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Non-Gaussian error statistics and ensemble data assimilation

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Computational Support	NCAR SCD (bluesky)

Framework for Assimilation/Prediction

- **Uncertainties (errors) are considered random variables**
  - Observations, Parameters, Model bias, Boundary conditions
  - Input forcing from atmospheric or climate models
  (e.g., temperature, precipitation, top soil moisture)

- **Normal (Gaussian) PDF generally used**
  - Variational methods (3D-Var, 4D-Var)
  - Kalman filters (extended, reduced-rank)
  - Ensemble Kalman filters
  - Least-square methods
  - Well understood
  - Relatively simple to use
  - Satisfactory results

$$PDF(\boldsymbol{x} = \boldsymbol{x}^f) \sim \exp\left[-\frac{1}{2} \left(\boldsymbol{x} - \boldsymbol{x}^f \right)^T \boldsymbol{P}_f^{-1} \left(\boldsymbol{x} - \boldsymbol{x}^f \right) \right]$$

$$J_b(\boldsymbol{x}) = -\ln\left[PDF(\boldsymbol{x} = \boldsymbol{x}^f) \right] = \frac{1}{2} \left(\boldsymbol{x} - \boldsymbol{x}^f \right)^T \boldsymbol{P}_f^{-1} \left(\boldsymbol{x} - \boldsymbol{x}^f \right)$$

Limitations of Normal (Gaussian) framework

- **Gaussian errors imply linear assumption**
  - Prediction models are nonlinear
  - Observation transformation operators are nonlinear
    - Remote sensing (radar, satellite)
    - Precipitation is a nonlinear function of T and q

- **Gaussian errors imply symmetric error structure**
  - Equally likely $\boldsymbol{x}=\boldsymbol{x}^f+\varepsilon$ and $\boldsymbol{x}=\boldsymbol{x}^f-\varepsilon$
  - Not all variables (observations) have symmetric errors
    - Moisture
    - Precipitation
    - Concentration (pollutant, aerosol)

- **Extreme events (floods, droughts)**
  - Belong to a non-Gaussian PDF (Tails of a Gaussian PDF)
  - Extremely large (positive/negative) system perturbations

- **Quality Control**
  - Large departures of observations from a forecast guess are typically rejected
  - Can belong to a non-Gaussian PDF, observations should be used

How to relax Gaussian PDF assumption ?

- **Develop non-Gaussian framework for assimilation/prediction**

  - Control variable errors can be mixed Gaussian/non-Gaussian

  - Observation errors can be mixed Gaussian/non-Gaussian

  - Improve understanding of nonlinear processes, prediction of extreme events

Further motivation for inclusion of non-Gaussian errors

- **Generality**

  - *non-Gaussian assimilation/prediction framework allows greater flexibility of the system*

- **Chaos**

  - Results from nonlinear dynamics suggest a *lognormal* error distribution of the initial ensemble perturbations (e.g., bred vectors, singular vectors)

  - Implication: the posterior PDF should be non-Gaussian (lognormal)

Ensemble Methodology

- **Maximum Likelihood Ensemble Filter (MLEF)**

- Originally developed to work with Normal (Gaussian) error assumption, extended for use with mixed Normal-Lognormal observation errors
- Estimate of the *conditional mode* of the posterior PDF
- Ensembles used to estimate the *uncertainty* of the conditional mode
- *Non-differentiable* cost-function minimization
- Implicit Hessian preconditioning
- 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

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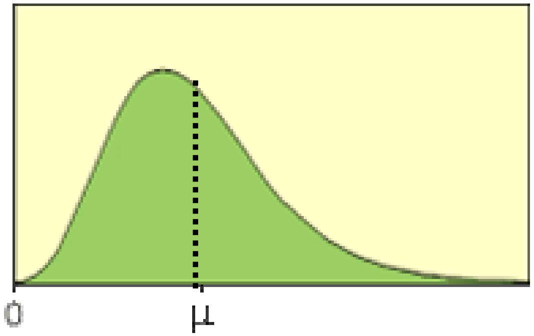
Zupanski and Zupanski 2005, *Mon. Wea. Rev.*
[ftp://ftp.cira.colostate.edu/milija/papers/MLEF_model_err.pdf]

Fletcher and Zupanski 2005, *Proc. Roy. Soc. London A*

[ftp://ftp.cira.colostate.edu/milija/papers/Steven_nongauss.pdf]

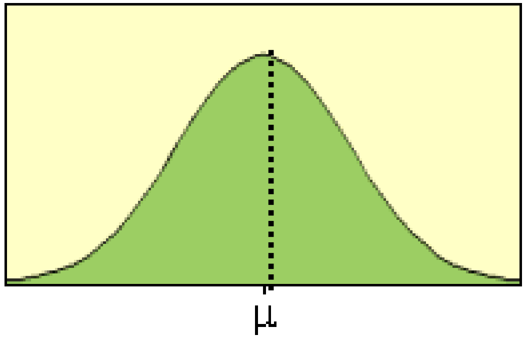
Non-Gaussian MLEF framework

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



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

Posterior conditional PDF:

$$\phi(X\mid Y)=\frac{\phi(X)\phi(Y\mid X)}{\phi(Y)}$$

***Log-likelihood cost-function*:**

$$J(x)=-\ln[\phi(x)]$$

Maximize posterior PDF ⇔ minimize cost function

Non-Gaussian MLEF framework
Lognormal height observation errors

- **Gaussian prior probability distribution (state vector)**

$$\phi(X) \sim Gaussian$$

- **Observations**

$$\phi(Y_{HEIGHT} \mid X) \sim Lognormal \Rightarrow \qquad \boxed{\frac{\boldsymbol{y}_{HEIGHT}}{\mathcal{H}(\boldsymbol{x})} = \boldsymbol{\varepsilon}_L}$$

$$\phi(Y_{WIND} \mid X) \sim Gaussian \Rightarrow \qquad \boxed{\boldsymbol{y}_{WIND} - \mathcal{H}(\boldsymbol{x}) = \boldsymbol{\varepsilon}_G}$$

- ***Minimize mixed Normal-Lognormal cost function:***

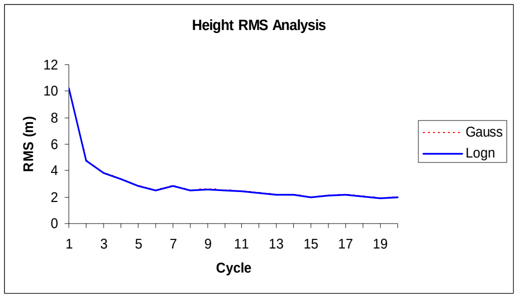
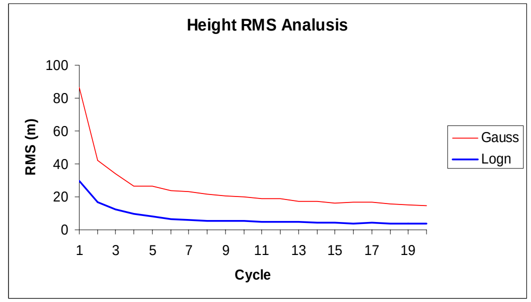
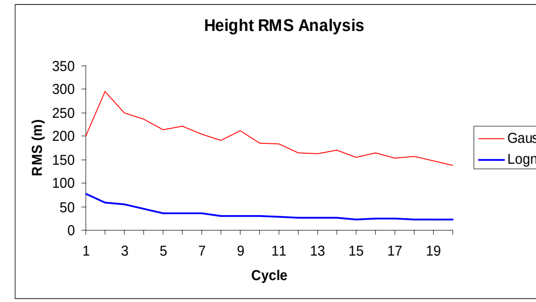
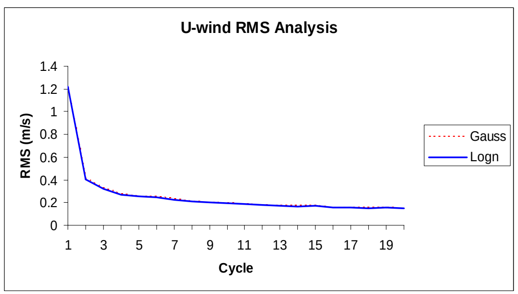
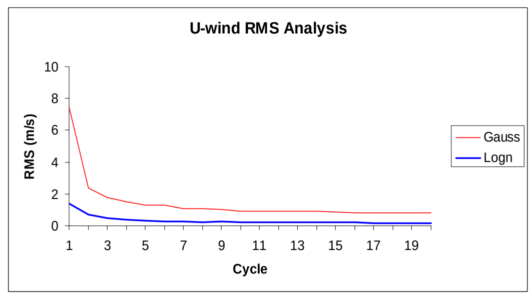
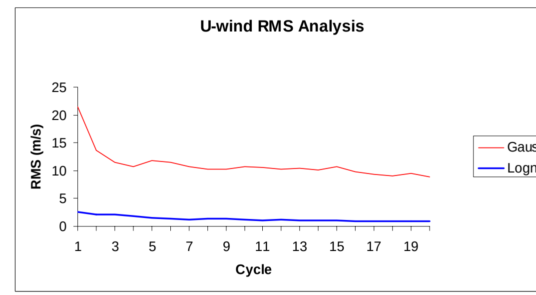
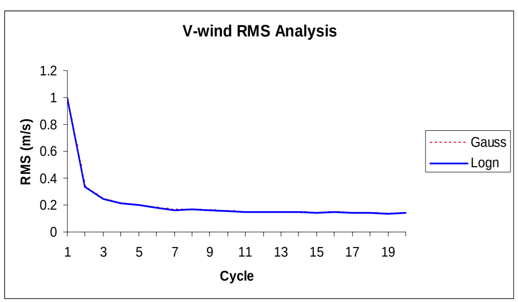
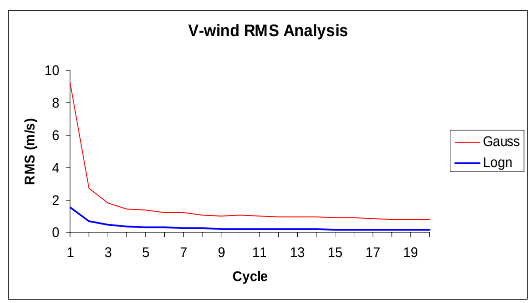
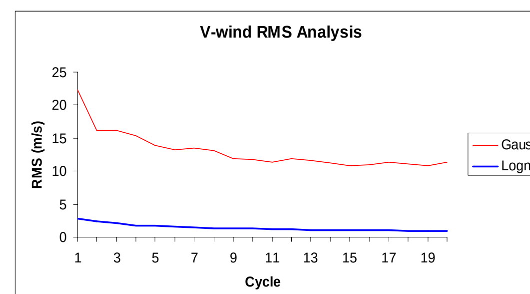
$$J(\boldsymbol{x}) = \frac{1}{2}\left(\boldsymbol{x} - \boldsymbol{x}^f\right)^T \boldsymbol{P}_f^{-1}\left(\boldsymbol{x} - \boldsymbol{x}^f\right) + \frac{1}{2}\left(y_{WIND} - \mathcal{H}(\boldsymbol{x})\right)^T \boldsymbol{R}^{-1}\left(y_{WIND} - \mathcal{H}(\boldsymbol{x})\right)$$

Normal

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

Lognormal
(additional nonlinear terms)

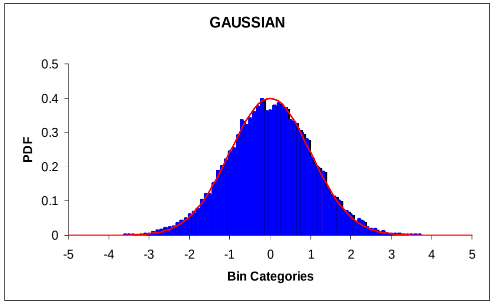
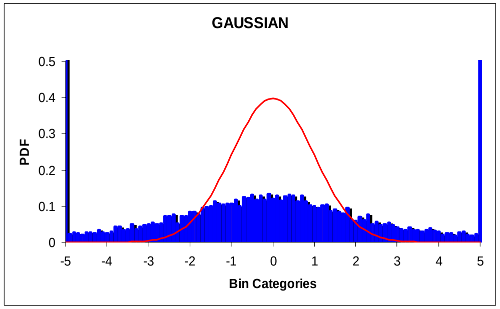
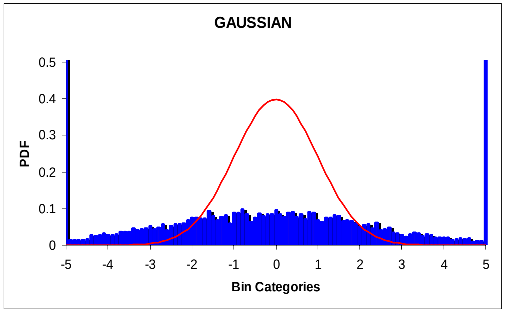
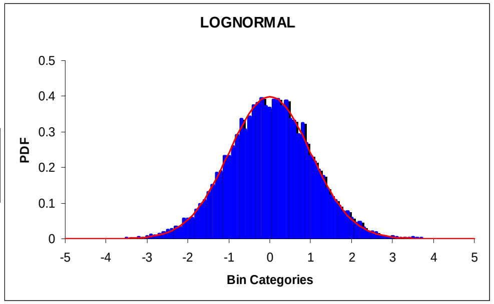
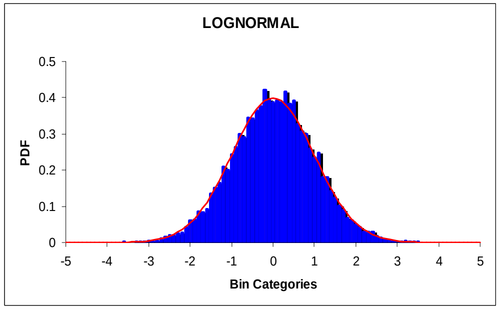
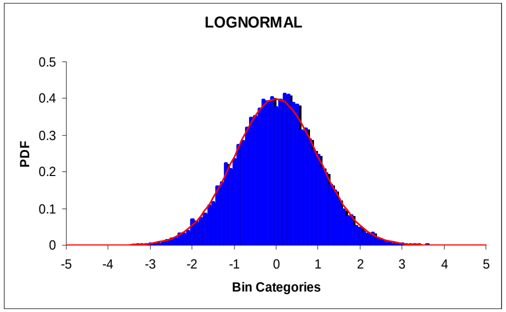
Results with CSU global shallow-water model:
Analysis RMS errors

	σ_{Logn}= 1.e-3 ~ σ_{Gauss}= 5 m	σ_{Logn}= 1.e-2 ~ σ_{Gauss}= 60 m	σ_{Logn}= 5.e-2 ~ σ_{Gauss}= 300 m
height			
U-wind			
V-wind			

Gaussian framework works only for *small* observation errors

Lognormal framework works for *all* error magnitudes

Results with CSU global shallow-water model:
Innovation Histogram (obs-fcst)

	σ_{Logn}= 1.e-3 ~ σ_{Gauss}= 5 m	σ_{Logn}= 1.e-2 ~ σ_{Gauss}= 60 m	σ_{Logn}= 5.e-2 ~ σ_{Gauss}= 300 m
Gaussian			
Lognormal			

$$\textit{Normalized} \quad \textit{Innovation} = \left[\boldsymbol{H}\boldsymbol{P}_f \boldsymbol{H}^{\mathrm{T}} + \boldsymbol{R}\right]^{-1/2} [\boldsymbol{y} - H(\boldsymbol{x}^a)]$$

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

Conclusions and Future Research Directions

Mixed Normal/Lognormal Observation errors

- Improved performance of a non-Gaussian algorithm
- Similar results for small errors, significant deficiencies of Gaussian error assumption for large errors

Development of a fully non-Gaussian algorithm

- Allow for non-Gaussian *state variable* errors (initial conditions, parameters)
- Generalized algorithm with a list of PDFs

Assume lognormal errors of initial ensemble perturbations

- Evaluate theoretical results from space-time chaos
- Improve robustness

THORPEX Research: MLEF with GFS and real observations

- NCEP observations with Global Forecasting System
- Double-resolution MLEF: high-resolution control, low-resolution ensembles

Thank you !

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MLEF Analysis Step

Use forecast (prior) error covariance square-root

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

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

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

Similar to variational, however:

❑ **Non-differentiable iterative minimization with preconditioning**

- No differentiability assumption: works for all bounded operators
- Generalized gradient, generalized Hessian

❑ **Solution in ensemble subspace**

- Reduced dimensions of the analysis correction subspace
- Focus on unstable, growing perturbations in the analysis
- Search for the attractor subspace (unstable manifold span-vectors)

Hessian preconditioning

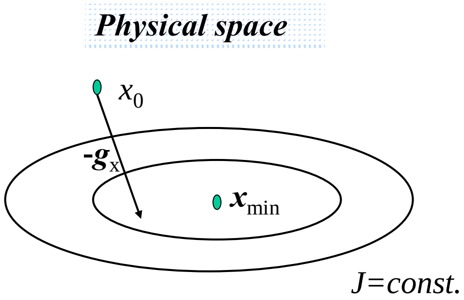
Change of variable (Hessian preconditioning)

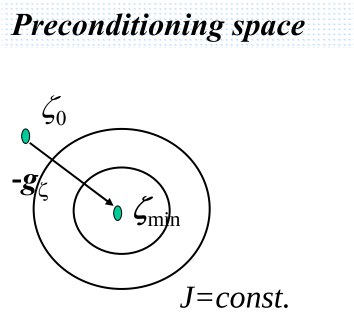
$$\boxed{\boldsymbol{x}_k = \boldsymbol{x}^f + \boldsymbol{P}_f^{1/2}\left[\boldsymbol{I} + \left(\boldsymbol{Z}^b\right)^T \boldsymbol{Z}^b\right]^{-1/2} \zeta_k}$$

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

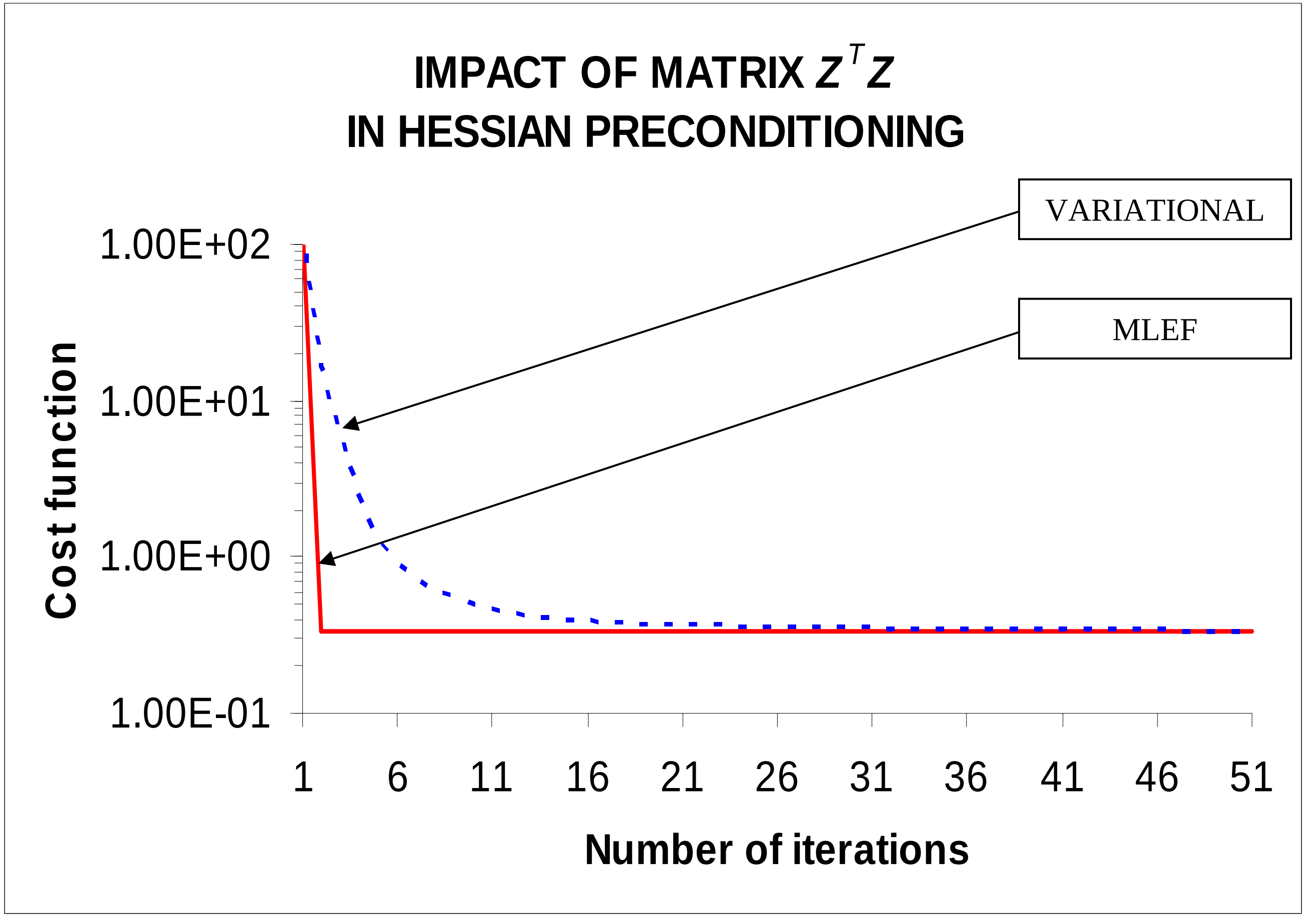
$$\boxed{\zeta_{k+1} = \zeta_k + \alpha_k \boldsymbol{d}_k}$$

k – iteration index





Hessian Preconditioning



$$\boldsymbol{P}_{VAR}^{-1} = \boldsymbol{P}_f$$

$$\mathrm{P}_{ENS}^{-1} = \boldsymbol{P}_f^{\,1/2}(\boldsymbol{I} + \boldsymbol{Z}^T \boldsymbol{Z})^{-1} \boldsymbol{P}_f^{\,T/2}$$

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**
- ***Assumption*: Inverse Hessian = Analysis error covariance**

How to make sure the assumption is valid?

- **$\|x^{true} - x^a\| < \varepsilon$: for small ε (compared to analysis errors)**
- **In practice, ε is only a fraction of the analysis error** (1-2 %)

Why is ε small?

- **Good Hessian preconditioning allows efficient and accurate minimization**
- **By monitoring minimization, assure the calculated solution is close to the true minimum**

Forecast (prior) error covariance

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

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

- **Control vector is the *most likely* forecast**
- **Square-root used in the algorithm** (full covariance can be calculated)
- **No sampling of error covariance**
- **Provides dynamic continuity between the analysis and forecast**