Ensemble Kalman filter methods

T.Janjić

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- We represent the atmosphere in terms of numerical models of the atmosphere, that is by discretizing nonlinear equations that govern the dynamics.
- Ongoing observations of the atmosphere using instruments with different spatial and temporal coverage as well as different accuracy give us valuable information on the current state of the atmosphere.
- Our objective is to combine these two sources of information and to produce an estimate on the grid of our numerical model.

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- The Kalman filter provides algebraic formulas for the change of mean and error covariance by the Bayesian update equation.
- In addition to the analysis we do get an estimate of analysis error consistent with the dynamics, prescribed model and observational error statistics.
- The Kalman filter provides us with formulas for advancing the error covariance matrix in time.

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- For large dimensional systems, the complete error structure of a time-evolving forecast error covariance is impossible to know or even to represent accurately.

Why the ensemble Kalman filter approach?

- The Kalman filter is difficult to implement in realistic systems because of:
  - computational costs,
  - the nonlinearity of dynamics and
  - poorly characterized error sources.
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- The ensemble Kalamn filter (EnKF) (Evensen 1994) uses ensembles (a sample) to calculate the uncertainty of the background and analysis error covariance.
- Ensembles are propagated with full nonlinear numerical model. This can be done over long time periods, and results in flow dependent error covariances.

Ensemble Kalman filter methods:

Step 1: Analysis

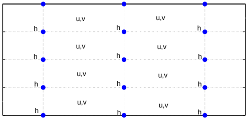
Step 2: Resampling

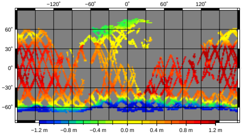
Step 3: Propagation of the ensembles

Ensemble Kalman filter methods:

Step 1: Analysis

$\mathbf{w}_k^b$





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Ensemble Kalman filter methods:

Step 1: Analysis

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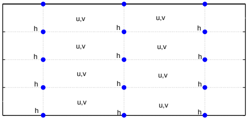

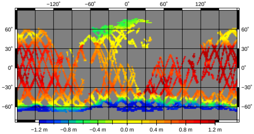

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Step 2: Resampling

The ensemble Kalman filter requires us to generate a number r of ensemble members $\mathbf{w}_k^{a,i}$, $i = 1, \ldots, r$:

$$\mathbf{w}_k^a, \mathbf{B}_k^a \Rightarrow \mathbf{w}_k^{a,1}, \mathbf{w}_k^{a,2}, \mathbf{w}_k^{a,r-1}, \ldots, \mathbf{w}_k^{a,r}$$

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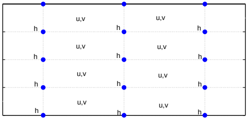

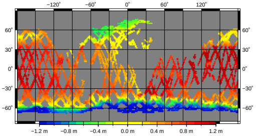

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Step 3: Propagation of the ensembles

$$\mathbf{w}_k^{a,1}, \mathbf{w}_k^{a,2}, \mathbf{w}_k^{a,r-1}, \ldots, \mathbf{w}_k^{a,r} \Rightarrow \mathbf{w}_k^{b,1}, \mathbf{w}_k^{b,2}, \mathbf{w}_k^{b,r-1}, \ldots, \mathbf{w}_k^{b,r} \Rightarrow \mathbf{w}_{k+1}^b, \mathbf{B}_{k+1}^b$$

Initial step of sequential data assimilation algorithm

The inputs to the Kalman filter are:

- An initial state at time t_0 and the corresponding covariance matrix $\mathbf{B}_0$
- Observations $\mathbf{f}_k^o$ and observational error covariance $\mathbf{R}_k$ at each analysis time
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We do not need to specify the covariances matrices of background error $\mathbf{B}_k^b$. It is generated and propagated by the filter using full nonlinear dynamics of the model.

However, we do need to specify $\mathbf{Q}_k$ and $\mathbf{R}_k$ for all k as well as $\mathbf{B}_0$.

Step 1: Analysis

$$\mathbf{w}_k^a = \mathbf{w}_k^b + \mathbf{K}_k(\mathbf{f}_k^o - \mathbf{H}_k\mathbf{w}_k^b),$$

$\mathbf{K}_k$ is taken as

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

or

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- $\mathbf{B}_k^b$ determines directly the quality of the analysis since it determines the weight each observation has.

Now we will consider how is $\mathbf{B}_k^b$ generated in the ensemble Kalman filter approach.

For EnKF background error covariance is calculated as sample covariance from the ensemble

Covariances represented through

$$\mathbf{B}_k^b = \frac{1}{r-1} \sum_{i=1}^{r} [\mathbf{w}_k^{b,i} - \mathbf{w}_k^b][\mathbf{w}_k^{b,i} - \mathbf{w}_k^b]^T.$$

$\mathbf{B}_k^b$ is the ensemble derived forecast error covariance;
$\mathbf{w}_k^{b,i}$ are ensemble members $i = 1, \dots, r$ of size n at time t_k;
$\mathbf{w}_k^b$ is the average over ensemble.

$$\mathbf{w}_k^b = \frac{1}{r} \sum_{i=1}^{r} \mathbf{w}_k^{b,i}$$

For EnKF nonlinear observation operators can be used on each ensemble member

Covariances are represented by

$$\mathbf{B}_k^b \approx \frac{1}{r-1}\sum_{i=1}^{r}[\mathbf{w}_k^{b,i} - \mathbf{w}_k^b][\mathbf{w}_k^{b,i} - \mathbf{w}_k^b]^T.$$

$$\mathbf{H}_k\mathbf{B}_k^b \approx \frac{1}{r-1}\sum_{i=1}^{r}[\mathbf{H}_k(\mathbf{w}_k^{f,i}) - \mathbf{H}_k(\mathbf{w}_k^b)][\mathbf{w}_k^{f,i} - \mathbf{w}_k^b]^T$$

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$\mathbf{H}_k$ operates on each of N ensemble members rather than on n columns of $\mathbf{B}_k^b$!

For EnKF background error covariance can be represented in square root form

- $\mathbf{B}_k^b$ is by definition positive semi-definite covariance.
- $\mathbf{B}_k^b$ has rank at most r.

$\mathbf{B}_k^b$ represented through

$$\mathbf{B}_k^b = \frac{1}{r-1}\sum_{i=1}^{r}[\mathbf{w}_k^{b,i} - \mathbf{w}_k^b][\mathbf{w}_k^{b,i} - \mathbf{w}_k^b]^T$$

can be written in matrix form as:

$$\mathbf{B}_k^b = \mathbf{W}_k^b(\mathbf{W}_k^b)^T$$

where $\mathbf{W}_k^b = \frac{1}{\sqrt{r-1}}[\mathbf{w}_k^{b,1} - \mathbf{w}_k^b \ldots \mathbf{w}_k^{b,r} - \mathbf{w}_k^b]$.

- Matrix $\mathbf{W}_k^b$ is of size $n \times r$, where $r \ll n$.

Different ensembles can span the same state space and have the same covariance

However this representation of $\mathbf{B}_k^b$ is not unique!

It is also true that

$$\mathbf{B}_k^b = \mathbf{W}_k^b \mathbf{U}_k (\mathbf{W}_k^b \mathbf{U}_k)^T$$

where $\mathbf{U}_k$ is any matrix of size $r \times r$ such that

$$\mathbf{U}_k \mathbf{U}_k^T = \mathbf{U}_k^T \mathbf{U}_k = \mathbf{I}_r.$$

Ensemble Transform Kalman Filter (ETKF) uses $\mathbf{U}_k = \mathbf{I}_r$.

For EnKF analysis error covariance can be calculated using the square root form

$$\mathbf{B}_k^a = \mathbf{B}_k^b - \mathbf{K}_k \mathbf{H}_k \mathbf{B}_k^b$$

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&= \mathbf{W}_k^b [\mathbf{I_r} - (\mathbf{W}_k^b)^T \mathbf{H}_k^T (\mathbf{H}_k \mathbf{B}_k^b \mathbf{H}_k^T + \mathbf{R}_k)^{-1} \mathbf{H}_k \mathbf{W}_k^b] (\mathbf{W}_k^b)^T
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&= \mathbf{W}_k^b(\mathbf{T}_k)(\mathbf{T}_k)^T(\mathbf{W}_k^b)^T \\
&= \mathbf{W}_k^a(\mathbf{W}_k^a)^T
\end{aligned}$$

where $\mathbf{T}_k$ is square root of matrix of size $r \times r$ given by

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- Matrix $\mathbf{W}_k^a \equiv \mathbf{W}_k^b \mathbf{T}_k$ is of size $n \times r$, where $r \ll n$ or
- $\mathbf{W}_k^a = \mathbf{W}_k^b \mathbf{T}_k \mathbf{U}_k$ where $\mathbf{U}_k$ is any orthogonal matrix of size $r \times r$.

Derivation of ETKF

- There are several different ensemble Kalman filter methods that differ by choice of square root matrix $\mathbf{T}_k$.
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Using the Shermann-Morrison-Woodbury identity

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Since the matrix $\mathbf{W}_k^{b\,T}\mathbf{H}_k^T\mathbf{R}_k^{-1}\mathbf{H}_k\mathbf{W}_k^b$ is positive definite, we can write it in terms of eigenvectors $\mathbf{C}_k^b$ and eigenvalues $\mathbf{D}_k$

$$(\mathbf{W}_k^b)^T\mathbf{H}_k^T\mathbf{R}_k^{-1}\mathbf{H}_k\mathbf{W}_k^b = \mathbf{C}_k^b\mathbf{D}_k(\mathbf{C}_k^b)^T$$

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$$\mathbf{I_r} + {\mathbf{W}_k^b}^T \mathbf{H}_k^T \mathbf{R}_k^{-1} \mathbf{H}_k \mathbf{W}_k^b = \mathbf{I_r} + \mathbf{C}_k^b \mathbf{D}_k (\mathbf{C}_k^b)^T = \mathbf{C}_k^b (\mathbf{I_r} + \mathbf{D}_k)(\mathbf{C}_k^b)^T.$$

Derivation of ETKF

In terms of unique nonnegative square root

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\begin{aligned}
\mathbf{I_r} + \mathbf{W}_k^b \mathbf{H}_k^T \mathbf{R}_k^{-1} \mathbf{H}_k \mathbf{W}_k^b &= \mathbf{C}_k^b (\mathbf{I_r} + \mathbf{D}_k)(\mathbf{C}_k^b)^T \\
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\end{aligned}
$$

This leads us to formula used for square root in ETKF for calculation of $\mathbf{B}_k^a$

$$\mathbf{W}_k^a = \mathbf{W}_k^b \mathbf{T}_k^{ETKF}$$

with

$$\mathbf{T}_k^{ETKF} = \mathbf{C}_k^b (\mathbf{I_r} + \mathbf{D}_k)^{-1/2} \qquad \text{(Bishop et al. 2001)}$$

$$\mathbf{T}_k^{LETKF} = \mathbf{C}_k^b (\mathbf{I_r} + \mathbf{D}_k)^{-1/2} {\mathbf{C}_k^b}^T \qquad \text{(Hunt et al. 2007)}$$

Derivation of ETKF

$$\mathbf{W}_k^a = \mathbf{W}_k^b \mathbf{T}_k^{ETKF}$$

$$\begin{aligned}\mathbf{K}_k &= \mathbf{B}_k^a \mathbf{H}_k^T \mathbf{R}_k^{-1} \\ &= \mathbf{W}_k^b \mathbf{T}_k^{ETKF} {\mathbf{T}_k^{ETKF}}^T (\mathbf{H}_k \mathbf{W}_k^b)^T \mathbf{R}_k^{-1}\end{aligned}$$

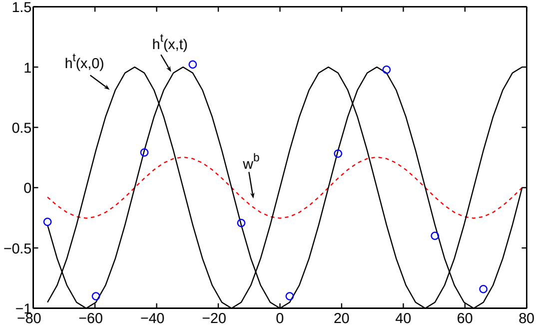
$$\mathbf{T}_k^{ETKF} = \mathbf{C}_k^b (\mathbf{I_r} + \mathbf{D}_k)^{-1/2} {\mathbf{C}_k^b}^T \quad \text{(Hunt et al. 2007)}$$

Example 1: How good is our analysis?

Let us consider simple passive advection equation

$$\frac{\partial h}{\partial t} + c\frac{\partial h}{\partial x} = 0$$
$$h(x,0) = sin(x)$$

Solution is given by $h^t(x,t) = sin(x - ct)$.



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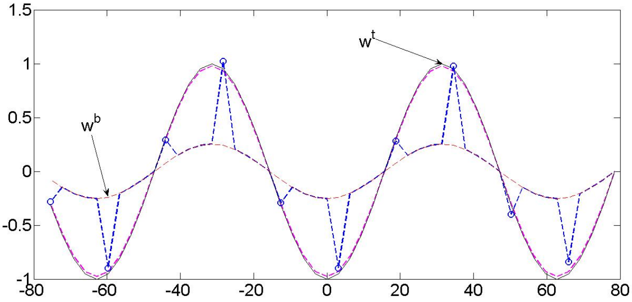

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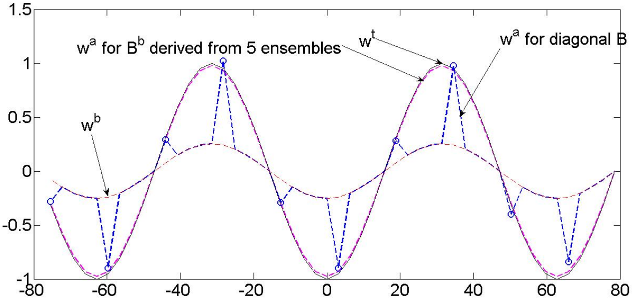

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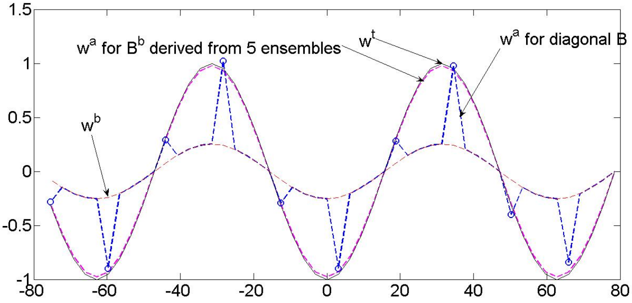

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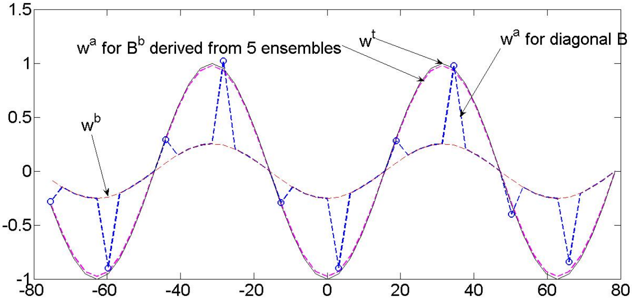

- Use of diagonal matrix does not propagate information about observations to the neighborhood grid points.
- Ensemble background error covariance incorporates information about the model, and this way produces an analysis consistent with it.
- RMS error calculations against data that is assimilated are misleading. In this case: RMS $= 0.0011$ for diagonal $\mathbf{B}_k^b$, RMS $= 0.0138$ for 5 ensemble members.

Example 2: How good are our unobserved variables?

$$\frac{\partial h}{\partial t} + c\frac{\partial h}{\partial x} = 0$$
$$u(x,t) = \frac{\partial h}{\partial x}$$
$$h(x,0) = sin(x)$$

Solution is given by $h^t(x,t) = sin(x - ct), u^t(x,t) = cos(x - ct)$.

- We observe only h as in Example 1.
- Our $\mathbf{w}_k = \begin{bmatrix} \mathbf{h} \\ \mathbf{u} \end{bmatrix}$
- Field u should be corrected through the background error covariance!

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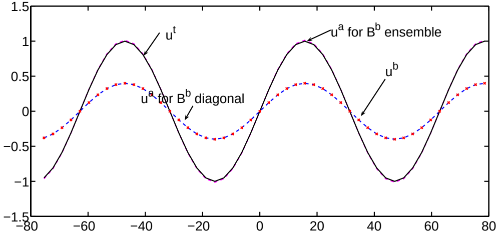

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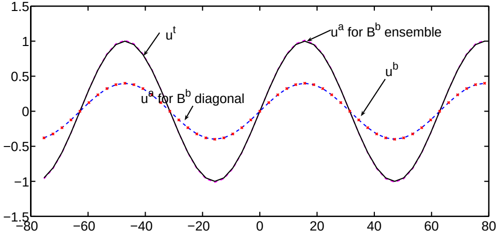

- Diagonal covariance matrix does not correct u since u is not observed.
- Field u was corrected through the ensemble background error covariance using the cross correlations between variables u and h as given by model dynamics!

Summary of analysis step

As result of the analysis step we obtain

$$\mathbf{w}_k^a, \mathbf{B}_k^a \text{ starting from } \mathbf{w}_k^b, \mathbf{B}_k^b \text{ and data } \mathbf{f}_k$$

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- reduced form are not unique resulting in different ensembles with same mean and covariance.
- The quality of the analysis is determined by the background error covariance. This is how the information from the data is transferred to the grid points of model.
- Ensemble background error covariance rely on the numerical model for cross-correlation between the variables.

Step 2: Generation of the ensembles

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Two ways

- stochastically by treating observations as random variables

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- stochastically by treating observations as random variables
- deterministic requiring that ensembles $\mathbf{w}_k^{a,i}$ are generated around state $\mathbf{w}_k^a$ using $\mathbf{B}_k^a$.

$$\mathbf{w}_k^{a,i} = \mathbf{w}_k^a + [\mathbf{W}_k^b \mathbf{T}_k \mathbf{U}]_i$$

where $\mathbf{Ue} = 0$ and $\mathbf{UU}^T = \mathbf{I}_r$, and $\mathbf{e} = [1 \dots 1]$.

Step 2: Resampling

If we generate $\mathbf{w}_k^{a,i}$ using

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$$\begin{aligned}
&\frac{1}{r-1}\sum_{i=1}^{r}[\mathbf{w}_k^{a,i} - \mathbf{w}_k^a][\mathbf{w}_k^{a,i} - \mathbf{w}_k^a]^T \\
= &\sum_{i=1}^{r}[\mathbf{W}_k^b \mathbf{T}_k \mathbf{U}]_i [\mathbf{W}_k^b \mathbf{T}_k \mathbf{U}]_i^T \\
= &\mathbf{W}_k^b \mathbf{T}_k \mathbf{U}[\mathbf{W}_k^b \mathbf{T}_k \mathbf{U}]^T \\
= &\mathbf{W}_k^a (\mathbf{W}_k^a)^T \\
= &\mathbf{P}_k^a
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Our best prior estimate of the state at time t_{k+1} is given by a forecast from proceeding analysis using fully nonlinear numerical model:

$$\mathbf{w}_{k+1}^b = M_{k+1,k}\mathbf{w}_k^a.$$

In majority of ensemble Kalman filter algorithms, full nonlinear numerical model is used to propagate each ensemble

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Step 3 is the expensive step of ensemble Kalman filter methods. It determines how many ensembles can be used for representing uncertainty.

Numerical model of atmosphere is not perfect

Instead of only propagating the analysis ensemble to obtain the new forecast ensemble, model error η_k^i can be added to:

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Modeling model error is very difficult!

Example 3: The effect of model error

- Setup follows Example 2 except that model has now wrong advection speed $c^m = c/2$.

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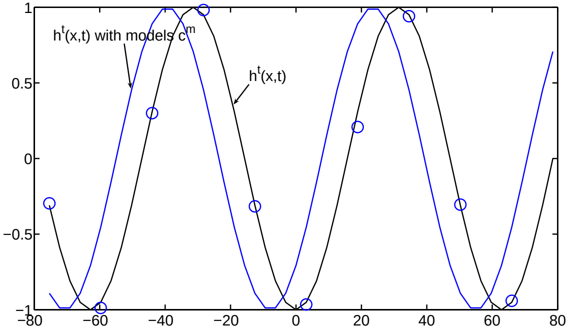

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- Analysis will be produced assuming
  1. model is perfect, $\eta_k^i = 0$;
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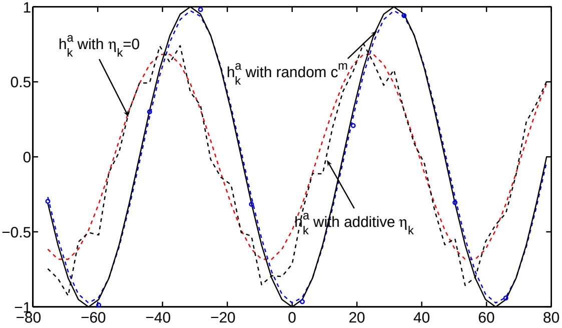

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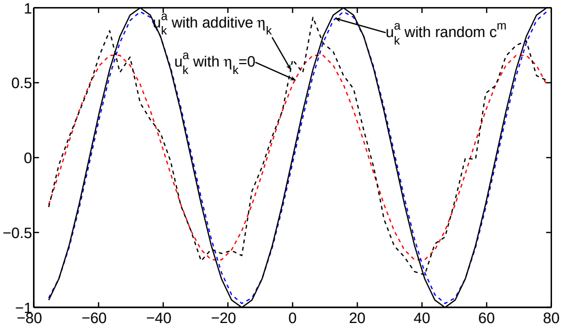

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- The inclusion of model error and observation error are still required.