

Ergodicity in data assimilation methods

David Kelly

Andy Majda Xin Tong

Courant Institute
New York University
New York NY
www.dtbkelly.com

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Part I: What is data assimilation?

What is data assimilation?

Suppose \mathbf{u} satisfies

$$\frac{d\mathbf{u}}{dt} = F(\mathbf{u})$$

with some **unknown** initial condition \mathbf{u}_0 . We are most interested in geophysical models, so think high dimensional, nonlinear, possibly stochastic.

Suppose we make *partial, noisy* observations at times $t = h, 2h, \dots, nh, \dots$

$$\mathbf{y}_n = H\mathbf{u}_n + \xi_n$$

where H is a linear operator (think low rank projection), $\mathbf{u}_n = \mathbf{u}(nh)$, and $\xi_n \sim N(0, \Gamma)$ iid.

The aim of **data assimilation** is to say something about the conditional distribution of \mathbf{u}_n given the observations $\{\mathbf{y}_1, \dots, \mathbf{y}_n\}$

Illustration (Initialization)

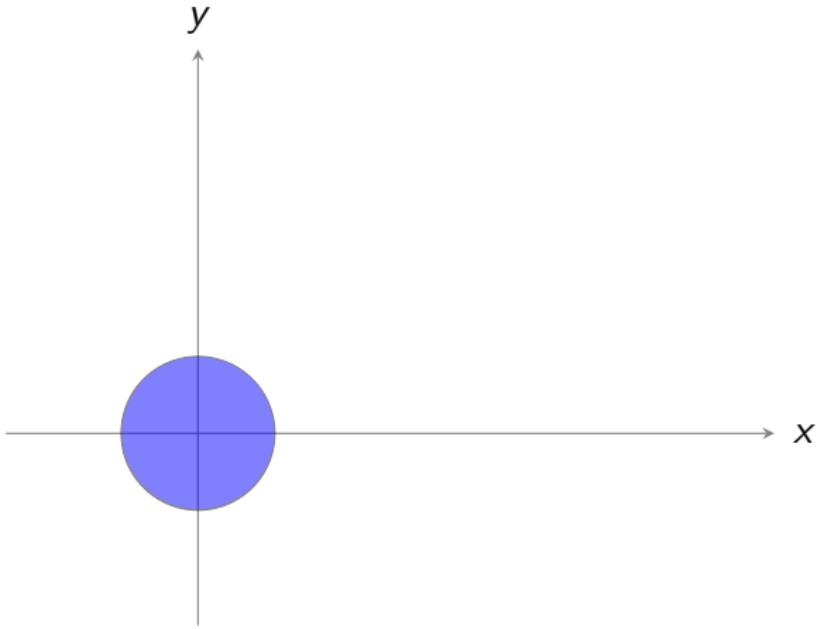


Figure: The blue circle represents our guess of u_0 . Due to the uncertainty in u_0 , this is a probability measure.

Illustration (Forecast step)

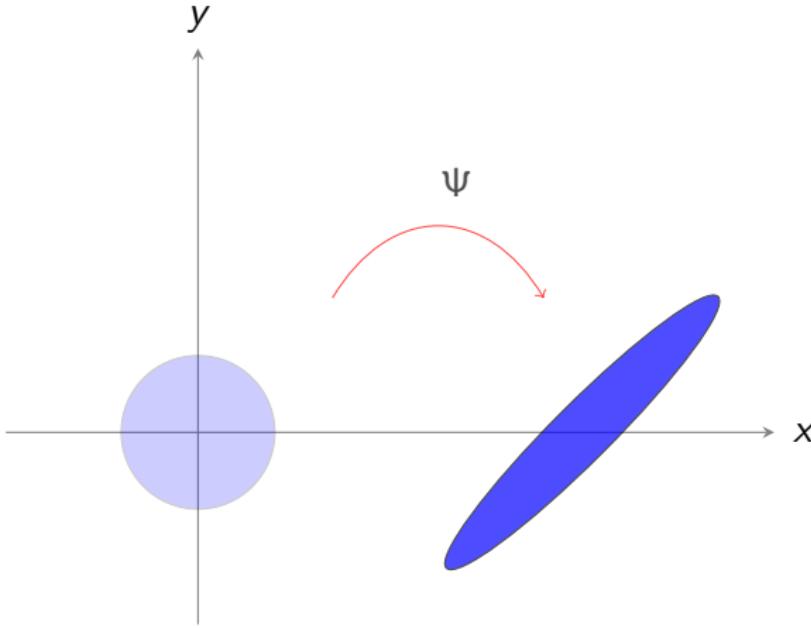


Figure: Apply the time h flow map Ψ . This produces a new probability measure which is our forecasted estimate of u_1 . This is called the forecast step.

Illustration (Make an observation)

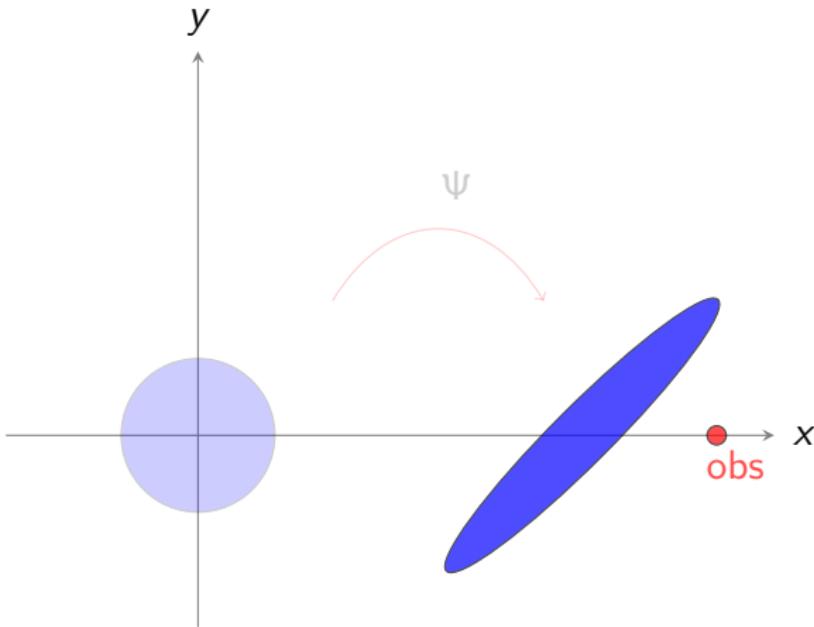


Figure: We make an observation
 $y_1 = H u_1 + \xi_1$. In the picture, we only observe the x variable.

Illustration (Analysis step)

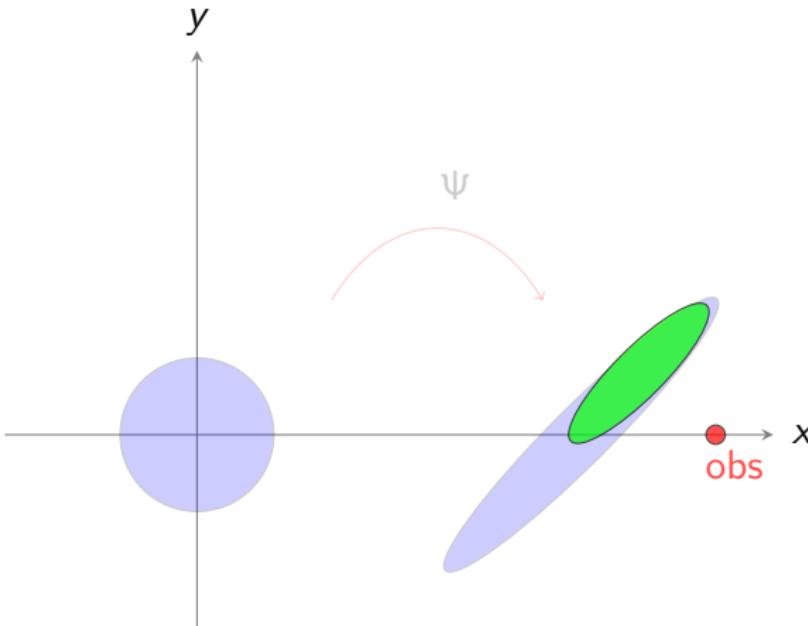


Figure: Using Bayes formula we compute the conditional distribution of $u_1|y_1$. This new measure (called the posterior) is the new estimate of u_1 . The uncertainty of the estimate is reduced by incorporating the observation. The forecast distribution steers the update from the observation.

Bayes' formula filtering update

Let $\mathbf{Y}_n = \{y_0, y_1, \dots, y_n\}$. We want to compute the conditional density $\mathbf{P}(u_{n+1} | \mathbf{Y}_{n+1})$, using $\mathbf{P}(u_n | \mathbf{Y}_n)$ and y_{n+1} .

By Bayes' formula, we have

$$\mathbf{P}(u_{n+1} | \mathbf{Y}_{n+1}) = \mathbf{P}(u_{n+1} | \mathbf{Y}_n, y_{n+1}) \propto \mathbf{P}(y_{n+1} | u_{n+1}) \mathbf{P}(u_{n+1} | \mathbf{Y}_n)$$

But we need to compute the integral

$$\mathbf{P}(u_{n+1} | \mathbf{Y}_n) = \int \mathbf{P}(u_{n+1} | \mathbf{Y}_n, u_n) \mathbf{P}(u_n | \mathbf{Y}_n) d u_n .$$

The ‘optimal filtering’ framework is **impractical** for high dimensional models, as the integrals are impossible to compute and densities impossible to store.

In **numerical weather prediction**, we have $O(10^9)$ variables for ocean-atmosphere models (discretized PDEs).

The Kalman Filter

For a linear model $\textcolor{red}{u}_{n+1} = M\textcolor{red}{u}_n + \eta_{n+1}$, the Bayesian integral is Gaussian and can be computed explicitly. The conditional density is characterized by its mean and covariance

$$\begin{aligned}\textcolor{red}{m}_{n+1} &= (1 - \textcolor{blue}{K}_{n+1}H)\hat{\textcolor{red}{m}}_n + \textcolor{blue}{K}_{n+1}\textcolor{red}{y}_{n+1} \\ \textcolor{blue}{C}_{n+1} &= (I - \textcolor{blue}{K}_{n+1}H)\hat{\textcolor{blue}{C}}_{n+1},\end{aligned}$$

where

- $(\hat{\textcolor{red}{m}}_{n+1}, \hat{\textcolor{blue}{C}}_{n+1})$ is the **forecast** mean and covariance.
- $\textcolor{blue}{K}_{n+1} = \hat{\textcolor{blue}{C}}_{n+1}H^T(\Gamma + H\hat{\textcolor{blue}{C}}_{n+1}H^T)^{-1}$ is the **Kalman gain**.

The procedure of updating $(\textcolor{red}{m}_n, \textcolor{blue}{C}_n) \mapsto (\textcolor{red}{m}_{n+1}, \textcolor{blue}{C}_{n+1})$ is known as the **Kalman filter**.

Extended Kalman filter

Suppose we have a nonlinear model:

$$\textcolor{red}{u}_{n+1} = \Phi(\textcolor{red}{u}_n) + \Sigma^{1/2} \eta_{n+1}$$

where Φ is a nonlinear map, η_n Gaussian. The **Extended Kalman filter** is given by the same update formulas

$$\begin{aligned}\textcolor{red}{m}_{n+1} &= (1 - \textcolor{blue}{K}_{n+1} H) \hat{\textcolor{red}{m}}_{n+1} + \textcolor{blue}{K}_{n+1} \textcolor{red}{y}_{n+1} \\ \textcolor{blue}{C}_{n+1} &= (I - \textcolor{blue}{K}_{n+1} H) \hat{\textcolor{blue}{C}}_{n+1},\end{aligned}$$

where $\hat{\textcolor{red}{m}}_{n+1} = \Phi(\textcolor{red}{m}_n)$ and $\hat{\textcolor{blue}{C}}_{n+1} = D\Phi(\textcolor{red}{m}_n) \textcolor{blue}{C}_n D\Phi(\textcolor{red}{m}_n)^T + \Sigma$.

Thus we approximate the forecast distribution with a Gaussian.
Still too expensive for $O(10^9)$ variables....

Ensemble Kalman filter (Evensen 94)

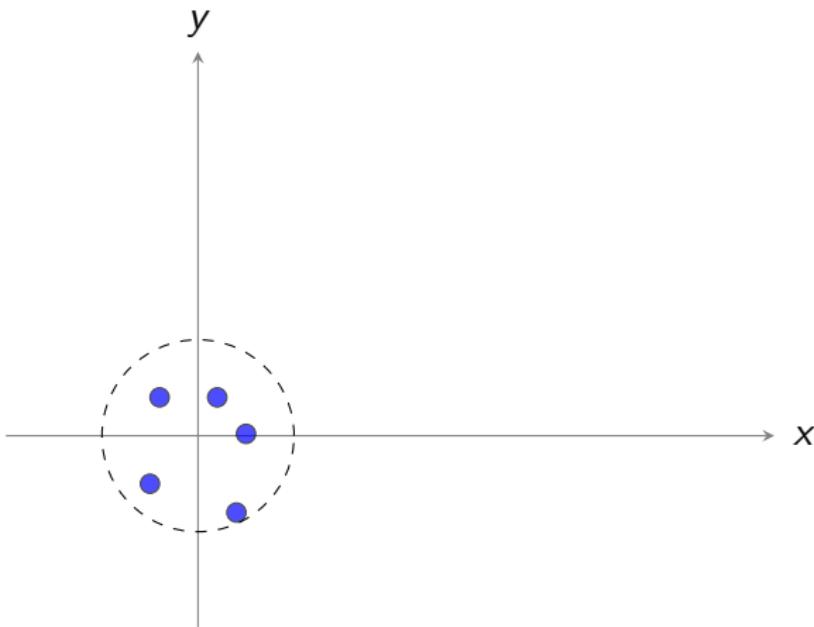


Figure: Start with K ensemble members drawn from some distribution. Empirical representation of u_0 . The ensemble members are denoted $u_0^{(k)}$.

Only KN numbers are stored. Better than Kalman if $K < N$.

Ensemble Kalman filter (Forecast step)

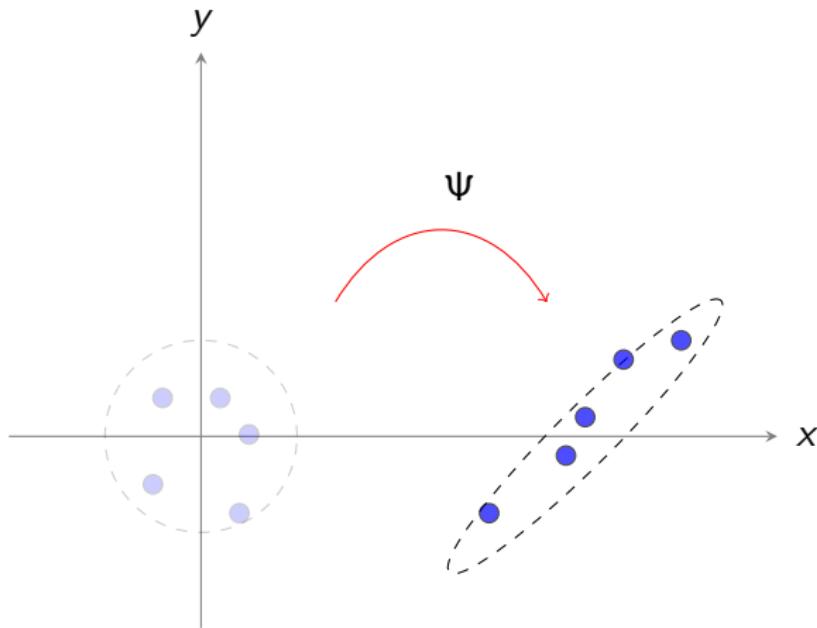


Figure: Apply the dynamics Ψ to each ensemble member.

Ensemble Kalman filter (Make obs)

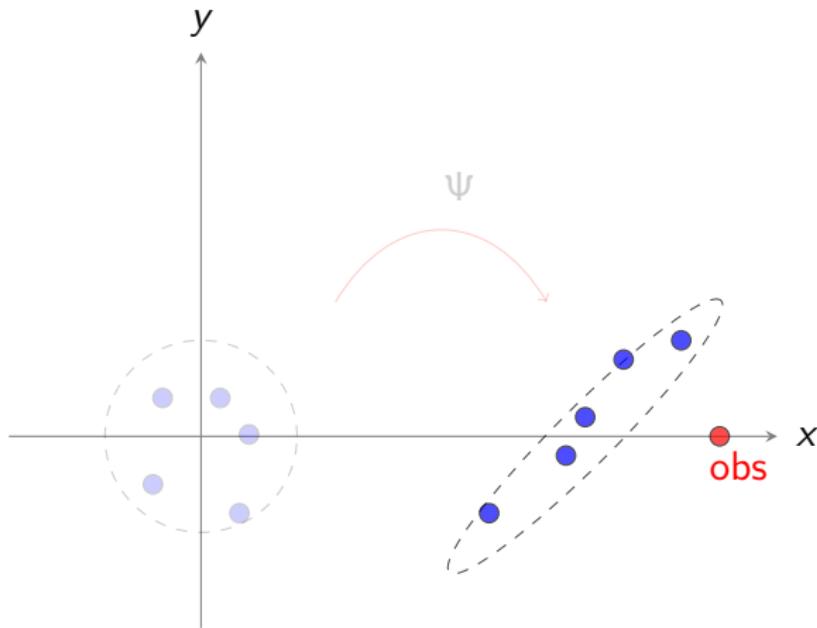


Figure: Make an observation.

Ensemble Kalman filter (Analysis step)

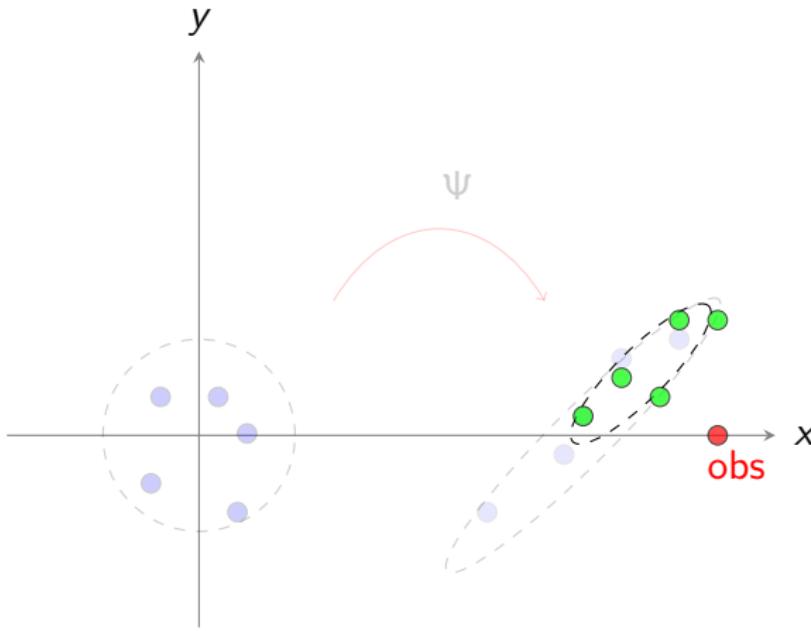


Figure: Approximate the forecast distribution with a Gaussian. Fit the Gaussian using the empirical statistics of the ensemble.

How to implement the Gaussian approximation

The naive method is to simply write:

$$\mathbf{P}(\mathbf{y}_1 | \mathbf{u}_1) \mathbf{P}(\mathbf{u}_1) \propto \exp\left(-\frac{1}{2} |\Gamma^{-1/2}(\mathbf{y}_1 - H\mathbf{u}_1)|^2\right) \exp\left(-\frac{1}{2} |\widehat{\mathbf{C}}^{-1/2}(\mathbf{u}_1 - \widehat{\mathbf{m}}_1)|^2\right)$$

with the empirical statistics

$$\widehat{\mathbf{m}}_1 = \frac{1}{K} \sum_{k=1}^K \Psi^{(k)}(\mathbf{u}_0^{(k)})$$

$$\widehat{\mathbf{C}}_1 = \frac{1}{K-1} \sum_{k=1}^K \left(\Psi^{(k)}(\mathbf{u}_0^{(k)}) - \widehat{\mathbf{m}}_1 \right) \left(\Psi^{(k)}(\mathbf{u}_0^{(k)}) - \widehat{\mathbf{m}}_1 \right)^T.$$

In the linear model case $\Psi(\mathbf{u}_n) = M\mathbf{u}_n + \boldsymbol{\eta}_n$, this produces an unbiased estimate of the posterior mean, but a biased estimate of the covariance.

How to implement the Gaussian approximation

A better approach is to sample using **Randomized Maximum Likelihood** (RML) method: Draw the sample $\textcolor{red}{u}_1^{(k)}$ by minimizing the functional

$$\frac{1}{2} |\Gamma^{-1/2}(\textcolor{red}{y}_1^{(k)} - Hu)|^2 + \frac{1}{2} |\widehat{\mathcal{C}}_1^{-1/2}(u - \Psi^{(k)}(\textcolor{red}{u}_0^{(k)}))|^2$$

where $\textcolor{red}{y}_1^{(k)} = y_1 + \xi_1^{(k)}$ is a perturbed observation.

In the linear case $\Psi(u_n) = M\textcolor{red}{u}_n + \eta_n$, this produces iid Gaussian samples with mean and covariance satisfying the Kalman update equations, with $\widehat{\mathcal{C}}$ in place of the true forecast covariance.

We end up with

$$\textcolor{red}{u}_1^{(k)} = (1 - \textcolor{blue}{K}_1 H) \Psi^{(k)}(\textcolor{red}{u}_0^{(k)}) + \textcolor{blue}{K}_1 H \textcolor{red}{y}_1^{(k)}$$

Ensemble Kalman filter (Perturb obs)

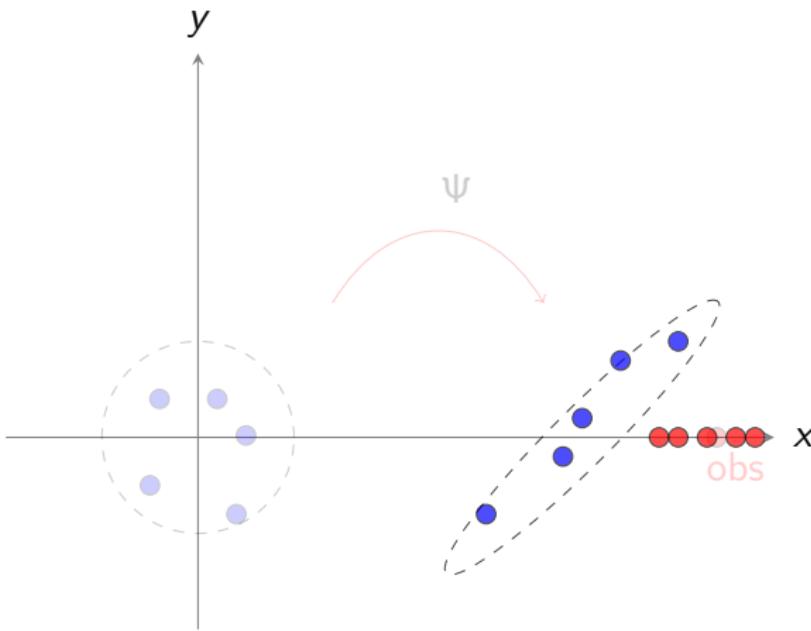


Figure: Turn the observation into K artificial observations by perturbing by the same source of observational noise.

$$y_1^{(k)} = y_1 + \xi_1^{(k)}$$

Ensemble Kalman filter (Analysis step)

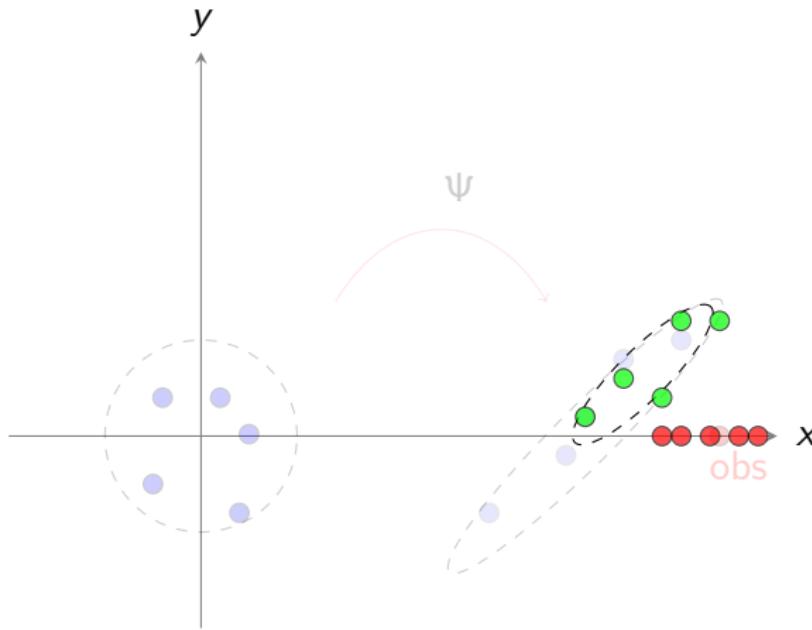


Figure: Update each member using the Kalman update formula. The Kalman gain K_1 is computed using the ensemble covariance.

$$\mathbf{u}_1^{(k)} = (1 - K_1 H) \psi(\mathbf{u}_0^{(k)}) + K_1 H \mathbf{y}_1^{(k)} \quad K_1 = \widehat{\mathbf{C}}_1 H^T (\Gamma + H \widehat{\mathbf{C}}_1 H^T)^{-1}$$

$$\widehat{\mathbf{C}}_1 = \frac{1}{K-1} \sum_{k=1}^K (\psi(\mathbf{u}_0^{(k)}) - \widehat{\mathbf{m}}_{n+1})(\psi(\mathbf{u}_0^{(k)}) - \widehat{\mathbf{m}}_{n+1})^T$$

Part II: Ergodicity for DA methods:

Why are we interested in ergodicity? And what kind?

Two types of ergodicity

- 1 - **Signal-Filter Ergodicity:** Ergodicity for the homogeneous Markov chain $(\mathbf{u}_n, \mathbf{u}_n^{(1)}, \dots, \mathbf{u}_n^{(K)})$.
- 2 - **Conditional ergodicity:** Let $\mathbf{P}_n^{Y_n}(\cdot; \mathbf{u}_0^{(1)}, \dots, \mathbf{u}_0^{(K)})$ be the law of $(\mathbf{u}_n^{(1)}, \dots, \mathbf{u}_n^{(K)})$, given the observations Y_n and initialization $(\mathbf{u}_0^{(1)}, \dots, \mathbf{u}_0^{(K)})$. We call the filter conditionally ergodic when any two such measures with different initialization, but same observations Y_n , converge as $n \rightarrow \infty$.

Two types of ergodicity

Signal-filter ergodicity tells us that:

- The filter will not **blow-up** (catastrophic filter divergence).
- The long-time statistics of the filter are **stable** with respect to **initialization**.
- The filter inherits ‘**physical properties**’ from the underlying model.

Conditional ergodicity suggests that the method is **accurate**, since all measures are synchronizing, they should be shadowing the true trajectory.

Animation I

The model $d\mathbf{u} = -\nabla V(\mathbf{u})dt + \sigma dW$, where $V(x, y) = (1 - x^2 - y^2)^2$. Observation $\mathbf{u}_x(t) + \xi(t)$. For EnKF, the process is signal-filter ergodic, but it is not conditionally ergodic.

Animation II

The model $d\textcolor{red}{u} = -\nabla V(\textcolor{red}{u})dt + \sigma dW$ where $V(x, y) = (1 - x^2 - y^2)^2$.

Observation $\textcolor{red}{y} = \textcolor{red}{u}_1 + \xi$. This filter (a type of particle filter) is both signal-filter ergodic and conditionally ergodic.

Today we focus on **signal-filter ergodicity**. Conditional ergodicity is much more difficult (but work in progress!).

The theoretical framework

A Markov chain $\{\mathbf{X}_n\}_{n \in \mathbb{N}}$ on a state space \mathcal{X} is called **geometrically ergodic** if it has a unique invariant measure π and for any initialization \mathbf{X}_0 we have

$$\left| \mathbf{E}_{\mathbf{X}_0} f(\mathbf{X}_n) - \int f(x) \pi(dx) \right| \leq C(\mathbf{X}_0) r^n$$

for some $r \in (0, 1)$ and any measurable bdd f .

The Meyn-Tweedie approach is to verify two assumptions that guarantee geometric ergodicity using a **coupling argument**:

- 1- **Lyapunov function / Energy dissipation:** $\mathbf{E}_n |\mathbf{X}_{n+1}|^2 \leq \alpha |\mathbf{X}_n|^2 + \beta$ with $\alpha \in (0, 1)$, $\beta > 0$.
- 2- **Minorization:** Find compact $C \subset \mathcal{X}$, measure ν supported on C , $\kappa > 0$ such that $P(x, A) \geq \kappa \nu(A)$ for all $x \in C$, $A \subset \mathcal{X}$.

Minorization is inherited

If we assume that the model and observational noise have nice densities (non-degenerate Gaussians, for instance) then the minorization condition is **inherited** from the model.

Is the same true of the **Lyapunov function**?

Lyapunov function: Inheriting an energy principle

Suppose we know the model satisfies an energy principle

$$\mathbf{E}_n |\Psi(\textcolor{red}{u})|^2 \leq \alpha |\textcolor{red}{u}|^2 + \beta$$

for $\alpha \in (0, 1)$, $\beta > 0$. Does the filter inherit the energy principle?

$$\mathbf{E}_n |\textcolor{red}{u}_{n+1}^{(k)}|^2 \leq \alpha' |\textcolor{red}{u}_n^{(k)}|^2 + \beta'$$

Observable energy (Tong, Majda, K. 15)

We have

$$\textcolor{red}{u}_{n+1}^{(k)} = (I - \textcolor{blue}{K}_{n+1} H) \Psi(\textcolor{red}{u}_n^{(k)}) + \textcolor{blue}{K}_{n+1} \textcolor{red}{y}_{n+1}^{(k)}$$

Start by looking at the observed part:

$$H \textcolor{red}{u}_{n+1}^{(k)} = (H - H \textcolor{blue}{K}_{n+1} H) \Psi(\textcolor{red}{u}_n^{(k)}) + H \textcolor{blue}{K}_{n+1} \textcolor{red}{y}_{n+1}^{(k)}.$$

But notice that

$$\begin{aligned} (H - H \textcolor{blue}{K}_{n+1} H) &= (H - H \widehat{\mathcal{C}}_{n+1} H^T (I + H \widehat{\mathcal{C}}_{n+1} H^T)^{-1} H) \\ &= (I + H \widehat{\mathcal{C}}_{n+1} H^T)^{-1} H \end{aligned}$$

Hence

$$|(H - H \textcolor{blue}{K}_{n+1} H) \Psi(\textcolor{red}{u}_n^{(k)})| \leq |H \Psi(\textcolor{red}{u}_n^{(k)})|$$

Observable energy (Tong, Majda, K. 15)

We have the energy estimate

$$\mathbf{E}_n |H\mathbf{\bar{u}}_{n+1}^{(k)}|^2 \leq (1 + \delta) |H\Psi(\mathbf{\bar{u}}_n^{(k)})|^2 + \beta'$$

for arb small δ . Unfortunately, the same trick doesn't work for the unobserved variables ... However, if we assume an observable energy criterion instead:

$$\mathbf{E}_n |H\Psi(\mathbf{\bar{u}}_n^{(k)})|^2 \leq \alpha |H\mathbf{\bar{u}}_n^{(k)}|^2 + \beta \quad (\star)$$

Then we obtain a Lyapunov function for the observed components of the filter:

$$\mathbf{E}_n |H\mathbf{\bar{u}}_n^{(k)}|^2 \leq \alpha' |H\mathbf{\bar{u}}_n^{(k)}|^2 + \beta'.$$

eg. (\star) is true for linear dynamics if there is no interaction between observed and unobserved variables at infinity.

Tells us that observed components will be statistically bounded, but not a Lyapunov function (unless we observe everything).

Can we get around the problem by
tweaking the algorithm?

Adaptive Covariance Inflation (Tong, Majda, K. 15)

We modify algorithm by introducing a **covariance inflation** :

$$\hat{\mathcal{C}}_{n+1} \mapsto \hat{\mathcal{C}}_{n+1} + \lambda_{n+1} I$$

where

$$\lambda_{n+1} \propto \Theta_{n+1} \mathbf{1}(\Theta_{n+1} > \Lambda)$$

$$\Theta_{n+1} = \sqrt{\frac{1}{K} \sum_{k=1}^K |\mathbf{y}_{n+1}^{(k)} - H\Psi(\mathbf{u}_n^{(k)})|^2}$$

and Λ is some constant threshold. If the predictions are near the observations, then there is no inflation.

Thm. The modified EnKF inherits an energy principle from the model.

$$\mathbf{E}_x |\Psi(x)|^2 \leq \alpha |x|^2 + \beta \Rightarrow \mathbf{E}_n |\mathbf{u}_{n+1}^{(k)}|^2 \leq \alpha' |\mathbf{u}_n^{(k)}|^2 + \beta'$$

Consequently, the modified EnKF is signal-filter ergodic.

Adaptive inflation schemes allows us to use **cheap** integration schemes in the forecast dynamics. These would usually lead to numerical blow-up.

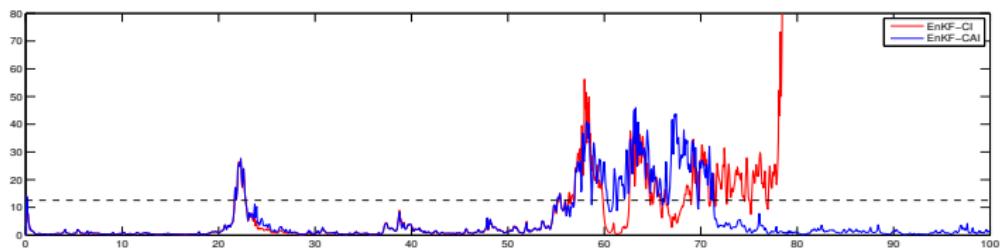
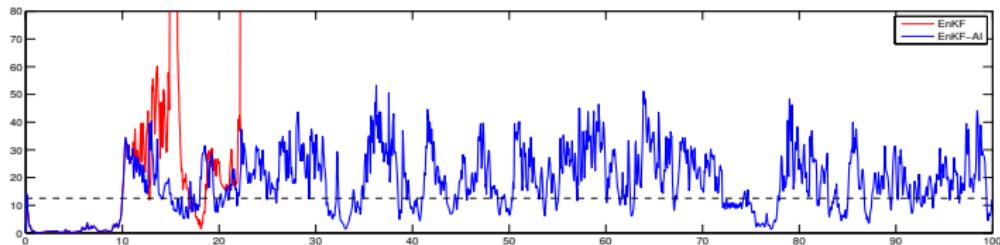


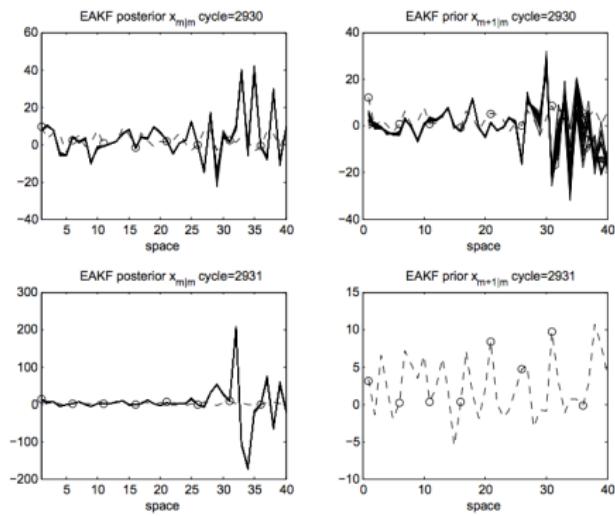
Figure: RMS error for EnKF on 5d Lorenz-96 with sparse obs (1 node), strong turbulence regime. Euler method with coarse step size. Lower panel has additional constant inflation which helps accuracy.

Applicable to more sophisticated geophysical models, such as 2-layer QG with course graining ([Lee, Majda 16'](#)).

Stability should not be taken for granted!

Catastrophic filter divergence

Lorenz-96: $\dot{u}_j = (u_{j+1} - u_{j-2})u_{j-1} - u_j + F$ with $j = 1, \dots, 40$. Periodic BCs. Observe every fifth node. (*Harlim-Majda 10, Gottwald-Majda 12*)



True solution in a bounded set, but filter **blows up** to machine infinity in finite time!

For complicated models, only heuristic arguments offered as explanation.

*Can we **prove** it for a simpler constructive model?*

The rotate-and-lock map (K., Majda, Tong. PNAS 15.)

The model $\Psi : \mathbb{R}^2 \rightarrow \mathbb{R}^2$ is a composition of two maps

$\Psi(x, y) = \Psi_{lock}(\Psi_{rot}(x, y))$ where

$$\Psi_{rot}(x, y) = \begin{pmatrix} \rho \cos \theta & -\rho \sin \theta \\ \rho \sin \theta & \rho \cos \theta \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix}$$

and Ψ_{lock} rounds the input to the nearest point in the grid

$$\mathcal{G} = \{(m, (2n + 1)\varepsilon) \in \mathbb{R}^2 : m, n \in \mathbb{Z}\}.$$

It is easy to show that this model has an **energy dissipation principle**:

$$|\Psi(x, y)|^2 \leq \alpha |(x, y)|^2 + \beta$$

for $\alpha \in (0, 1)$ and $\beta > 0$.

(a)

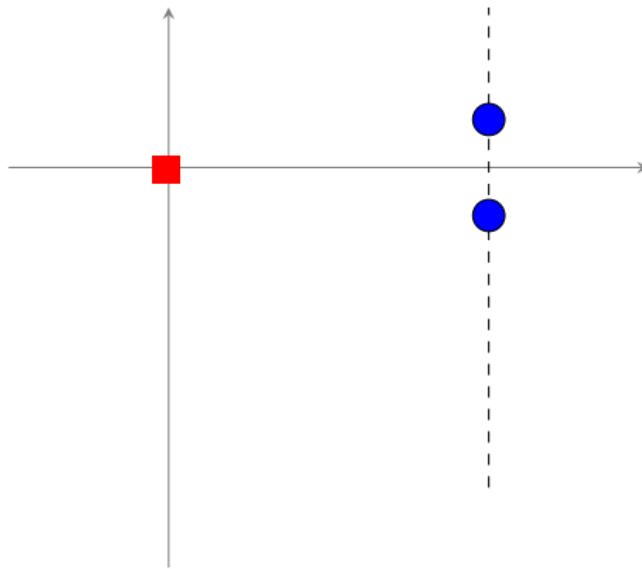


Figure: The red square is the trajectory $u_n = 0$. The blue dots are the positions of the forecast ensemble $\Psi(u_0^+)$, $\Psi(u_0^-)$. Given the locking mechanism in Ψ , this is a natural configuration.

(b)

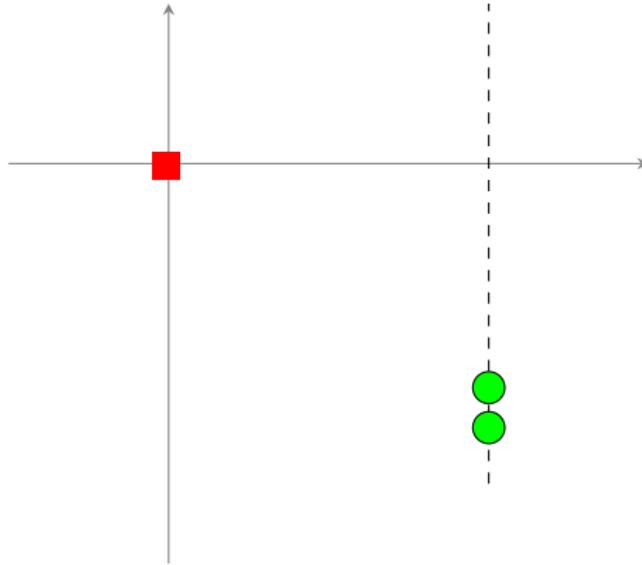


Figure: We make an observation (H shown below) and perform the analysis step. The green dots are u_1^+ , u_1^- .

Observation matrix

$$H = \begin{bmatrix} 1 & 0 \\ \varepsilon^{-2} & 1 \end{bmatrix}$$

Truth $u_n = (0, 0)$.

The filter is certain that the x-coordinate is \hat{x} (the dashed line). The filter thinks the observation must be $(\hat{x}, \varepsilon^{-2}\hat{x} + u_{1,y})$, but it is actually $(0, 0) + \text{noise}$. The filter concludes that $u_{1,y} \approx -\varepsilon^{-2}\hat{x}$.

(c)

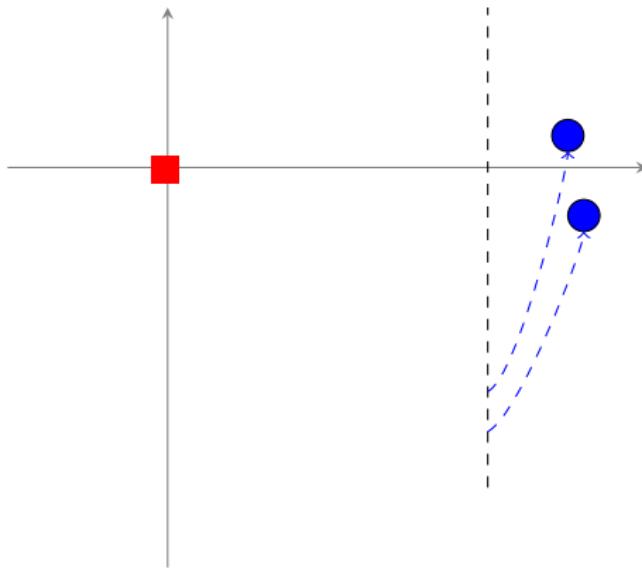


Figure: Beginning the next assimilation step. Apply Ψ_{rot} to the ensemble (blue dots)

(d)

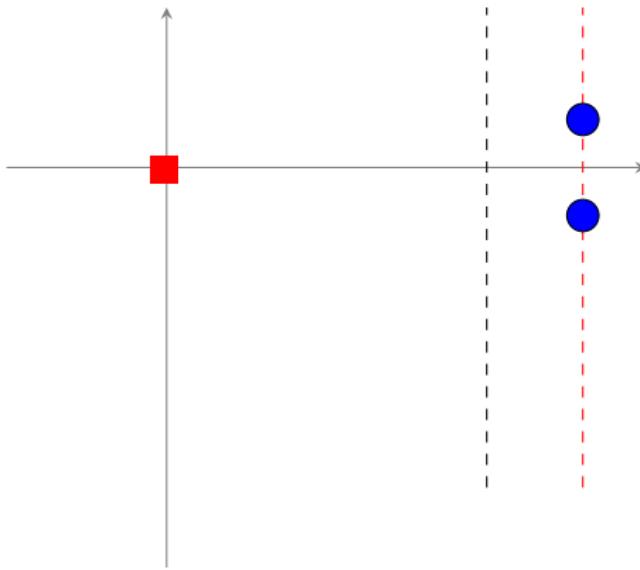


Figure: Apply Ψ_{lock} .
The blue dots are the forecast ensemble $\Psi(u_1^+), \Psi(u_1^-)$. Exact same as frame 1, but higher energy orbit. The cycle repeats leading to **exponential growth**.

Theorem (K.-Majda-Tong 15 PNAS)

For any $N > 0$ and any $p \in (0, 1)$ there exists a choice of parameters such that

$$\mathbf{P} \left(|\textcolor{red}{u}_n^{(k)}| \geq M_n \text{ for all } n \leq N \right) \geq 1 - p$$

where M_n is an exponentially growing sequence.

ie - The filter can be made to grow exponentially for an arbitrarily long time with an arbitrarily high probability.

References

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All my slides are on my website (www.dtbkelly.com) **Thank you!**