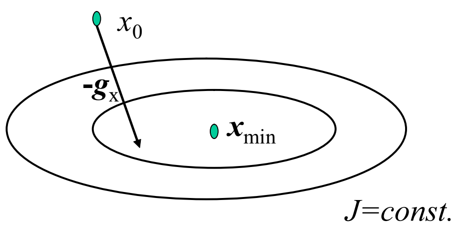
$$\boldsymbol{Z}^b = \left[\boldsymbol{z}_1^b \quad \boldsymbol{z}_2^b \quad \cdot \quad \cdot \quad \boldsymbol{z}_{N_E}^b\right] \qquad \boldsymbol{z}_i^b = \boldsymbol{R}^{-1/2}\left[\mathcal{H}(\boldsymbol{x}^b + \boldsymbol{p}_i^f) - \mathcal{H}(\boldsymbol{x}^b)\right]$$

Change of variable (Hessian preconditioning)

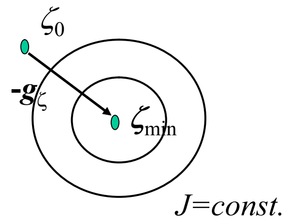
$$\boldsymbol{x}_k = \boldsymbol{x}^b + \boldsymbol{P}_f^{1/2}\left[\boldsymbol{I} + \left(\boldsymbol{Z}^b\right)^T \boldsymbol{Z}^b\right]^{-1/2} \zeta_k$$

$$\zeta_{k+1} = \zeta_k + \alpha_k \boldsymbol{d}_k$$

Physical space



Preconditioning space



Generalized **gradient**

$$\left(\nabla_G J\right)_k = \left[\boldsymbol{I} + \left(\boldsymbol{Z}^b\right)^T \boldsymbol{Z}^b\right]^{-1/2} \zeta_k - \left(\boldsymbol{Z}^k\right)^T \boldsymbol{R}^{-1}\left(\boldsymbol{y} - \mathcal{H}(\boldsymbol{x}_k)\right)$$

$$\boldsymbol{Z}^k = \left[\boldsymbol{z}_1^k \quad \boldsymbol{z}_2^k \quad \cdot \quad \cdot \quad \boldsymbol{z}_s^k\right] \qquad \boldsymbol{z}_i^k = \boldsymbol{R}^{-1/2}\left[\mathcal{H}(\boldsymbol{x}_k + \boldsymbol{p}_i^f) - \mathcal{H}(\boldsymbol{x}_k)\right]$$

k – iteration index

MLEF Mathematical Framework

Analysis (posterior) error covariance

$$\boldsymbol{P}_a^{1/2} = \boldsymbol{P}_f^{1/2}(\boldsymbol{I} + \boldsymbol{Z}^T\boldsymbol{Z})^{-1/2}$$

$$\boldsymbol{z}_i = \boldsymbol{R}^{-1/2}\mathcal{H}(\boldsymbol{x} + \boldsymbol{p}_i^f) - \boldsymbol{R}^{-1/2}\mathcal{H}(\boldsymbol{x})$$

- **Analysis error covariance estimated from minimization algorithm**
- **Inverse Hessian = Analyis error covariance (linear assumption)**

How to apply linear result to nonlinear problem?

- **If the Hessian is calculated at the minimum, it is close to the truth**
- $\|x^{true} - x^a\| < \varepsilon$ **: for small** ε **linear theory is valid**
- **Avoid sample error covariance calculations**
  - noisy for limited sample
  - inflation factors

• For good Hessian preconditioning, expect superior minimization convergence
• Valid for arbitrary nonlinear operators and cost functions

Prediction models

(1) Korteweg-de Vries-Burgers (KdVB)

- one-dimensional, one variable, two solitons
- nonlinear advection, dispersion, diffusion

(2) NASA GEOS-5 column precipitation model

- one-dimensional, two variables (tempertaure, specific humidity)
- forced by the global GEOS-5 model

(3) CSU global shallow-water model

- two-dimensional, three variables (height, stream function, velocity potential)
- finite-difference, on a twisted icosahedral grid

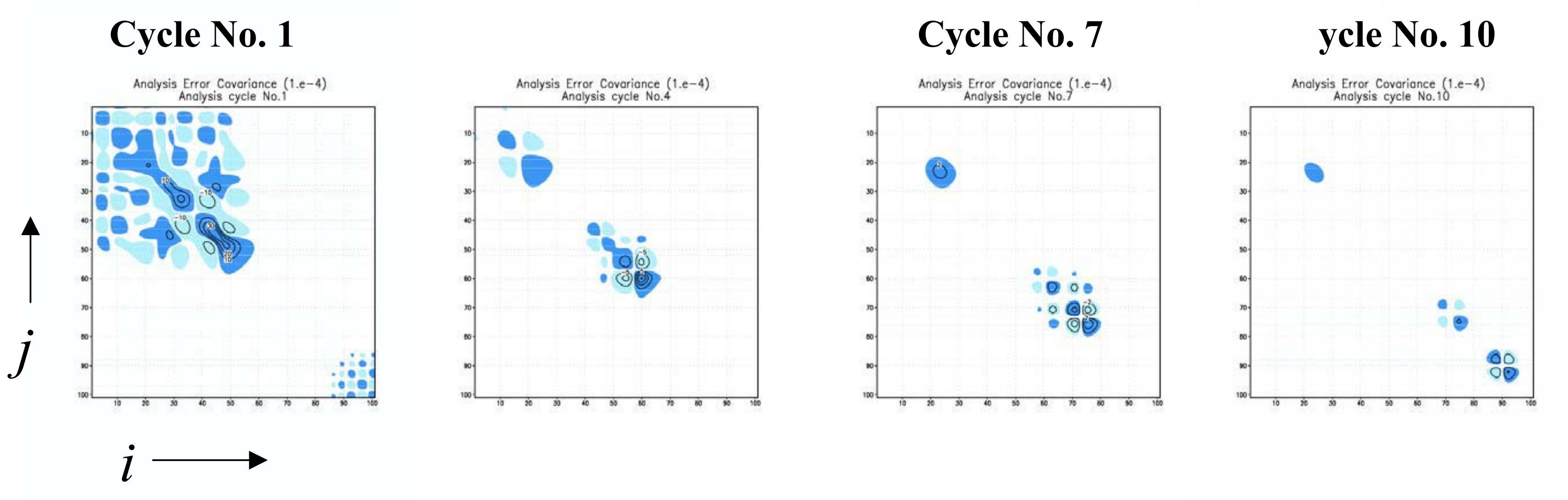
(4) CSU RAMS – non-hydrostatic model with explicit microphysics

- Exner function, potential temperature, winds, specific humidity, rain, graupel, hail, aggregates, pristine ice, snow
- finite-difference, Arakawa C-grid

KdVB model: covariance localization

• **KdVB model**

$$\frac{\partial u}{\partial t} + u\frac{\partial u}{\partial x} + 6\frac{\partial^3 u}{\partial x^3} = \nu\frac{\partial^2 u}{\partial x^2}$$



• **Initial error covariance noisy, but quickly becomes spatially localized**

• **No need to artificially force error covariance localization**

Why does the localization happens by itself ?

Error covariance localization

$n = 1$

$$\left(P_f^{1/2}\right)_1 = M_1 P_0^{1/2}$$

$$\left(P_a^{1/2}\right)_1 = \left(P_f^{1/2}\right)_1 \left(I + Z_1^T Z_1\right)^{-1/2} = \left[M_1 P_0^{1/2}\right]\left(I + Z_1^T Z_1\right)^{-1/2}$$

$n = 2$

$$\left(P_f^{1/2}\right)_2 = M_2 \left(P_a^{1/2}\right)_1 = \left[M_2 M_1 P_0^{1/2}\right]\left(I + Z_1^T Z_1\right)^{-1/2}$$

$$\left(P_a^{1/2}\right)_2 = \left(P_f^{1/2}\right)_2 \left(I + Z_2^T Z_2\right)^{-1/2} = \left[M_2 M_1 P_0^{1/2}\right]\left(I + Z_1^T Z_1\right)^{-1/2}\left(I + Z_2^T Z_2\right)^{-1/2}$$

$n = N$

$$\left(P_f^{1/2}\right)_N = M_N \left(P_a^{1/2}\right)_{N-1} = \left[M_N \ldots M_2 M_1 P_0^{1/2}\right]\left(I + Z_1^T Z_1\right)^{-1/2}\left(I + Z_2^T Z_2\right)^{-1/2} \cdots \left(I + Z_{N-1}^T Z_{N-1}\right)^{-1/2}$$

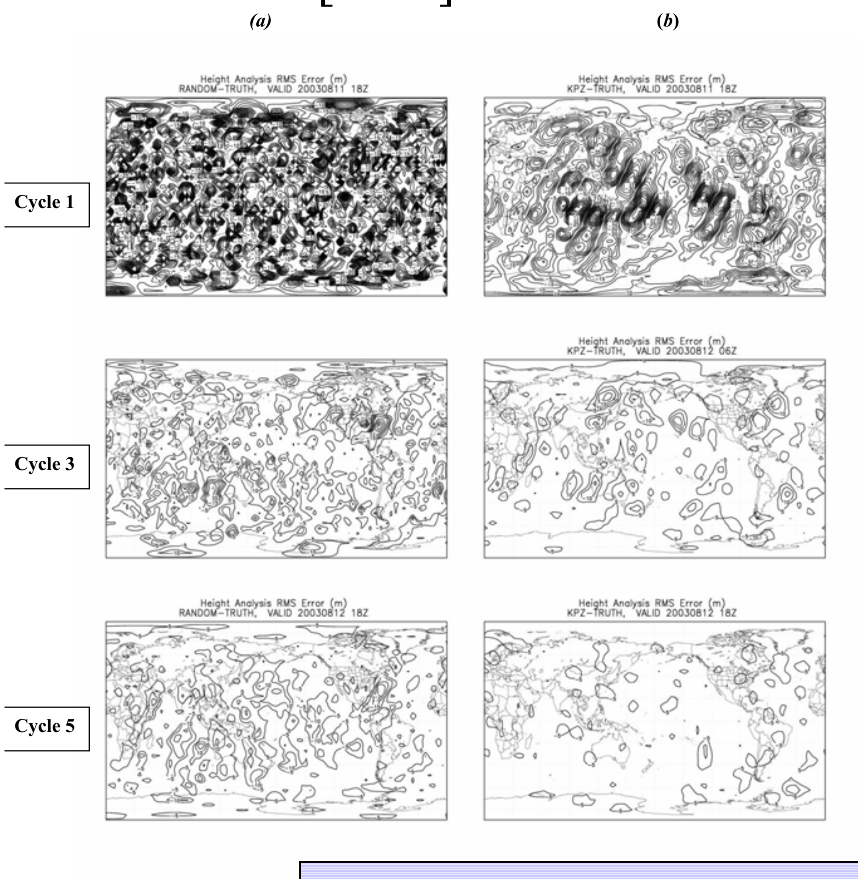
$$\left(P_a^{1/2}\right)_N = \underbrace{\left[M_N \ldots M_2 M_1 P_0^{1/2}\right]}_{\text{Lyapunov vector}}\left(I + Z_1^T Z_1\right)^{-1/2}\left(I + Z_2^T Z_2\right)^{-1/2} \cdots \left(I + Z_N^T Z_N\right)^{-1/2}$$

Possible explanation for error covariance localization:

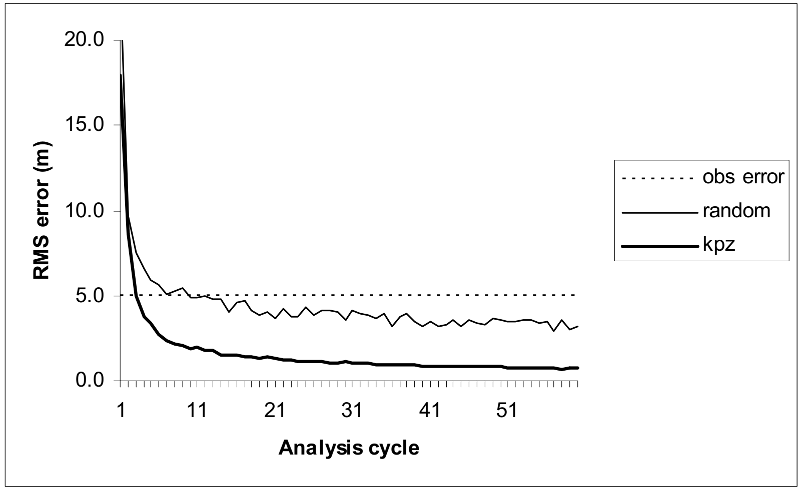
Dynamic localization of Lyapunov vectors

MLEF with CSU global shallow-water model

Height analysis increment
$[x^a - x^b]$



Height RMS error $[x^a - x^t]$



Impact of the initial choice for ensemble perturbations:
Correlated initial ensemble perturbations can significantly improve algorithm performance (Kardar-Parisi-Zhang equation + correlations)

Analysis increment

• **Analysis increment is a linear combination of the square-root forecast error covariance column-vectors:**

$$\boldsymbol{x}^a - \boldsymbol{x}^b = \boldsymbol{P}_f^{1/2}\boldsymbol{w} = w_1\boldsymbol{p}_1^f + w_2\boldsymbol{p}_2^f + \cdots + w_{N_E}\boldsymbol{p}_{N_E}^f$$

$$\boldsymbol{w} = \left(\boldsymbol{I} + \boldsymbol{Z}^T\boldsymbol{Z}\right)^{-1/2}\zeta$$

• If the column-vectors are smooth, the analysis increment will be smooth

• Due to the $\boldsymbol{P}_f$ dynamic localization, need to improve the initial error covariance fast

Impact of dynamics:

• **smoothness of the analysis**

• **localization of error covariance**

Model error and parameter estimation in MLEF

State augmentation approach

$$\mathbf{z}_n = \begin{bmatrix} \mathbf{x}_n \\ \mathbf{b}_n \\ \boldsymbol{\gamma}_n \end{bmatrix} = \begin{bmatrix} M_{n,n-1} & (1-\alpha^n)G & 0 \\ 0 & \mathbf{I} & 0 \\ 0 & 0 & \mathbf{I} \end{bmatrix} \begin{bmatrix} \mathbf{x}_{n\text{-}1} \\ \mathbf{b}_{n\text{-}1} \\ \boldsymbol{\gamma}_{n-1} \end{bmatrix} + \begin{bmatrix} \alpha^n \\ 0 \\ 0 \end{bmatrix} \Phi_0$$

$\mathbf{x}$ – state vector (initial conditions) ; $\mathbf{b}$ – model bias ; γ – empirical parameters

Augmented control variable:

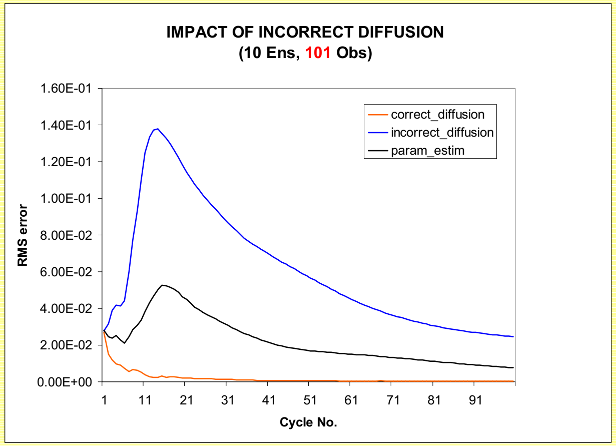
$$\mathbf{z} = (\mathbf{x}_0, \mathbf{b}, \gamma)$$

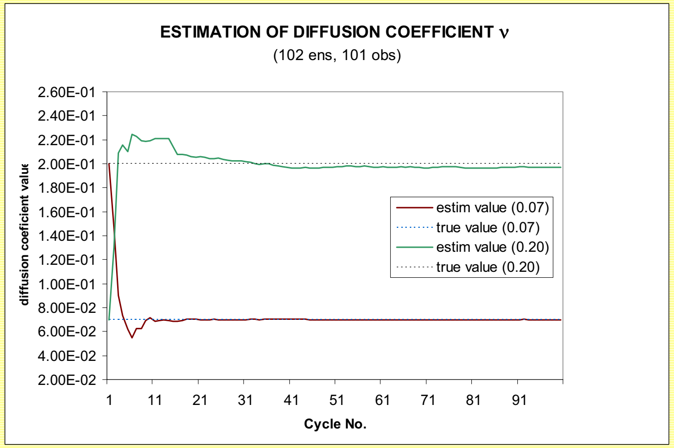
Augmented error covariance:

$$\mathbf{P} = \begin{pmatrix} P_{x_0,x_0} & P_{x_0,b} & P_{x_0,\gamma} \\ P_{b,x_0} & P_{b,b} & P_{b,\gamma} \\ P_{\gamma,x_0} & P_{\gamma,b} & P_{\gamma,\gamma} \end{pmatrix}$$

Model error and parameter estimation with KdVB model

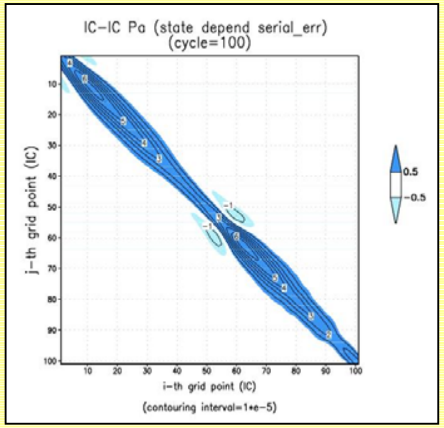
Parameter estimation (diffusion coefficient)

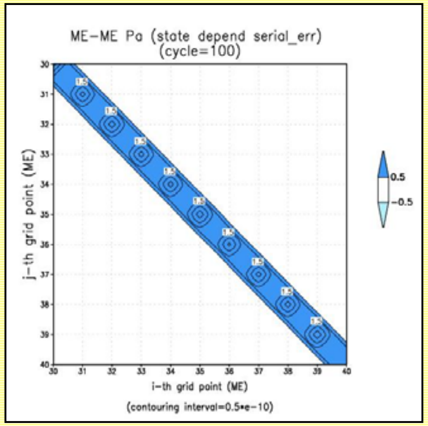


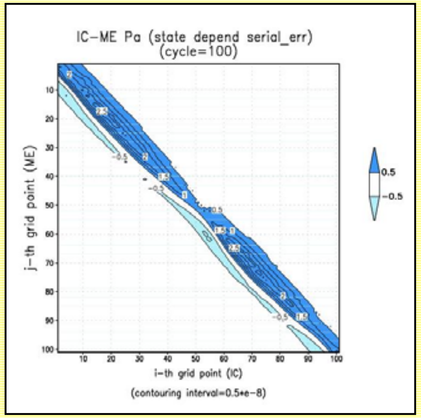


Error covariance block matrices

IC-IC **ME-ME** **IC-ME**



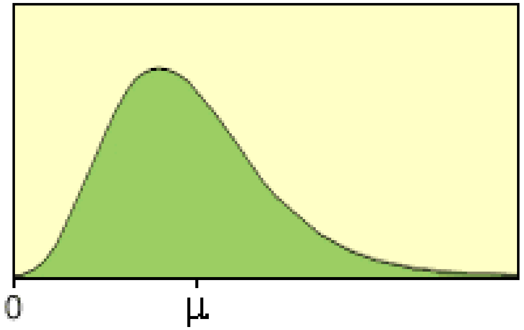




Significant cross-correlation between initial conditions and model error

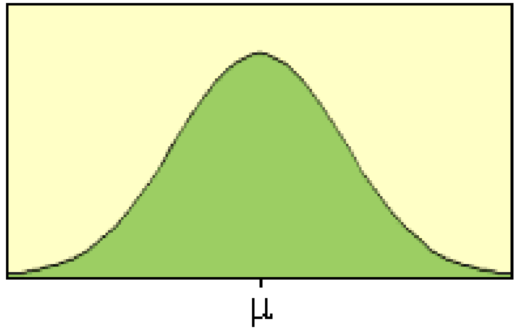
Non-Gaussian MLEF framework

Log-Normal PDF



$$\phi(x)=\begin{cases}\dfrac{exp\left(-\dfrac{1}{2}\left(\dfrac{log(x)-m}{s}\right)^2\right)}{xs\sqrt{2\pi}} & x>0\\ 0 & \text{otherwise}\end{cases}$$

Gaussian PDF



$$\phi(x)=\frac{exp\left(-\dfrac{1}{2}\left(\dfrac{x-\mu}{\sigma}\right)^2\right)}{\sigma\sqrt{2\pi}}$$

***Log-likelihood cost-function*:** $J(x)=-\ln[\phi(x)]$

Maximize posterior PDF ⇔ minimize cost function

Posterior conditional PDF $\phi(X\mid Y)=\dfrac{\phi(X)\phi(Y\mid X)}{\phi(Y)}$

$$\boldsymbol{max}\{\phi(X\mid Y)\}\propto \boldsymbol{max}\{\phi(X)\phi(Y\mid X)\}=\boldsymbol{min}\{-\ln[\phi(X)]-\ln[\phi(Y\mid X)]\}$$

Non-Gaussian MLEF framework:
Lognormal height observation errors

Assume:

- **Gaussian prior probability distribution (state vector)** $\phi(X) \sim Gaussian$

- **Observations: Height (Lognormal), Wind (Gaussian)**

$\phi(Y_{HEIGHT} \mid X) \sim Lognormal$

$\phi(Y_{WIND} \mid X) \sim Gaussian$

$$\frac{\boldsymbol{y}_{HEIGHT}}{\mathcal{H}(\boldsymbol{x})} = \boldsymbol{\varepsilon} \Rightarrow \ln[\boldsymbol{y}_{HEIGHT}] - \ln[\mathcal{H}(\boldsymbol{x})] = \ln \boldsymbol{\varepsilon}$$

$$\boldsymbol{y}_{WIND} - \mathcal{H}(\boldsymbol{x}) = \boldsymbol{\varepsilon}$$

Minimize mixed Normal-Lognormal cost function:

$$J(\boldsymbol{x}) = \frac{1}{2}\left(\boldsymbol{x} - \boldsymbol{x}^b\right)^T \boldsymbol{P}_f^{-1}\left(\boldsymbol{x} - \boldsymbol{x}^b\right) + \frac{1}{2}\left(y_{WIND} - \mathcal{H}(\boldsymbol{x})\right)^T \boldsymbol{R}^{-1}\left(y_{WIND} - \mathcal{H}(\boldsymbol{x})\right)$$

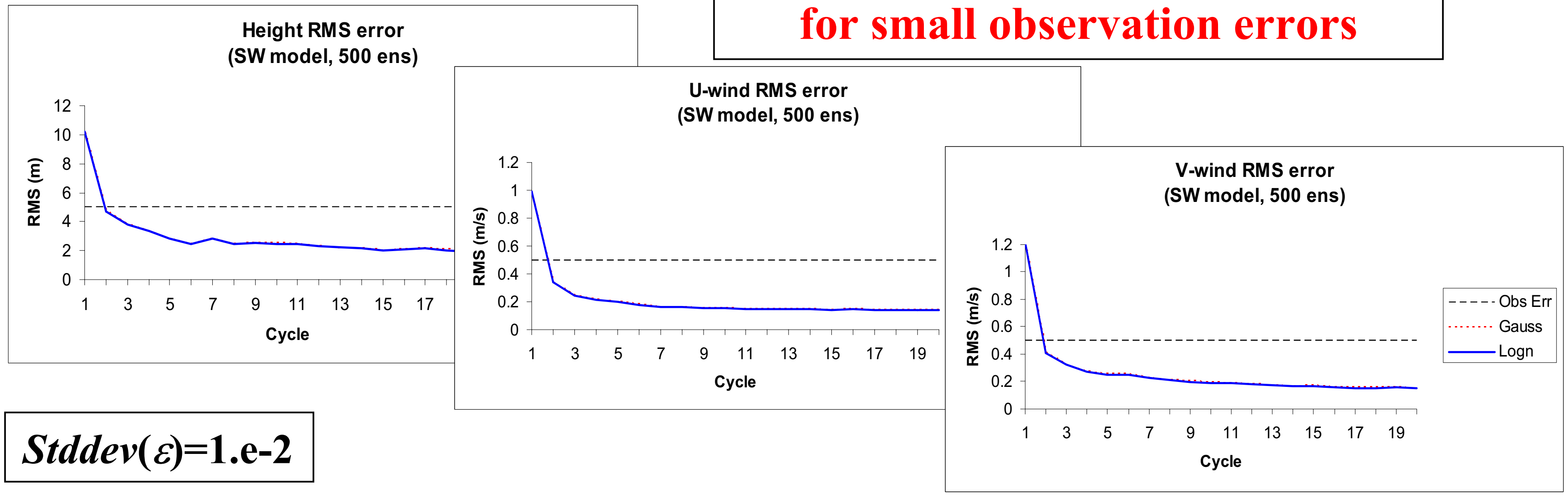
$$+ \frac{1}{2}\left(\ln\left[\frac{y_{HEIGHT}}{\mathcal{H}(\boldsymbol{x})}\right] - m\right)^T \boldsymbol{R}_S^{-1}\left(\ln\left[\frac{y_{HEIGHT}}{\mathcal{H}(\boldsymbol{x})}\right] - m\right) + \sum_{i=1}^{N_{obs}} \ln\left[\frac{y_{HEIGHT}}{\mathcal{H}(\boldsymbol{x})}\right]_i$$

Higher nonlinearity of the cost function compared to the Gaussian

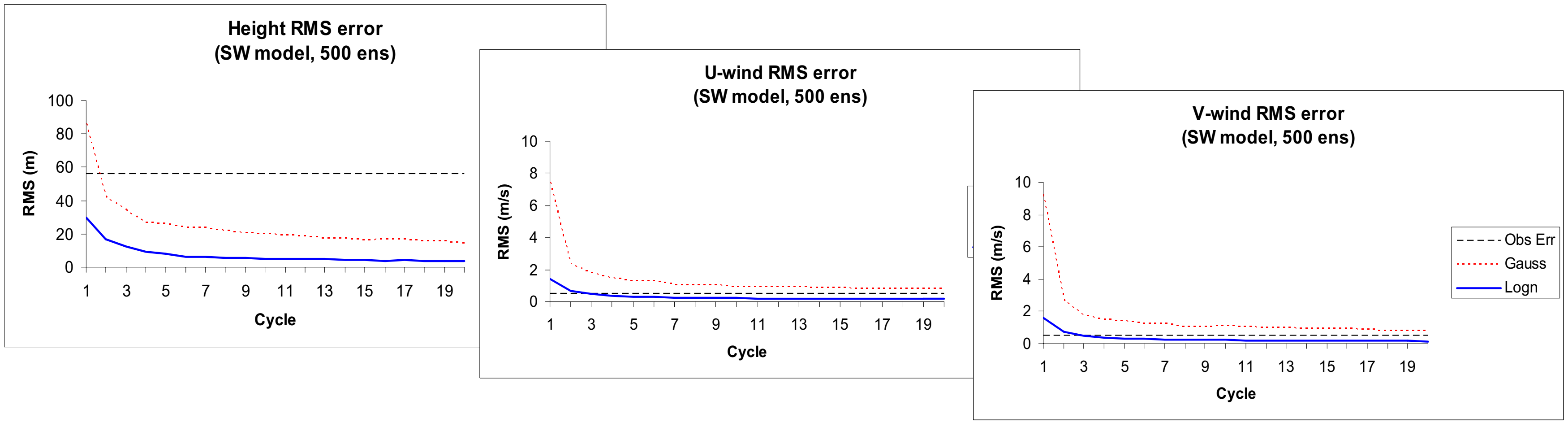
Impact of Lognormal observation erros:
Analysis RMS errors

Stddev(ε)=1.e-3

Gaussian framework works only for small observation errors



Stddev(ε)=1.e-2

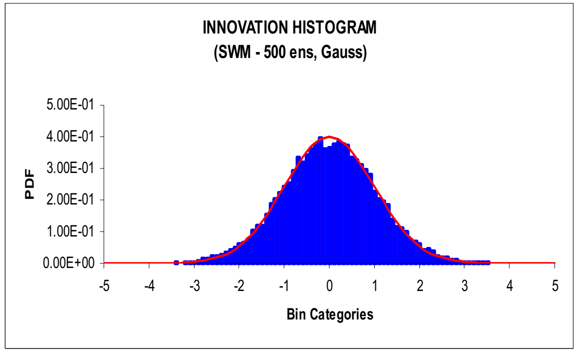


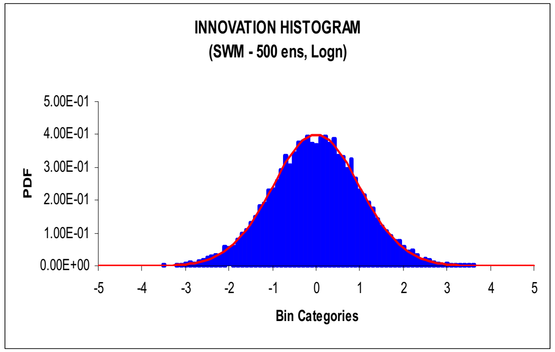
Lognormal framework works for all error magnitudes

Impact of Lognormal height observation errros:
Innovation histogram

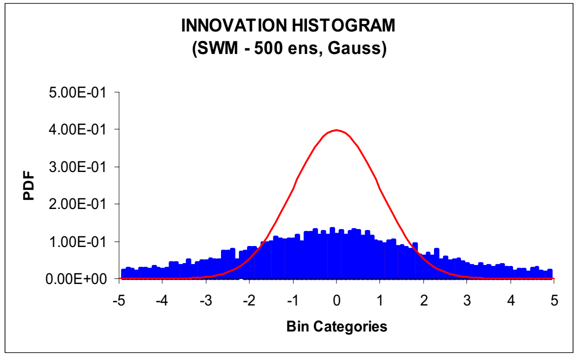
Gaussian framework | **Lognormal framework**

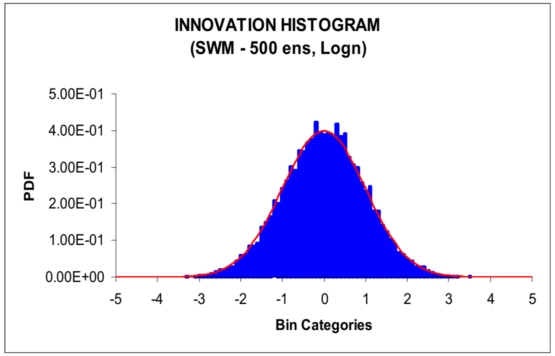
Stddev(ε)=1.e-3





Stddev(ε)=1.e-2





Height innovations → $y - \mathcal{H}(\mathbf{x})$ | $\ln\left[\frac{y}{\mathcal{H}(\mathbf{x})}\right] - m$

Generalized non-Gaussian framework can handle Gaussian, Lognormal, or mixed PDF errors !

Ongoing work

❑ **NCEP Global Forecasting System model and real data**

- Apply MLEF with GFS and compare with other EnKF algorithms
- Compare (and combine) the conditional mean and mode PDF estimates
- Develop and test *double-resolution* MLEF
  - Operational (high) resolution control analysis/forecast
  - Low (coarse) resolution ensembles – error covariance

❑ **Carbon Cycle data assimilation**

- Apply MLEF with fully coupled SiB-CASA-RAMS atmospheric-carbon-biomass model
- Assimilate carbon concentration globally and locally
- Empirical parameter estimation in carbon models

❑ **GOES-R Risk Reduction**

- Evaluate the impact of GOES-R measurements in applications to severe weather and tropical cyclones
- Information content of GOES-R measurements

Future Research Directions

Algorithmic and theoretical aspects:

Development of a fully non-Gaussian algorithm
- Allow for non-Gaussian *state variable* components
- Generalized algorithm with a list of PDFs

Representativeness error
- How well the ensembles represent the truth
- Improve robustness of the algorithm

Model bias and parameter estimation
- Improve prediction models by learning about its errors and uncertainties
- Develop as a probabilistic tool for new model development

Initiation of ensemble perturbations ("cold" start)
- Competition between the rate of covariance localization and the development of a representative ensemble basis
- Kardar-Parisi-Zhang equation + correlations
- Tikhonov regularization as a criteria for ensemble size reduction

  (B. Uzunoglu: reduction from 1000 ensembles to about 200 in few cycles !)

Future Research Directions

Applications:

Climate models

- Assimilation of clouds and precipitation – MMF (Multiscale Modeling Framework)
- Coupled climate-ocean models
- Predictability

Microscale models

- Boundary layer, 100m-500m horizontal resolution
- Probabilistic transfer and interaction between scales

Carbon data assimilation

- Exploit assimilation of new measurements (OCO-Orbiting Carbon Observatory)

Cross-over the existing scientific boundaries

- Apply probabilistic assimilation/prediction to other science disciplines
- General, adaptive, algorithmically simple algorithm opens new possibilities