Data assimilation: the seamless integration of data into computational models

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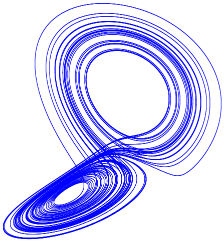
A toy atmospheric model

Lorenz equations:

$$\dot{x} = \sigma(y - x)$$
$$\dot{y} = x(\rho - z) - y$$
$$\dot{z} = xy - \beta z$$



Uncertainty in initial conditions

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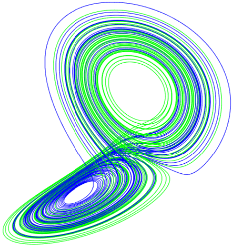

Uncertainty in parameters

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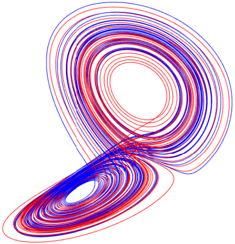

Numerical discretization and differentiation

Lorenz equations:

$$x_n = x_{n-1} + [\sigma(y_{n-1} - x_{n-1})]\mathrm{dt}$$
$$y_n = y_{n-1} + [x_{n-1}(\rho - z_{n-1}) - x_{n-1}]\mathrm{dt}$$
$$z_n = z_{n-1} + [x_{n-1}y_{n-1} - \beta z_{n-1}]\mathrm{dt}$$

Model (deterministic)

Evolution equation

$$z_n = \Psi(z_{n-1}, \lambda)$$

where

$$z_0 \sim \mathcal{N}(m_0, C_0)$$

Model

Evolution equation

$$z_n = \Psi(z_{n-1}, \lambda) + \xi_{n-1}$$

where

$$\begin{aligned} z_0 &\sim \mathcal{N}(m_0, C_0) \\ \xi_n &\sim \mathcal{N}(0, B) \quad \text{i.i.d.} \quad \forall\ n \end{aligned}$$

Parameter estimation

Augmented state space

$$\begin{aligned} z_n &= \Psi(z_{n-1}, \lambda_{n-1}) + \xi_{n-1} \\ \lambda_n &= \lambda_{n-1} \end{aligned}$$

where

$$\begin{aligned} [z_0, \lambda_0]^\top &\sim \mathcal{N}(m_0, C_0) \\ \xi_n &\sim \mathcal{N}(0, B) \quad \text{i.i.d.} \quad \forall\ n \end{aligned}$$

L63 example

Augmented state space

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Observations

Partial and noisy data:

$$y_n = h(z_n) + \eta_n$$

where

$$\eta_n \sim \mathcal{N}(0, R) \quad \text{i.i.d.} \quad \forall\ n$$

Conditional probability

Definition (Conditional probability)

For a probability space $(\Omega, \mathcal{F}, \mathbb{P})$ and events $A, B \in \mathcal{F}$ the conditional probability of B given A is

$$\mathbb{P}(A|B) = \frac{\mathbb{P}(A, B)}{\mathbb{P}(B)}.$$

Bayes theorem

Theorem (Bayes)

For a given probability space $(\Omega, \mathcal{F}, \mathbb{P})$ *the following holds for two events* A *and* B *in* $\mathcal{F}$

$$\mathbb{P}(A|B) = \frac{\mathbb{P}(B|A)\mathbb{P}(A)}{\mathbb{P}(B)}.$$

Bayesian data assimilation ansatz

$$\mathbb{P}(\text{Model}|\text{Obs}) = \frac{\mathbb{P}(\text{Obs}|\text{Model})\mathbb{P}(\text{Model})}{\mathbb{P}(\text{Obs})}$$

Bayesian data assimilation ansatz

$$\mathbb{P}(\mathsf{Model}|\mathsf{Obs}) \propto \mathbb{P}(\mathsf{Obs}|\mathsf{Model})\mathbb{P}(\mathsf{Model})$$

Bayesian data assimilation for densities

$$\begin{aligned}
\pi(z_{n+1}|y_{1:n+1}) &= \pi(z_{n+1}|y_{1:n}, y_{n+1}) \\
&= \frac{\pi(y_{n+1}|y_{1:n}, z_{n+1})\pi(z_{n+1}|y_{1:n})}{\pi(y_{n+1}|y_{1:n})} \\
&= \frac{\pi(y_{n+1}|z_{n+1})\pi(z_{n+1}|y_{1:n})}{\pi(y_{n+1}|y_{1:n})}
\end{aligned}$$

$$\implies \pi(z_{n+1}|y_{1:n+1}) \propto \pi(y_{n+1}|z_{n+1})\pi(z_{n+1}|y_{1:n}) \tag{1}$$

Special case

Linear model: Ψ is linear, e.g.,

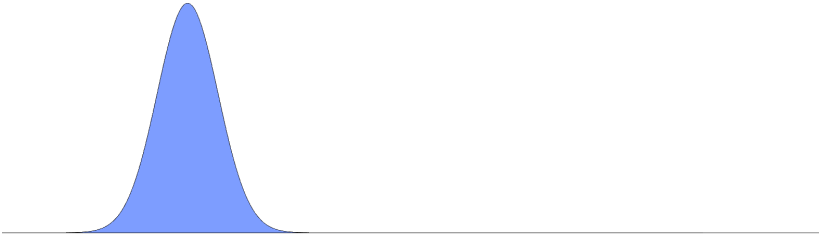
$$z_n = Az_{n-1} + \xi_{n-1} \tag{2}$$

with $A \in \mathbb{R}^{N_z} \times \mathbb{R}^{N_z}$

Linear observation operator

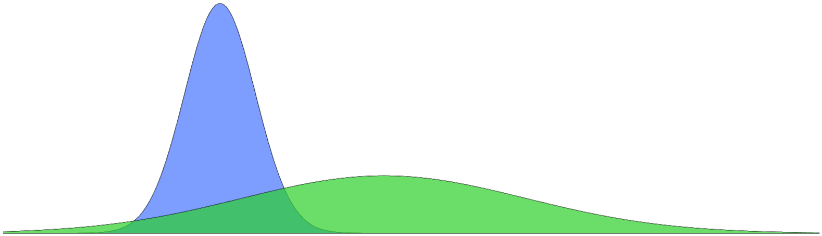
$$h = H \quad \text{with} \quad H \in \mathbb{R}^{N_y} \times \mathbb{R}^{N_y}$$

Linear Model



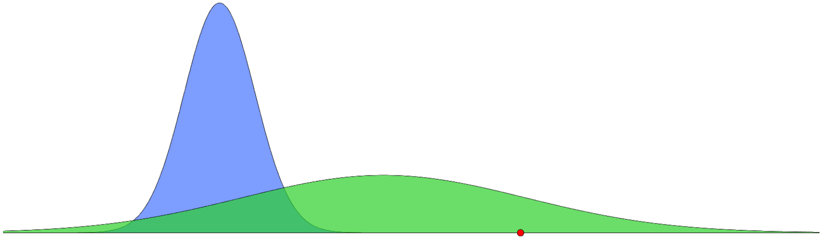
Initial distribution: $z_0 \sim \mathcal{N}(m_0, C_0)$

Linear Model



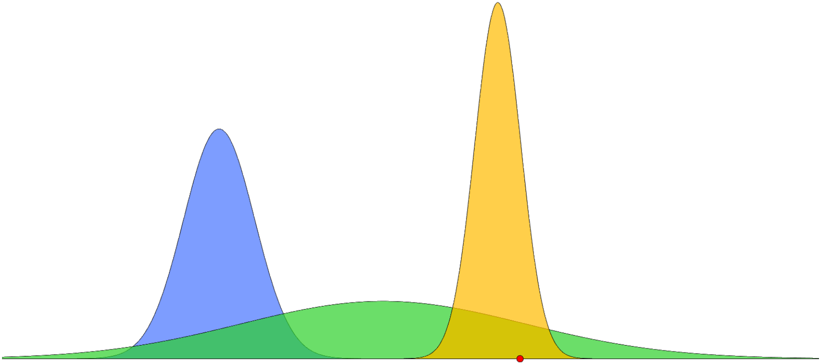
Prior distribution: $\mathcal{N}(\hat{m}_1, \hat{C}_1)$

Linear Model



Likelihood: $\mathcal{N}(H\hat{z}_1, R)$

Linear Model



Posterior: $\mathcal{N}(m_1, C_1) \propto \mathcal{N}(H\hat{z}_1, R)\mathcal{N}(\hat{m}_1, \hat{C}_1)$

Kalman filter

Two steps:

Kalman filter

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Forecast formulas

$$\hat{m}_{n+1} = A m_n$$
$$\hat{C}_{n+1} = A C_n A^\top + B$$

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Forecast formulas

$$\hat{m}_{n+1} = Am_n$$
$$\hat{C}_{n+1} = AC_nA^\top + B$$

Analysis formulas

$$m_{n+1} = \hat{m}_{n+1} - K_{n+1}(H\hat{m}_{n+1} - y_{n+1})$$
$$C_{n+1} = \hat{C}_{n+1} - K_{n+1}H\hat{C}_{n+1}$$

Kalman gain

$$K_{n+1} = \hat{C}_{n+1}H^\top(R + H\hat{C}_{n+1}H^\top)^{-1}$$

Nonlinear Model

Problem: Kalman Filter is not applicable anymore

Ansatz: approximative Algorithms

1. **Extended Kalman Filter**: linearize model function

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1. **Extended Kalman Filter**: linearize model function
2. **Monte Carlo Approximation**:

$$\pi(z_n|y_{1:n}) = \frac{1}{M}\sum_{i=1}^{M}\delta(z - z_n^i)$$

where

$$z_n^i \sim \pi(z_n|y_n)$$

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- Particle filters (curse of dimensionality)
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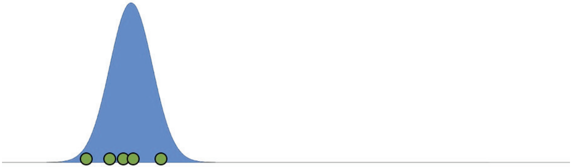
- Particle filters (curse of dimensionality)
- Ensemble Kalman filter(underlying Gaussian assumption)

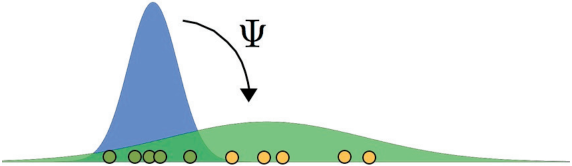
Ensemble Kalman Filter



$$\mathcal{N}(m_0, C_0) \text{ with } m_0 \approx \frac{1}{M}\sum_{i=1}^{M} z_0^i$$

$$C_0 \approx \frac{1}{M}\sum_{i=1}^{M}(z_0^i - m_0)(z_0^i - m_0)^\top$$

Ensemble Kalman Filter



$$\mathcal{N}(\hat{m}_1, \hat{C}_1) \text{ with } \hat{m}_1 \approx \frac{1}{M}\sum_{i=1}^{M} \hat{z}_1^i = \frac{1}{M}\sum_{i=1}^{M} \Psi(z_0^i)$$

$$\hat{C}_1 \approx \frac{1}{M}\sum_{i=1}^{M} (\hat{z}_1^i - \hat{m}_1)(\hat{z}_1^i - \hat{m}_1)^\top$$

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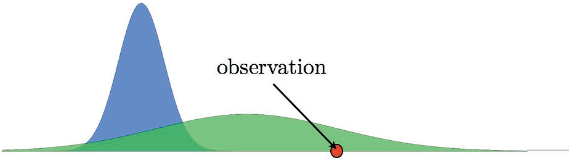

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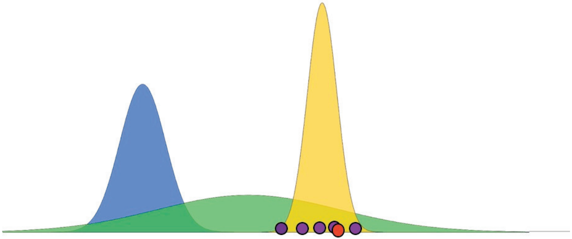

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Ansatz:: propagate samples $\hat{z}^i_{n+1}$ with Kalman formula

$$z^i_{n+1} = \hat{z}^i_{n+1} - K_{n+1}(H\hat{z}^i_{n+1} - \tilde{y}^i_{n+1})$$

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Need:: perturbed observations

$$\tilde{y}^i_{n+1} = y_{n+1} + \epsilon^i_{n+1}$$

with $\epsilon^i_{n+1} \sim \mathcal{N}(0, R)$ i.i.d. to get the correct mean and covariance in the linear case for $M \to \infty$

Ensemble Kalman Filter

Works well in practice:: e.g., EnKF is used for operational NWP for z_n^i with dimension 10^9 only using $M = 100$

Yet: mathematical foundation largely missing

Recent study: accuracy results for EnKF for idealized setting: $H = Id$ and observational error small

Particle Filter

Problem: sampling from $\pi(z_n|y_{1:n})$ to approximate posterior via

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Idea: sampling from $\pi(z_n|y_{1:n-1})$ instead i.e.,

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Bayes:

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Weighting: unnormalized weights

$$\tilde{w}_n^i = \pi(y_n|z_n^i)w_n^i \text{ with } w_0^i = \frac{1}{M}$$

and normalized weights

$$w_n^i = \frac{\tilde{w}_n^i}{\sum_{j=1}^{M}\tilde{w}_n^j}$$

Resampling

Problem: weights w_n^i become very small
Ansatz: resampling

Input: w_n^i
For$(k = 1 : M)$

1. Draw a number $u \in [0, 1]$ from the uniform distribution $U[0, 1]$
2. Compute $i^* \in \{1, \ldots, M\}$ which satisfies

$$i^* = \arg\min_{i \geq 1} \sum_{j=1}^{i} w_j \geq u \tag{4}$$

3. Set $\xi_{i^*} = \xi_i^* + 1$

Return ξ_i