Hybrid Variational/Ensemble Data Assimilation

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Outline

- Hybrid formulation in variational framework
- Overview of ensemble generation methods
- Introduction to hybrid practice

Motivation of Hybrid DA

- 3D-Var uses static ("climate") BE

$$J(\delta x) = \frac{1}{2}\delta x^{\mathrm{T}}\mathrm{B}^{-1}\delta x + \frac{1}{2}[\mathrm{H}\delta x - d]^{\mathrm{T}}\mathrm{R}^{-1}[\mathrm{H}\delta x - d]$$

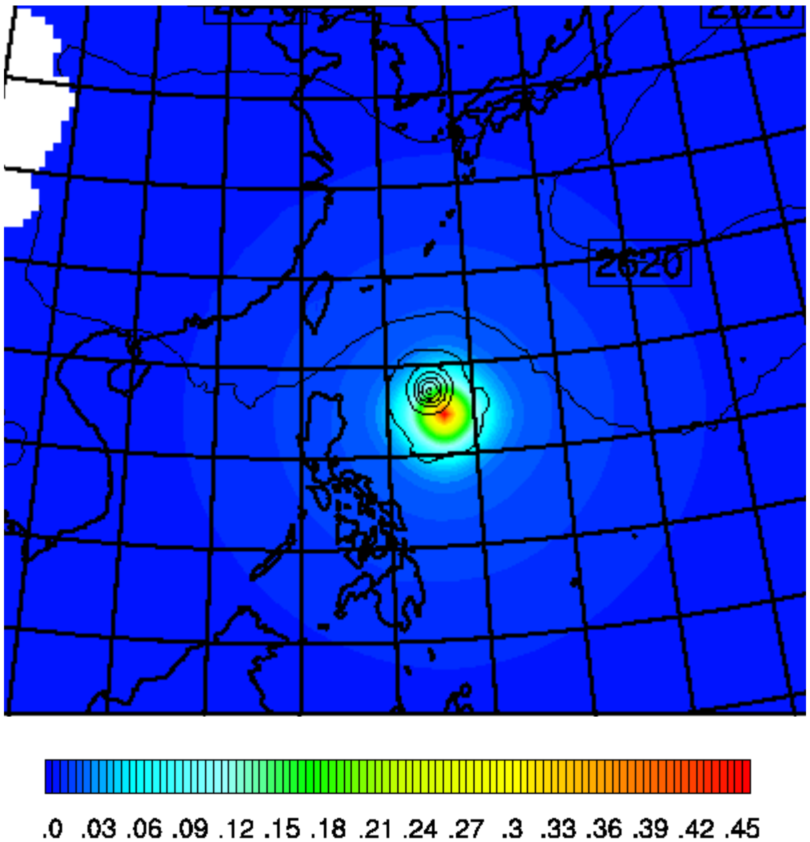
- 4D-Var implicitly uses flow-dependent information, but still starts from static BE

$$J(\delta x) = \frac{1}{2}\delta x^{\mathrm{T}}\mathrm{B}^{-1}\delta x + \frac{1}{2}\sum_{i=1}^{I}[\mathrm{HM}_i\delta x - d_i]^{\mathrm{T}}\mathrm{R}^{-1}[\mathrm{HM}_i\delta x - d_i]$$

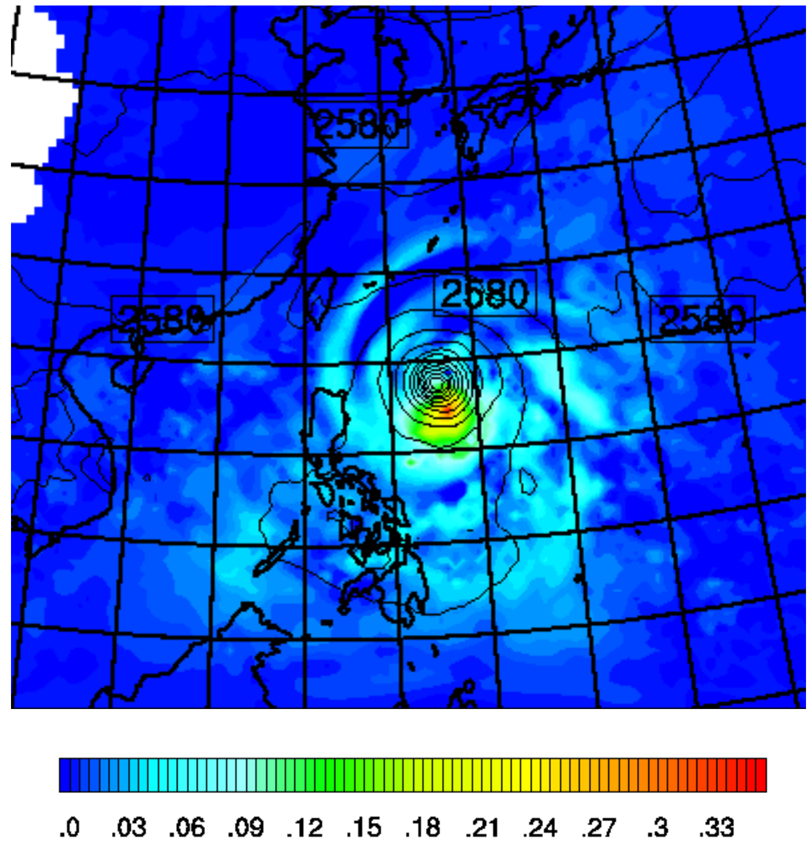
- Hybrid uses flow-dependent background error covariance from forecast ensemble perturbation in a variational DA system

T Analysis increments from a single obs at 750mb near Typhoon center

3DVAR



HYBRID
(32 ensemble members)



What is the Hybrid DA?

- Ensemble mean is analyzed by a variational algorithm (i.e., minimize a cost function).
  - It combines (so “hybrid”) the 3DVAR “climate” background error covariance and “error of the day” from ensemble perturbation.

- Hybrid algorithm (again in a variational framework) itself usually does not generate ensemble analyses.

- Need a separate system to update ensemble
  - Could be ensemble forecasts already available from NWP centers
  - Could be an Ensemble Kalman Filter-based DA system
  - Or multiple model/physics ensemble

- Ensemble needs to be good to well represent “error of the day”

Vector/Matrix expression of Ensemble

- Consider an ensemble of the model state vector of dimension M

  $\mathbf{X} = (\mathbf{x_1}, \mathbf{x_2}, ..., \mathbf{x_N})$, N is the ensemble size

  then $\mathbf{X}$ *is* a $\mathrm{M} \times \mathrm{N}$ matrix. $\mathrm{M} \sim \mathrm{O}(10^{6\sim7})$, $\mathrm{N} \sim \mathrm{O}(100)$.

- Ensemble mean is simply a column vector of Mx1

$$\bar{\mathbf{x}} = \frac{1}{N-1} \sum_{i=1}^{N} \mathbf{x}_i$$

- (Normalized) Ensemble perturbation matrix also a MxN matrix

$$\mathbf{X}' = \frac{1}{\sqrt{N-1}} (\mathbf{x_1} - \bar{\mathbf{x}}, ..., \mathbf{x_N} - \bar{\mathbf{x}}) = (\mathbf{x}'_1, ..., \mathbf{x}'_N)$$

- Sample covariance matrix (MxM) formed by

$$\mathbf{B}_e = \mathbf{X}'(\mathbf{X}')^{\mathrm{T}}$$

  – it is a low-rank matrix (i.e., only have at most N non-zero eigenvalues)

Hybrid formulation (1)

(Hamill and Snyder, 2000)

- 3DVAR cost function

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

- Idea: replace **B** by a weighted sum of static $\mathbf{B}_{\mathrm{s}}$ and the ensemble $\mathbf{B}_{\mathrm{e}}$

$$\mathbf{B} = a_s \mathbf{B}_{\mathrm{s}} + a_e \mathbf{B}_{\mathrm{e}},\ a_s = 1 - a_{\mathrm{e}}$$

  - Has been demonstrated on a simple model.
  - Difficult to implement for large NWP model.

Hybrid formulation (2): used in WRFDA
(Lorenc, 2003)

• Ensemble covariance is included in the 3DVAR cost function through augmentation of control variables

$$J(\mathbf{x},\alpha) = \beta_s \frac{1}{2}(\mathbf{x}-\mathbf{x}_b)^{\mathbf{T}}\mathbf{B}^{-1}(\mathbf{x}-\mathbf{x}_b) + \overbrace{\beta_e \frac{1}{2}\sum_{i=1}^{\mathrm{N}} \alpha_i^{\mathbf{T}}\mathbf{C}^{-1}\alpha_i}^{\text{ensemble control variable } \alpha_i \ (M \times 1)}$$

$$+\frac{1}{2}[\mathbf{y}-H(\mathbf{x}+\mathbf{x}_e^{'})]^{\mathbf{T}}\mathbf{R}^{-1}[\mathbf{y}-H(\mathbf{x}+\mathbf{x}_e^{'})]$$

$\mathbf{x}_e^{'} = \sum_{\mathrm{i}=1}^{\mathrm{N}} \alpha_i \circ \mathbf{x}_i^{'}$, where $\mathbf{x}_i^{'}$ is the ensemble perturbation for the ensemble member i.

$\circ$ denote element - wise product. α_{i} is in effect the ensemble weight.

$\mathbf{C}$: correlation matrix (effectively loclization of ensemble perturbations)

• In practical implementation, α_i can be reduced to horizontal 2D fields (i.e., use same weight in different vertical levels) to save computing cost.

• β_s and β_e ($1/\beta_s$ + $1/\beta_e$ =1) can be tuned to have different weight between static and ensemble part.

Similarity to radiance VarBC equation

Modeling of errors in satellite radiances:

$$y = H(x_t) + B(\beta) + \varepsilon \qquad \begin{cases} \langle \varepsilon \rangle = 0 \\ B(\beta) = \sum_{i=1}^{N} \beta_i p_i \end{cases}$$

Bias-correction coefficients

Predictors:

- **Offset (i.e., 1)**
- **1000-300mb thickness**
- **200-50mb thickness**
- **Surface skin temperature**
- **Total column water vapor**
- **Scan, Scan^2, Scan^3**

Bias parameters can be estimated within the variational assimilation, jointly with the atmospheric model state.

Inclusion of the bias parameters in the control vector : $\mathbf{x}^{\mathrm{T}} \rightarrow [\mathbf{x}, \beta]^{\mathrm{T}}$

$$\mathbf{J}(\mathbf{x},\beta) = \underbrace{(\mathbf{x}_\mathrm{b} - \mathbf{x})^\mathrm{T} \mathbf{B}_\mathrm{x}^{-1} (\mathbf{x}_\mathrm{b} - \mathbf{x})}_{\mathrm{J_b}\text{: background term for x}} + \underbrace{[\mathbf{y} - H(\mathbf{x}) - B(\beta)]^\mathrm{T} \mathbf{R}^{-1} [\mathbf{y} - H(\mathbf{x}) - B(\beta)]}_{\mathrm{J_o}\text{: corrected observation term}}$$
$$+ \underbrace{(\beta_\mathrm{b} - \beta)^\mathrm{T} \mathbf{B}_\beta^{-1} (\beta_\mathrm{b} - \beta)}_{\mathrm{J_p}\text{: background term for } \beta}$$

Hybrid formulation (3)

- Equivalently can write in another form (Wang et al., 2008)

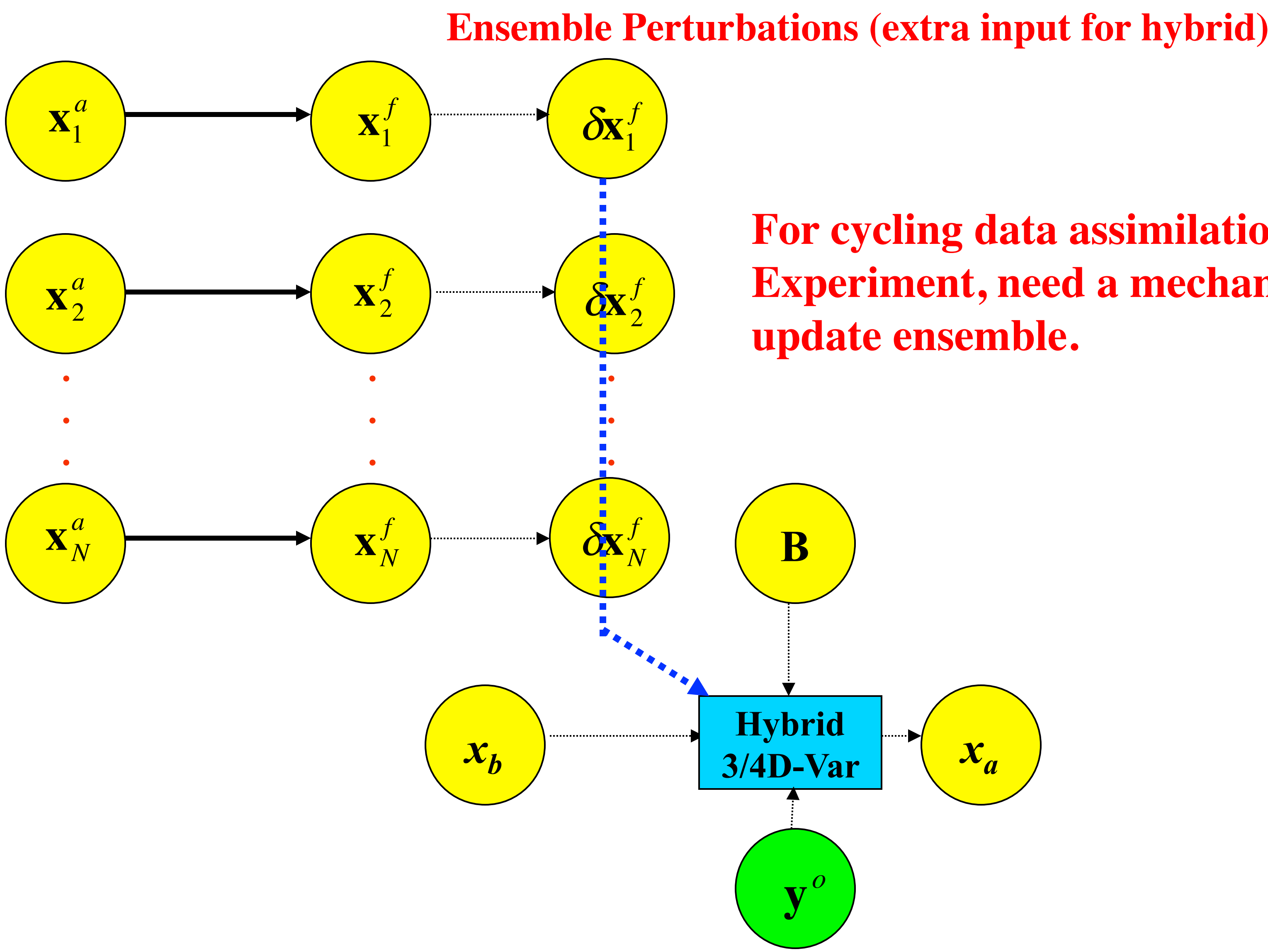
$$J(\mathbf{x},\alpha) = \frac{1}{2}(\mathbf{x} + \mathbf{x}_e - \mathbf{x}_b)^{\mathbf{T}} \left(\frac{1}{\beta_s}\mathbf{B} + \frac{1}{\beta_e}\mathbf{B}_e \circ \mathbf{C}\right)^{-1} (\mathbf{x} + \mathbf{x}_e - \mathbf{x}_b)$$

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

- This explains why **C** is for localization.

- This is also equivalent to Hamill and Snyder (2000).

Hybrid DA data flow



For cycling data assimilation/forecast Experiment, need a mechanism to update ensemble.

EnKF-based Ensemble Generation

- EnKF with perturbed observations

- EnKF without perturbed observations
  - All based on square-root filter
  - Ensemble Transformed Kalman Filter (ETKF)
  - Ensemble Adjustment Kalman Filter (EAKF)
  - Ensemble Square-Root Filter (EnSRF)

- Most implementation assimilates obs sequentially (i.e., one by one, or box by box)
  - can be parallelized

Common practice of EnKF

- Kalman Filter equation for mean analysis

$$\overline{\mathbf{x}_a} = \overline{\mathbf{x}_b} + \mathbf{B}\mathbf{H}^{\mathrm{T}}(\mathbf{H}\mathbf{B}\mathbf{H}^{\mathrm{T}} + \mathbf{R})^{-1}[\mathbf{y} - H(\overline{\mathbf{x}_b})] = \overline{\mathbf{x}_b} + \mathbf{K}[\mathbf{y} - H(\overline{\mathbf{x}_b})]$$

- EnKF uses forecast ensemble $\mathbf{x}_i^b$ (i=1~N) to estimate covariance matrices (Evensen, 1994)

$$\mathbf{B}\mathbf{H}^{\mathrm{T}} \approx \mathbf{X}_b^{'}(\mathbf{H}\mathbf{X}_b^{'})^{\mathrm{T}} = \frac{1}{\mathrm{N}-1}[\mathbf{X}_b - \overline{\mathbf{X}_b}][H(\mathbf{X}_b) - \overline{H(\mathbf{X}_b)}]^{\mathrm{T}}$$

$$\mathbf{H}\mathbf{B}\mathbf{H}^{\mathrm{T}} \approx (\mathbf{H}\mathbf{X}_b^{'})(\mathbf{H}\mathbf{X}_b^{'})^{\mathrm{T}} = \frac{1}{\mathrm{N}-1}[H(\mathbf{X}_b) - \overline{H(\mathbf{X}_b)}][H(\mathbf{X}_b) - \overline{H(\mathbf{X}_b)}]^{\mathrm{T}}$$

- Problem left: how to obtain analysis perturbations (thus analysis ensemble) from forecast ensemble? $\mathbf{X}_b^{'} \xrightarrow{\textit{ensemble update}} \mathbf{X}_a^{'}$
  - With relationship

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

$$\mathbf{X}_{\mathbf{a}}^{'}(\mathbf{X}_{\mathbf{a}}^{'})^{\mathbf{T}} = (\mathbf{I} - \mathbf{K}\mathbf{H})\mathbf{X}_b^{'}(\mathbf{X}_b^{'})^{\mathbf{T}}$$

Ensemble update: original implementation for ocean DA (Evensen, 1994)

- Perform an "ensemble of analyses" with each analysis using the same set of observations.

$$\mathbf{x}_i^a = \mathbf{x}_i^b + \mathbf{B}\mathbf{H}^{\mathrm{T}}(\mathbf{H}\mathbf{B}\mathbf{H}^{\mathrm{T}} + \mathbf{R})^{-1}[\mathbf{y} - H(\mathbf{x}_i^b)],\ \mathrm{i} = 1,\ldots,\mathrm{N}$$

- Does not take into account uncertainty in observations, and cause underestimation of analysis error covariance.

Ensemble update: Perturbed observations (Houtekamer & Mitchell, 1998)

- Perform an "ensemble of analyses" with each analysis using the randomly perturbed observations.

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

$$\mathbf{y}_i = \mathbf{y} + \varepsilon_i,$$

ε_i is Gaussian random error with zero mean and covariance $\mathbf{R}$.

Used by Environment Canada

Ensemble update: ETKF

(Bishop et al., 2001; Wang et al., 2007)

$$\mathbf{X}_a^{'} = \mathbf{X}_b^{'}\mathbf{T}$$

$$\mathbf{T} = r\mathbf{E}(\rho\lambda + \mathbf{I})^{\mathbf{-1/2}}\mathbf{E}^{\mathbf{T}} \;\; (\mathrm{N} \times \mathrm{N} \text{ matrix})$$

- Where **E** and **λ** contain eigenvectors and eigenvalues of a NxN (N is ensemble size) matrix

$$(\mathbf{HX}_b^{'})^T \mathbf{R}^{-1} (\mathbf{HX}_b^{'})$$

- r and ρ are tunable inflation factors.

ETKF is a simple/fast scheme.
It is within WRFDA release.

Exist localized version: LETKF (Hunt et al., 2007)

Ensemble update: EAKF (built in DART)
(Anderson, 2003; Liu et al., 2012)

- a two-step square-root filter
  - adjustment step (shift+compact) for observation space analysis

$$\mathbf{y}_i^a = \mathbf{A}_y^{1/2}(\mathbf{HBH}^\mathbf{T})^{-1/2}\left(\mathbf{y}_i^b - \overline{\mathbf{y}^b}\right) + \overline{\mathbf{y}^a},\ \ i = 1,\ldots,N$$

  - regression step from observation space to model space analysis increment

$$\mathbf{x}_i^a - \mathbf{x}_i^b = \mathbf{BH}^\mathbf{T}(\mathbf{HBH}^\mathbf{T})^{-1}\left(\mathbf{y}_i^a - \mathbf{y}_i^b\right)$$

Ensemble update: EnSRF (Whitaker & Hamill, 2002)

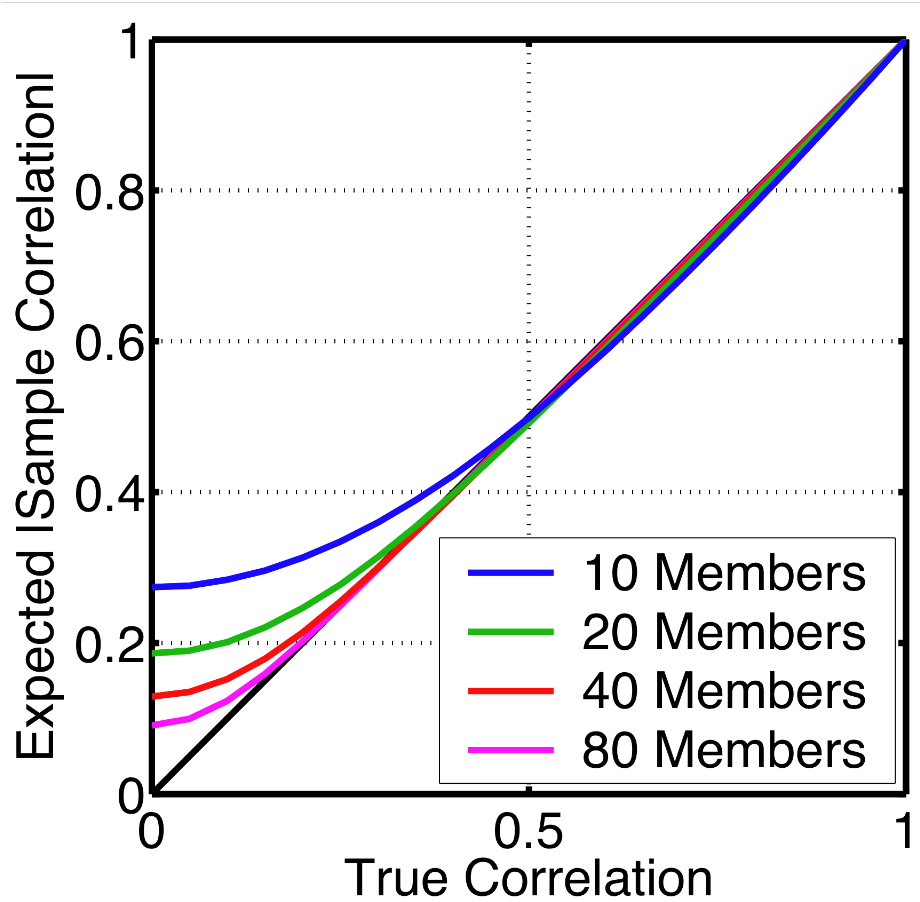
$$\mathbf{x}_i^a = (\mathbf{I} - \tilde{\mathbf{K}}\mathbf{H})\mathbf{x}_i^b,\ \mathrm{i} = 1,\ldots,\mathrm{N}$$

$$\tilde{\mathbf{K}} = \left(\mathbf{I} + \sqrt{\frac{\mathbf{R}}{\mathbf{H}\mathbf{B}\mathbf{H}^T + \mathbf{R}}}\right)^{-1}\mathbf{K}$$

Should take scalar form for serial algorithm assimilating obs. one by one

Used by NOAA/NCEP

Sampling Error: noise in sample covariance



Sampling errors lead to spurious correlation for two distant points.

This can result in filter divergence.

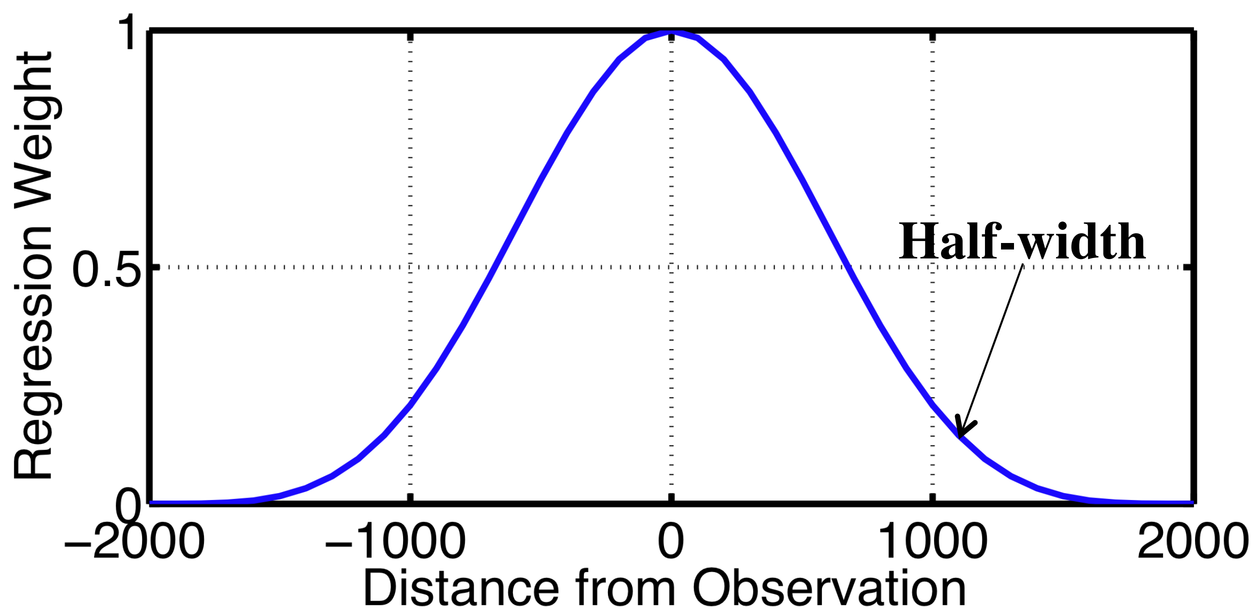
Low-rank covariance (less degree of freedom), can not well fit dense/detailed observations.

Deal with sampling error (increase rank)

1. Use larger ensembles; expensive for large models.

2. Variance Inflation: increase ensemble spread.

3. Localization: reduce correlation as function of distance. Compactly supported correla tion function (Gaspari-Cohn) is most commonly used.



Advantages of the Hybrid DA

- Hybrid localization is in model space while EnKF localization is usually in observation space.

- For some observations type, e.g., radiances, localization is not well defined in observation space

- Easier to make use of existing radiance VarBC in hybrid

- For small-size ensemble, use of static B could be beneficial to have a higher-rank covariance.

Hybrid practice

- **Computation steps:**
  - Computing ensemble mean (**gen_be_ensmean.exe**).
  - Extracting ensemble perturbations (**gen_be_ep2.exe**).
  - Running WRFDA in "hybrid" mode (**da_wrfvar.exe**).
  - Displaying results for: ens_mean, std_dev, ensemble perturbations, hybrid increments, cost function and, etc.
  - If time permits, play with different namelist settings: "je_factor" and "alpha_corr_scale".
- **Scripts to use:**
  - Some NCL scripts to display results.

- **Ensemble generation part not included in current practice**

Namelist for WRFDA in hybrid mode

&wrfvar7
je_factor=2, # half/half for Jb and Je term

&wrfvar16
alphacv_method=2, # ensemble part is in model space (u,v,t,q,ps)

ensdim_alpha=10,

alpha_corr_type=3, # 1=Exponential; 2=SOAR; 3=Gaussian

alpha_corr_scale=750., # correlation scale in km

alpha_std_dev=1.,

alpha_vertloc=true, (use program “**gen_be_vertloc.exe 42” to generate file**)

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