# An Introduction to Ensemble Kalman Filtering

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#### **Overview**

- **1. The Data Assimilation Problem**
- 2. A Bayesian View of Ensemble Kalman Filtering
- **3.** Challenges to Ensemble Filters
- 4. Adaptive Ensemble Filter Algorithms
- **5.** Model and Observing System Development with Ensembles

A (Physical) system:

Atmosphere, coupled climate system...

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### A model of the physical system:

Represents system with discrete vector: the model 'state vector'. Approximates time evolution of system (poorly).

#### Observations of the system:

Have a (sometimes poor) estimate of observation error. Could be sparse and irregular in time (and space). Relation to model 'state vector' may be complicated. May have very low information content.

### (Physical) system:

Estimates of state (analyses, posteriors...). Initial conditions for forecasts. Enhanced (physical) understanding.

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Estimates of model errors. Relative characteristics of different models. Improved model (find good values for model 'parameters').

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## **Observations:**

Estimates of observation errors.

- Information content of existing or planned observations.
- Observing system designs that provide increased information.



#### **Ensemble Filter Products now Available to Forecasters**

### **Environment Canada Operational GEM 16 member ENKF**

#### **Ensemble Filter Products now Available to Forecasters**



500 hPa heights and height spread initialized 2007061812 valid 2007061912

#### **Ensemble Filter Products now Available to Forecasters**

- **1.** Many other ensemble forecast products are available.
- 2. Most suffer from the same challenges outlined below.
- 3. Other ensemble generation methods may have additional issues.

### **An introduction to Ensemble Filtering.**

- 1: Single variable and observation of that variable.Let's think of it as temperature at SLC.(Slides are for a mid-winter ski day...inversion in the valley)
- 2: Single observed variable, single unobserved variable. SLC temperature, Park City temperature.

That's all there is... (without loss of generality).





- A: Prior estimate based on all previous information, C.
- B: An additional observation.





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### Consistent Color Scheme Throughout

**<u>Green = Prior</u>** 

**<u>Red = Observation</u>** 

**Blue = Posterior** 

Bayes rule: 
$$p(A|BC) = \frac{p(B|AC)p(A|C)}{p(B|C)} = \frac{p(B|AC)p(A|C)}{\int p(B|x)p(x|C)dx}$$

This product is closed for Gaussian distributions.



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Product of d-dimensional normals with means  $\mu_1$  and  $\mu_2$  and covariance matrices  $\Sigma_1$  and  $\Sigma_2$  is normal.

 $\mathbf{N}(\boldsymbol{\mu}_{1},\boldsymbol{\Sigma}_{1})N(\boldsymbol{\mu}_{2},\boldsymbol{\Sigma}_{2}) = c\mathbf{N}(\boldsymbol{\mu},\boldsymbol{\Sigma})$ 

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 $N(\mu_{1}, \Sigma_{1})N(\mu_{2}, \Sigma_{2}) = cN(\mu, \Sigma)$ Covariance:  $\Sigma = (\Sigma_{1}^{-1} + \Sigma_{2}^{-1})^{-1}$ Mean:  $\mu = (\Sigma_{1}^{-1} + \Sigma_{2}^{-1})^{-1}(\Sigma_{1}^{-1}\mu_{1} + \Sigma_{2}^{-1}\mu_{2})$ 

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$$N(\mu_{I}, \Sigma_{I})N(\mu_{2}, \Sigma_{2}) = cN(\mu, \Sigma)$$
  
Covariance:  $\Sigma = (\Sigma_{I}^{-1} + \Sigma_{2}^{-1})^{-1}$   
Mean:  $\mu = (\Sigma_{I}^{-1} + \Sigma_{2}^{-1})^{-1}(\Sigma_{I}^{-1}\mu_{I} + \Sigma_{2}^{-1}\mu_{2})$   
Weight:  $c = \frac{1}{(2\Pi)^{d/2}|\Sigma_{I} + \Sigma_{2}|^{1/2}} \exp\left\{-\frac{1}{2}[(\mu_{2} - \mu_{I})^{T}(\Sigma_{I} + \Sigma_{2})^{-1}(\mu_{2} - \mu_{I})]\right\}$ 

We'll ignore the weight since we immediately normalize products to be PDFs.

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Easy to derive for 1D (d=1); just do products of exponentials.

Bayes rule: 
$$p(A|BC) = \frac{p(B|AC)p(A|C)}{p(B|C)} = \frac{p(B|AC)p(A|C)}{\int p(B|x)p(x|C)dx}$$

Ensemble filters: Prior is available as finite sample.



How can we take product of sample with continuous likelihood?



Observation likelihood usually continuous (nearly always Gaussian).



Product of prior Gaussian fit and Obs. likelihood is Gaussian.



#### **Sampling Posterior PDF:**



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# Ensemble Adjustment (Kalman) Filter.



# Ensemble Adjustment (Kalman) Filter.



Ensemble Adjustment (Kalman) Filter.



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### Ensemble Adjustment (Kalman) Filter.

First, 'shift' ensemble to have exact mean of posterior.
#### Ensemble Filter Algorithms:



#### Ensemble Adjustment (Kalman) Filter.

Second, use linear contraction to have exact variance of posterior.

Ensemble Filter Algorithms:



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Ensemble Filter Algorithms:



Ensemble Adjustment (Kalman) Filter.

Bimodality maintained, but not appropriately positioned or weighted. No problem with random outliers.

# **2: Single observed variable, single unobserved variable** SLC temperature, temperature at Park City.

So far, have known observation likelihood for single variable.

Now, suppose model state vector has an additional variable.

Will examine how ensemble methods update additional variable.

Basic method generalizes to any number of additional variables.

Related to Kalman filter in subtle ways.





















Assume that all we know is prior joint distribution.

One variable is observed.

Using only increments guarantees that if observation had no impact on observed variable, unobserved variable is unchanged (highly desirable).



























Now have an updated (posterior) ensemble for the unobserved variable.



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Fitting Gaussians shows that mean and variance have changed.



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Fitting Gaussians shows that mean and variance have changed.

Other features of the prior distribution may also have changed.



Dynamical system governed by (stochastic) Difference Equation:

$$dx_t = f(x_t, t) + G(x_t, t)d\beta_t, \quad t \ge 0$$
(1)

Observations at discrete times:

$$y_k = h(x_k, t_k) + v_k; k = 1, 2, ...; t_{k+1} > t_k \ge t_0$$
 (2)

Observational error white in time and Gaussian (nice, not essential).

$$v_k \to N(0, R_k) \tag{3}$$

Complete history of observations is:

$$Y_{\tau} = \{ y_l; t_l \le \tau \}$$

$$\tag{4}$$

Goal: Find probability distribution for state at time t:

$$p(x, t | Y_t) \tag{5}$$

State between observation times obtained from Difference Equation. Need to update state given new observation:

$$p(x, t_k | Y_{t_k}) = p(x, t_k | y_k, Y_{t_{k-1}})$$
(6)

Apply Bayes rule:

$$p(x, t_k | Y_{t_k}) = \frac{p(y_k | x_k, Y_{t_{k-1}}) p(x, t_k | Y_{t_{k-1}})}{p(y_k | Y_{t_{k-1}})}$$
(7)

Noise is white in time (3) so:

$$p(y_k | x_k, Y_{t_{k-1}}) = p(y_k | x_k)$$
(8)

Integrate numerator to get normalizing denominator:

$$p(y_k|Y_{t_{k-1}}) = \int p(y_k|x)p(x,t_k|Y_{t_{k-1}})dx$$
(9)

Probability after new observation:

$$p(x, t_k | Y_{t_k}) = \frac{p(y_k | x) p(x, t_k | Y_{t_{k-1}})}{\int p(y_k | \xi) p(\xi, t_k | Y_{t_{k-1}}) d\xi} (10)$$

Exactly analogous to earlier derivation except that x and y are vectors.

EXCEPT, no guarantee we have prior sample for each observation.

SO, let's make sure we have priors by 'extending' state vector.

Extending the state vector to joint state-observation vector.

Recall: 
$$y_k = h(x_k, t_k) + v_k; k = 1, 2, ...; \quad t_{k+1} > t_k \ge t_0$$
 (2)

Applying h to x at a given time gives expected values of observations.

Get prior sample of obs. by applying h to each sample of state vector x.

Let z = [x, y] be the combined vector of state and observations.

NOW, we have a prior for each observation:

$$p(z, t_k | Y_{t_k}) = \frac{p(y_k | z) p(z, t_k | Y_{t_{k-1}})}{\int p(y_k | \xi) p(\xi, t_k | Y_{t_{k-1}}) d\xi}$$
(10.ext)

One more issue: how to deal with many observations in set  $y_k$ ?

Let  $y_k$  be composed of s subsets of observations:  $y_k = \{y_k^1, y_k^2, ..., y_k^s\}$ 

Observational errors for obs. in set i independent of those in set j.

Then: 
$$p(y_k|z) = \prod_{i=1}^{s} p(y_k^i|z)$$

Can rewrite (10.ext) as series of products and normalizations.
#### Phase 3: Generalize to geophysical models and observations

One more issue: how to deal with many observations in set  $y_k$ ?

Implication: can assimilate observation subsets sequentially.

If subsets are scalar (individual obs. have mutually independent error distributions), can assimilate each observation sequentially.

If not, have two options:

- 1. Repeat everything above with matrix algebra.
- Do singular value decomposition; diagonalize obs. error covariance. Assimilate observations sequentially in rotated space. Rotate result back to original space.

Good news: Most geophysical obs. have independent errors!

1. Use model to advance ensemble (3 members here) to time at which next observation becomes available.

Ensemble state estimate after using previous observation (analysis). Ensemble state at time of next observation (prior).

 $t_k$ 

k+1

2. Get prior ensemble sample of observation, y=h(x), by applying forward operator h to each ensemble member.



Theory: observations from instruments with uncorrelated errors can be done sequentially.

3. Get observed value and observational error distribution from observing system.



4. Find increment for each prior observation ensemble (this is a scalar problem for uncorrelated observation errors).



5. Use ensemble samples of y and each state variable to linearly regress observation increments onto state variable increments.



6. When all ensemble members for each state variable are updated, have a new analysis. Integrate to time of next observation...





Observation in red.

Prior ensemble in green.

Observing all three state variables.

Obs. error variance = 4.0.

4 20-member ensembles.



Observation in red.

Prior ensemble in green.



Observation in red.

Prior ensemble in green.



Observation in red.

Prior ensemble in green.



Observation in red.

Prior ensemble in green.

Ensemble is passing through unpredictable region.



Observation in red.

Prior ensemble in green.

Part of ensemble heads for one lobe, the rest for the other.



Observation in red.

Prior ensemble in green.

The prior is not linear here.

Standard regression might be pretty bad.



Observation in red.

Prior ensemble in green.

The prior is not linear here.

On the other hand...

20 Hard to contrive examples this bad.

Behavior like this not apparent in real assimilations.



















- 1. Ignore it: if number of unrelated observations is small and there is some way of maintaining variance in priors.
- 2. Use larger ensembles to limit sampling error.
- 3. Use additional *a priori* information about relation between observations and state variables.
- 4. Try to determine the amount of sampling error and correct for it.





Weight regression as function of horizontal *distance* from observation. Gaspari-Cohn: 5th order compactly supported polynomial.



Distance from Observation (Km?) Can use other functions to weight regression. Unclear what *distance* means for some obs./state variable pairs. Referred to as LOCALIZATION.

- 4. Try to determine the amount of sampling error and correct for it:
  - A. Could weight regressions based on sample correlation.Limited success in tests.For small true correlations, can still get large sample correl.
  - B. Do bootstrap with sample correlation to measure sampling error.Limited success.Repeatedly compute sample correlation with a sample removed.
  - C. Use hierarchical Monte Carlo.Have a 'sample' of samples.Compute expected error in regression coefficients and weight.

<u>Ways to deal with regression sampling error:</u> 4C. Use hierarchical Monte Carlo: ensemble of ensembles.



M groups of N-member ensembles.

Compute obs. increments for each group.

For given obs. / state pair:

- 1. Have M samples of regression coefficient,  $\beta$ .
- 2. Uncertainty in  $\beta$  implies state variable increments should be reduced.
- 3. Compute regression confidence factor,  $\alpha$ .

4C. Use hierarchical Monte Carlo: ensemble of ensembles.

# Split ensemble into M independent groups. For instance, 80 ensemble members becomes 4 groups of 20.

With M groups get M estimates of regression coefficient,  $\beta_i$ .

Find regression confidence factor  $\alpha$  (weight) that minimizes:

$$\sqrt{\sum_{j=1}^{M} \sum_{i=1, i \neq j}^{M} [\alpha \beta_i - \beta_j]^2}$$

Minimizes RMS error in the regression (and state increments).

4C. Use hierarchical Monte Carlo: ensemble of ensembles.





#### Localization in GCM can be very complex. Surface Pressure Obs. at 20N, 60E

#### **Dealing With Ensemble Filter Errors**



Often smoothly decrease impact to 0 as function of distance.

#### Model/Filter Error; Filter Divergence and Variance Inflation

1. History of observations and physical system => 'true' distribution.



## Model/Filter Error; Filter Divergence and Variance Inflation

History of observations and physical system => 'true' distribution.
Sampling error, some model errors lead to insufficient prior variance.



3. Can lead to 'filter divergence': prior is too confident, obs. ignored

## Model/Filter Error; Filter Divergence and Variance Inflation

History of observations and physical system => 'true' distribution.
Sampling error, some model errors lead to insufficient prior variance.



3. Naive solution is Variance inflation: just increase spread of prior

4. For ensemble member i,  $inflate(x_i) = \sqrt{\lambda}(x_i - \bar{x}) + \bar{x}$ .
#### Model/Filter Error; Filter Divergence and Variance Inflation

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## Model/Filter Error; Filter Divergence and Variance Inflation

History of observations and physical system => 'true' distribution.
Most model errors also lead to erroneous shift in entire distribution.



# Model/Filter Error; Filter Divergence and Variance Inflation

History of observations and physical system => 'true' distribution.
Most model errors also lead to erroneous shift in entire distribution.



- 4. Inflating can ameliorate this
- 5. Obviously, if we knew E(error), we'd correct for it directly

### **Physical Space Variance Inflation**

Inflate all state variables by same amount before assimilation

# Capabilities:

- 1. Can be very effective for a variety of models.
- 2. Can maintain linear balances.
- 3. Stays on local flat manifolds.
- 4. Simple and inexpensive.

# Liabilities:

 State variables not constrained by observations can 'blow up'. For instance unobserved regions near the top of AGCMs.
Magnitude of λ normally selected by trial and error.



After inflating, observation is in prior cloud: filter divergence avoided







Adjunct Algorithms Developed for DART Can Tolerate Errors.

1. Adaptive Error Tolerant Filters.

Automatically detect error in assimilation system. Add uncertainty when model disagrees with observations. Can deal with LARGE model, observation, and filter error.

### Variance inflation for Observations: An Adaptive Error Tolerant Filter

1. For observed variable, have estimate of prior-observed inconsistency



Assumes that prior and observation are supposed to be unbiased. Is it model error or random chance?

## Variance inflation for Observations: An Adaptive Error Tolerant Filter

1. For observed variable, have estimate of prior-observed inconsistency



2. Expected(prior mean - observation) =  $\sqrt{\sigma_{prior}^2 + \sigma_{obs}^2}$ .

3. Inflating increases expected separation. Increases 'apparent' consistency between prior and observation. Adjunct Algorithms Developed for DART Can Tolerate Errors.

1. Adaptive Error Tolerant Filters.

Automatically detect error in assimilation system. Add uncertainty when model disagrees with observations. Can deal with LARGE model, observation, and filter error.

 Hierarchical filters detect and avoid small ensemble sampling errors. Ensemble of ensembles for tuning period. Limit impact of observations as required. Eliminate unnecessary calculation.

# **Can apply filters without tuning to large problems.**

# 1. Get an improved estimate of state of physical system.

# Initial conditions for forecasts.

Includes time evolution and 'balances'. High quality analyses (re-analyses).

# 2. Get better estimates of observing system error characteristics.

Estimate value of existing or planned observations. Design observing systems that provide increased information.

# 3. Improve model of physical system.

Evaluate model systematic errors.

Forward and backward sensitivity analysis (adjoint and linear tangent replacement). Select appropriate values for model parameters. DART/CAM NWP Assimilation: January, 2003

# Model: CAM 3.1 T85L26.

Initialized from a climatological distribution (huge spread).

## **Observations: Radiosondes, ACARS, Satellite Winds.**

Subset of observations used in NCAR/NCEP reanalysis.

Compare to NCEP operational, T254L64, uses radiances.







#### NCEP

#### Difference.



# CAM gains zonal structure.



# NH converged. SH poorly observed.

## 6-Hour Forecast Observation Space Temperature RMS



DART/CAM competitive with operational NWP system.

Assimilation increases information about all three pieces:

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Initial conditions for forecasts.Includes time evolution and 'balances'.High quality analyses (re-analyses).

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Evaluate model systematic errors.

Forward and backward sensitivity analysis (adjoint and linear tangent replacement). Select appropriate values for model parameters. High-quality analysis of CO in Finite Volume CAM-CHEM model.

Assimilate standard observations plus MOPITT CO observations.

Work by Ave Arellano and Peter Hess supported by Kevin Raeder.

# Impact of Assimilation in Modeled CO



Suggests the utility of assimilation in providing better initial/boundary conditions to regional CO forecasts. Assimilating MOPITT CO provides important constraints to regional CO distribution in the troposphere.



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# Estimate value of existing or planned observations.

Design observing systems that provide increased information.

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Forward and backward sensitivity analysis (adjoint and linear tangent replacement). Select appropriate values for model parameters. Assimilating GPS Radio Occultation Observations in WRF Assimilated as refractivity along beam path. Complicated function of T, Q, P and ionospheric electric field.



#### Get a sounding as GPS satellite sets relative to low earth satellite.

Assimilating GPS Radio Occultation Observations in WRF

Weather Research and Forecasting Model. Regional Weather Prediction model. Configured for CONUS domain, 50 km grid.

Several hundred profiles available from CHAMP satellite.



Assimilating GPS Radio Occultation Observations in WRF

Evaluating Impact of GPS Observations.

Case 1: Assimilate radiosondes EXCEPT those close to GPS profiles. Case 2: Also assimilate GPS profiles.

Look at reduction in error from close (unused) radiosonde profiles.

NOTE: Identical code allows assimilation in CAM, GFDL, GFS...

# <u>GPS Radio Occultation Impact on T and Q Errors in WRF</u> Each plot displays bias (left pair) and RMS (right pair). Red curves include GPS: reduced bias and RMS.



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Forward and backward sensitivity analysis (adjoint and linear tangent replacement). Select appropriate values for model parameters.

# Example of low-resolution assimilation comparisons. CAM spectral vs. FV for January, 2003: Temperature Bias



Anderson: NSF August, 2006

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2. Get better estimates of observing system error characteristics.

Estimate value of existing or planned observations. Design observing systems that provide increased information.

# 3. Improve model of physical system.

Evaluate model systematic errors.

Forward/backward sensitivity analysis (adjoint/linear tangent proxy).

Select appropriate values for model parameters.

### **Ensemble Sensitivity Analysis**

Can compute correlation (covariance) between ANY forecast or analysis quantity and ALL other forecast and analysis quantities or functions thereof at any time lag.

Can get same information as unlimited number of adjoint and linear tangent integrations over arbitrary periods.

Explore relations between variables, observations, or functions thereof.

Example 1: Base point is 500 hPa mid-latitude temperature. Look at impact on evolution of 500hPa temperatures.

Similar to linear tangent integration. Significant correlations from 20 member T85 ensemble.

Time lag 00 hours: 500 hPa Temperature to 500 hPa Temperature



Time lag 06 hours: 500 hPa Temperature to 500 hPa Temperature



Time lag 12 hours: 500 hPa Temperature to 500 hPa Temperature



Time lag 18 hours: 500 hPa Temperature to 500 hPa Temperature


## Forward in Time Sensitivity (Linear Tangent equivalent)

Time lag 24 hours: 500 hPa Temperature to 500 hPa Temperature



# Forward in Time Sensitivity (Linear Tangent equivalent)

# Time lag 30 hours: 500 hPa Temperature to 500 hPa Temperature



# **Ensemble Sensitivity Analysis**

Can compute correlation (covariance) between ANY forecast or analysis quantity and ALL other forecast and analysis quantities or functions thereof.

Can get same information as unlimited number of adjoint and linear tangent integrations over arbitrary periods.

Explore relations between variables, observations, or functions thereof.

Example 2: Base point is 500 hPa mid-latitude zonal velocity. Look at impact of previous 500 hPa temperature.

Compare to an adjoint integration.

# Time lag -00 hours: 500 hPa Zonal Velocity to 500 hPa Temperature



# Time lag -06 hours: 500 hPa Zonal Velocity to 500 hPa Temperature



# Time lag -12 hours: 500 hPa Zonal Velocity to 500 hPa Temperature



# Time lag -18 hours: 500 hPa Zonal Velocity to 500 hPa Temperature



#### Time lag -24 hours: 500 hPa Zonal Velocity to 500 hPa Temperature



Time lag -30 hours: 500 hPa Zonal Velocity to 500 hPa Temperature



# Assimilation increases information about all three pieces:

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Initial conditions for forecasts. Includes time evolution and 'balances'. High quality analyses (re-analyses).

2. Get better estimates of observing system error characteristics.

Estimate value of existing or planned observations. Design observing systems that provide increased information.

# 3. Improve model of physical system.

Evaluate model systematic errors. Forward and backward sensitivity analysis (adjoint and linear tangent replacement). Select appropriate values for model parameters. Climate Model Parameter Estimation via Ensemble Data Assimilation.



T21 CAM assimilation of gravity wave drag efficiency parameter.

Oceanic values are noise (should be 0).

0< efficiency< ~4 suggested by modelers.

Positive values over NH land expected.

Problem: large negative values over tropical land near convection.

May reduce wind bias in tropical troposphere, but for 'Wrong Reason'.

# Assimilation tries to use free parameter to fix ALL model problems

# Data Assimilation Research Testbed (DART)



Software to do everything here (and more) is in DART.

Requires F90 compiler, Matlab.

Available from www.image.ucar.edu/DAReS/.