

The Data Assimilation Research Testbed: An Intro to Powerful Nonlinear and Non-Gaussian Data Assimilation Tools Jeff Anderson, NCAR/DAReS







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Prediction Model

Prediction Model

Observing System







Observations combined with a Model forecast...



Data Assimilation: What can it do?

- Analyses and forecasts of state variables.
- Smoothing estimates of state variables.
- Estimate model parameters.
- Estimate model errors.
- Estimate observing system errors.
- Quantitatively design observing systems.
- Estimate external forcing.
- Estimate anything correlated with model/observations.

A General Description of the Forecast Problem

A 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:

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

$$Y_{\tau} = \left\{ y_l; t_l \le \tau \right\} \tag{4}$$

Goal: Find probability distribution for state:

$$p(x,t | Y_t)$$
 Analysis $p(x,t^+ | Y_t)$ Forecast (5)

A General Description of the Forecast Problem

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

$$p(x,t_k \mid Y_{t_k}) = p(x,t_k \mid y_k,Y_{t_{k-1}})$$
(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:

$$p\left(y_{k} \mid x_{k}, Y_{t_{k-1}}\right) = p\left(y_{k} \mid x_{k}\right)$$
(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)

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A General Description of the Forecast Problem

Probability after new observation:





Gaussian state

linear forward operator,

$$y_{k} = h(x_{k}, t_{k}) + v_{k}; \qquad k = 1, 2, ...; \qquad t_{k+1} > t_{k} \ge t_{0}$$

Gaussian observation error

Product of Two Gaussians

Product of d-dimensional normals with means μ_1 and μ_2 and covariance matrices \sum_1 and \sum_2 is normal.

 $N(\mu_1, \Sigma_1)N(\mu_2, \Sigma_2) = cN(\mu, \Sigma)$

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Covariance:
$$\Sigma = (\Sigma_1^{-1} + \Sigma_2^{-1})^{-1}$$

Mean:

$$\mu = \sum (\sum_{1}^{-1} \mu_1 + \sum_{2}^{-1} \mu_2)$$

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$$\Sigma = (\Sigma_1^{-1} + \Sigma_2^{-1})^{-1}$$

Mean:
$$\mu = \sum (\sum_{1}^{-1} \mu_1 + \sum_{2}^{-1} \mu_2)$$

Weight:
$$c = \frac{1}{(2\Pi)^{d/2} |\Sigma_1 + \Sigma_2|^{1/2}} \exp\left\{-\frac{1}{2} \left[(\mu_2 - \mu_1)^T (\Sigma_1 + \Sigma_2)^{-1} (\mu_2 - \mu_1) \right] \right\}$$

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

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

Numerator is just product of two Gaussians.

Denominator just normalizes posterior to be a PDF.

(10)



(10)



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(10)

Product of d-dimensional normals with means μ_1 and μ_2 and covariance matrices \sum_1 and \sum_2 is normal.

$$N(\mu_1, \Sigma_1)N(\mu_2, \Sigma_2) = cN(\mu, \Sigma)$$

Covariance:
$$\Sigma = (\Sigma_1^{-1} + \Sigma_2^{-1})^{-1}$$

Mean: $u = (\sum_{1}^{-1} + \sum_{2}^{-1})^{-1} (\sum_{1}^{-1} \mu_1 + \sum_{2}^{-1} \mu_2)$

Must store and invert covariance matrices. Too big to store for large problems. Too costly to invert, > $O(n^2)$.

1. Start with ensemble of forecasts.



2. Fit a normal to ensemble.



3. Do standard Kalman filter.



Have continuous posterior; need an ensemble.



4. Can create an ensemble with exact sample mean and covariance of continuous posterior.



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



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.

Can think about single observation without (too much) loss of generality.

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



4. Find the increments for the 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, integrate to time of next observation ...



Ensemble Kalman Filter Step 1: Observation Increments







Fit a Gaussian to the sample.



Get the observation likelihood.



Compute the continuous posterior PDF.


Use a deterministic algorithm to 'adjust' the ensemble.



First, 'shift' the ensemble to have the exact mean of the posterior.



First, 'shift' the ensemble to have the exact mean of the posterior. Second, linearly contract to have the exact variance of the posterior. Sample statistics are identical to Kalman filter.

Linear regression of observation increments onto each state variable independently (used for parallelism in DART).





Assume that all we know is the prior joint distribution.

One variable is observed.

What should happen to the unobserved variable?







Have joint prior distribution of two variables.

Next, regress the observed variable increments onto increments for the unobserved variable.

Equivalent to first finding image of increment in joint space.



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Regression: Equivalent to first finding image of increment in joint space.

Then projecting from joint space onto unobserved priors.



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

Fitting Gaussians shows that mean and variance have changed.



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

Fitting Gaussians shows that mean and variance have changed.

Other features of the prior distribution may also have changed.

Some Error Sources in Ensemble Filters



Some Error Sources in Ensemble Filters



Ensemble Kalman Filter: Conclusions

- Basic Ensemble Kalman Filter is trivial.
- ➢ Good ensemble filters require inflation, localization, ...
- 'Automated' inflation, localization algorithms exist.
- Parallel implementations for 100,000 cores for large models.
- Calibration and validation essential.
- > Hybrids with variational methods.
- > Other enhancements in the pipeline.

The Data Assimilation Research Testbed (DART)

DART provides data assimilation 'glue' to build ensemble forecast systems for the atmosphere, ocean, land, ...



Data Assimilation Research Testbed (DART)

- > A state-of-the-art Data Assimilation System for Geoscience
 - Flexible, portable, well-tested, extensible, free!
 - > Works with many models.
 - > Works with any observations: Real, synthetic, novel.
- A Data Assimilation Research System
 - > Theory based, widely applicable general techniques.
 - Localization, Sampling Error Correction, Adaptive Inflation,
- Professional software engineering
 - Carefully constructed and verified.
 - Excellent performance.
 - Comprehensive documentation, examples, tutorials.
- People: The DAReS Team





48 UCAR member universities, More than 100 other sites, (More than 1500 registered users).



DART Accelerates Forecast System Development

- Works with nearly all NCAR community models (dozens of other models, too).
- New models can be added in weeks.
- Adding new observations is even easier.
- Modular: models, observations and assimilation tools easily combined.
- Enables DA use by prediction scientists. Doesn't require assimilation expertise.
- Fast & efficient software: laptops to supers.

Example: NCAR Real-time ensemble prediction system



Keyboard commands: toggle county overlay (regions only) [o] --- previous image [<] --- next image [>] --- hide header [h]

Forecasts sponsored by the National Science Foundation, National Center for Atmospheric Research/Mesoscale and Microscale Meteorology Laboratory, and Computational Information Systems Laboratory

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Example: NCAR Real-time ensemble prediction system

Severe weather forecast for two days compared to NWS warnings



- WRF, 10 member ensemble, GFS for boundary conditions
- Continuous operation from April 2015 to December 2017
- 48 hour forecasts at 3km resolution
- First continuously cycling ensemble system for CONUS

DART Applications with CESM Earth System Models

DART interfaces exist for many components of NCAR's Community Earth System Model:

- Lower atmosphere: CAM-FV, CAM-SE, MPAS
- Upper atmosphere, ionosphere: WACCM, WACCMX
- Atmospheric Chemistry: CAM/Chem
- Ocean: POP
- Land surface / biosphere: CLM
- Sea Ice: CICE
- Weakly coupled DA combinations of the above

Multiple Component POP/CAM Coupled DA

Comparisons to HADISST and HADSLP.

Correlation high where observations existed.

DART did not assimilate SST products or observations.

Produces competitive reanalysis.



Novel Algorithm 1: General Method for Observation Increments



Bayes' Rule: Combining Forecast with Observation



Bayes' Rule: Combining Forecast with Observation



Bayes' Rule: Combining Forecast with Observation



Should I Worry About Ice Going Down the Hill?



Have 10 forecasts of NCAR temperature.

Use Bayes to combine with uncertain NCAR temperature observation.
Should I Worry About Ice Going Down the Hill?



Original DART: Fit a normal to the forecast ensemble.

Should I Worry About Ice Going Down the Hill?



Bayes product gives continuous normal posterior.

Should I Worry About Ice Going Down the Hill?



Get a posterior ensemble.

Until now, we only knew how to do this for normal distributions.

Normal may work okay for applications like NWP.

Should I Worry About Air Quality Going Down the Hill?



Forecast model knows ozone must be positive.

Fitting a normal leads to probability of negative.

Should I Worry About Air Quality Going Down the Hill?



Doing the DA can lead to negative ensemble members.

What does that mean? Not sure, but nothing good.

Putting these back into model to make new forecasts is a problem, too.

Should I Worry About Air Quality Going Down the Hill?



Now can do any distribution using quantile conserving ensemble algorithms.

Example: Gamma for bounded quantity like ozone.

Posterior ensemble no longer crazy.

Novel Algorithm 1: Observation Increment Quantile Conserving Filter

DART now provides nearly general solutions for this step (Anderson, 2022, MWR150, 1061-1074).



Novel Algorithm 2: Nonlinear constraint-preserving regression

Linear regression can cause inconsistent updates for other variables.



Prior for normal-gamma distribution with 100 member ensemble.



Contours are correct distribution.

Prior for normal-gamma distribution with 100 member ensemble.



Example: Use observation of temperature to improve estimate of ozone.

Prior for normal-gamma distribution with 100 member ensemble.

Posterior ensemble has problems.



Example regression increment vectors: Don't respect bounds, Struggle with nonlinearity.



Doesn't violate prior PDF constraints like bounds. Also deals with curvature (nonlinearity).



Crucially important for things like chemical tracers, streamflow, sea ice concentration, snow cover,...

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Algorithm

 y_n^p , y_n^a , x_n^p , n=1, ...N are prior and posterior (analysis) ensembles of observed variable y and unobserved variable x

 F_x^p and F_y^p are continuous CDFs appropriate for x and y $\Phi(z)$ is the CDF of the standard normal, $\Phi^{-1}(p)$ is the probit function $\tilde{x}_n^p = \Phi^{-1}[F_x^p(x_n^p)]$, $\tilde{y}_n^p = \Phi^{-1}[F_y^p(y_n^p)]$ and $\tilde{y}_n^a = \Phi^{-1}[F_y^p(y_n^a)]$ are probit space $\Delta \tilde{y}_n = \tilde{y}_n^a - \tilde{y}_n^p$ is probit space observation increment

 $\Delta \tilde{x}_n = \frac{\tilde{\sigma}_{x,y}}{\tilde{\sigma}_{y,y}} \Delta \tilde{y}_n$ regress increments in probit space (eq. 5 Anderson 2003)

 $\tilde{x}_n^a = \tilde{x}_n^p + \Delta \tilde{x}_n$ is posterior ensemble in probit space

 $x_n^a = (F_x^p)^{-1}[\Phi(\tilde{x}_n^a)]$ is posterior ensemble

Example 2: Normal observed, beta unobserved

Application: Sea ice fraction, bounded between 0 and 1.



Example 3: Normal observed, binormal unobserved

Application: Convection initiation. Either convection is occurring or it is not, partially convecting is not possible.



Example 4: Gamma observed, normal unobserved

Application: Impact of tracer observations on free atmosphere variables.



DART is Uniquely Able to Use These New Methods

• Works with DART's sequential ensemble algorithms.

• Compatible with existing DART parallel implementation.

• Works with all (dozens) of DART supported models.

Important for Many High-Impact DA Science Collaborations

- Estimating and Predicting Bounded Quantities:
 - Atmospheric chemistry,
 - Streamflow and flooding,
 - Ocean biogeochemistry,
 - Sea ice (ASP Postdoc Chris Riedel already pushing forward),
 - Snow and land ice,
 - Land surface and biosphere,
 - Source and sink estimation, CO2, pollutants, Accidental/intentional releases,
 - Model parameter estimation.
- Non-Gaussian distributions:
 - Convection,
 - Radiation remote sensing.

DART: The Next Generation

Breakthroughs in ensemble DA algorithms being implemented in DART provide powerful and unique nonlinear and non-Gaussian capabilities for Earth system applications.

RESISTANCE IS FUTILE

YOU WILL BE ASSIMILATED

Major improvements for: Tracers / bounded quantities; Remote sensing observations; Model parameter estimation. DAReS is looking forward to an exciting and busy future accelerating science progress with these powerful new methods.



Anderson, J., Hoar, T., Raeder, K., Liu, H., Collins, N., Torn, R., Arellano, A., 2009: *The Data Assimilation Research Testbed: A community facility.* BAMS, **90**, 1283—1296, doi: 10.1175/2009BAMS2618.1

Given a prior ensemble estimate of an observed quantity, y



Fit a continuous PDF from an appropriate distribution family and find the corresponding CDF



Compute the quantile of ensemble members; just the value of CDF evaluated for each member.



Continuous likelihood for this observation.



Bayes tells us that the continuous posterior PDF is the product of the continuous likelihood and prior.



Normal times normal is normal.

Posterior ensemble members have same quantiles as prior. This is quantile function, inverse of posterior CDF.



For normal prior and likelihood, this is identical to existing deterministic Ensemble Adjustment Kalman Filter (EAKF)



Localization of Quantile (or Probit) Increments: Normal-binormal example

Standard increment localization may ignore prior constraints. Quantile increment localization 'knows' prior was binormal.



What about the normal-normal case?

$$\begin{split} \tilde{y}_{n}^{p} &= \Phi^{-1} \big[F_{y}^{p} \big(y_{n}^{p} \big) \big] \quad \text{and} \ \tilde{y}_{n}^{a} &= \Phi^{-1} \big[F_{y}^{p} \big(y_{n}^{a} \big) \big] \\ F_{y}^{p} \text{ is for } Normal \left[\mu_{y}^{p}, \big(\sigma_{y}^{p} \big)^{2} \right] \\ \text{This means that} \ y_{n}^{p} &= \sigma_{y}^{p} \tilde{y}_{n}^{p} + \mu_{y}^{p}, \quad y_{n}^{a} &= \sigma_{y}^{p} \tilde{y}_{n}^{a} + \mu_{y}^{p} \\ \text{Similarly} \ x_{n}^{p} &= \sigma_{x}^{p} \tilde{x}_{n}^{p} + \mu_{x}^{p} \end{split}$$

Differences are $\Delta y_n = \sigma_y^p \Delta \tilde{y}_n$ and $\Delta x_n = \sigma_x^p \Delta \tilde{x}_n$ Covariance $\sigma_{x,y} = \sigma_x^p \sigma_y^p \tilde{\sigma}_{x,y}$ Variance $\sigma_{y,y} = \sigma_y^p \sigma_y^p \tilde{\sigma}_{y,y}$

The standard increment regression is $\Delta x_n = \frac{\sigma_{x,y}}{\sigma_{y,y}} \Delta y_n$

Substituting for all terms $\sigma_x^p \Delta \tilde{x}_n = \frac{\sigma_x^p \sigma_y^p \tilde{\sigma}_{x,y}}{\sigma_y^p \sigma_y^p \tilde{\sigma}_{y,y}} \sigma_y^y \Delta \tilde{y}_n$ Cancels to give $\Delta \tilde{x}_n = \frac{\tilde{\sigma}_{x,y}}{\tilde{\sigma}_{y,y}} \Delta \tilde{y}_n$

What about the normal-normal case?

Computing increments in regular space is equivalent to computing increments in probit space.

For normal-normal, just do what we have always done (and for any normal in a bivariate pair???).

Recall that the QCEFF normal filter in observation space is equivalent to our traditional EAKF in observation space.

Similarly, the method here is identical to the EAKF for unobserved updates.

The EAKF is equivalent to the Kalman Filter for normal/Gaussian cases.

The QCEFF normal combined with regression here is an ensemble generalization of the EAKF and the Kalman filter.

Caveat: quantile increment localization is NOT the same as standard increment localization even in the normal-normal case.

Inverting quantile functions can be expensive.

As described, have to do that for each observation/unobs pair.

More efficient workflows are possible; stay in probit space:

- 1. Compute all forward operators for a window.
- 2. Compute prior probit for all joint state ensembles.
- 3. Loop through observations (sequential_obs loop):
 - a. Invert prior probit for observed variable,
 - b. Compute posterior for observed,
 - c. Do probit conversion for posterior obs,
 - d. Do regression of obs probit increments for each joint unobs,
- 4. Back to regular space for all state only at the end of all obs

Number of quantile/probit inversions down to one per extended state.