Mathematics and numerics for data assimilation and state estimation – Lecture 15

Summer semester 2020

Overview

On the course's oral exam

- Time and place: between 10:00 and 18:00 on July 31, Kackertstrasse 9, room C301,
- Preparation: Will give you a list of 20-25 topics for you to prepare on on July 17.
- The exam: Will randomly draw 5 topics from list which you will be asked to expand upon.
- Duration: Roughly 20 minutes.

Information on the student presentation

- Presentations planned on Thursday 02.07 and Friday 03.07.
- Structure: Roughly 20 minutes presentation, most likely over Zoom, either alone or in pairs.
- Please email me before 21.06 with information on:
  1. What paper/topic you would like to present
  2. your preferred time for presenting
  3. and possibly, whom you'd like to present together with.
- I will try to avoid multiple presentations on the same topic, so email me early if you have found an interesting topic.

Summary lecture 14 and plan for today

- For a linear-Gaussian filtering problem

$$
\begin{aligned}
V_{j+1} &= \Psi(V_j) + \xi_j, \\
Y_{j+1} &= h(V_{j+1}) + \eta_{j+1}, \quad j = 1, 2, \ldots,
\end{aligned}
$$

  we described iterative formulas for the pdf of $V_n | Y_{1:n} = y_{1:n}$.

- Plan for today: develop Approximate Gaussian filters for settings where Ψ is nonlinear.

Summary of Kalman filtering

For linear-Gaussian dynamics

$$\begin{aligned} V_{j+1} &= AV_j + \xi_j, \quad j = 0, 1, \ldots \\ V_0 &\sim N(m_0, C_0) \end{aligned} \tag{1}$$

with $\xi_j \overset{iid}{\sim} N(0, \Sigma)$.

Observations:

$$Y_j = HV_j + \eta_j, \quad j = 1, 2, \ldots, \tag{2}$$

with $\eta_j \overset{iid}{\sim} N(0, \Gamma)$.

And independence assumptions:

$$\{\eta_j\} \perp \{\xi_j\} \perp \{V_0\}$$

We derived the ...

Kalman filtering algorithm

Given any sequence $y_1, y_2, \ldots$ and $V_j | Y_{1:j} = y_{1:j} \sim N(m_j, C_j)$ the next-time filtering distributions are iteratively determined by

Prediction step

$$\begin{aligned} \hat{m}_{j+1} &= A m_j \\ \hat{C}_{j+1} &= A C_j A^T + \Sigma \end{aligned}$$

Analysis step

$$\begin{aligned} K_{j+1} &= \hat{C}_{j+1} H^T (H \hat{C}_{j+1} H^T + \Gamma)^{-1} \qquad \textbf{Kalman gain} \\ m_{j+1} &= (I - K_{j+1} H) \hat{m}_{j+1} + K_{j+1} y_{j+1} \\ C_{j+1} &= (I - K_{j+1} H) \hat{C}_{j+1} \end{aligned}$$

Alternative Bayesian view of Kalman filtering

In Lecture 14, using that

$$V_{n+1}|Y_{1:j} = y_{1:j} \sim N(\hat{m}_{j+1}, \hat{C}_{j+1})$$

and

$$Y_{j+1}|V_{j+1} = v_{j+1} \sim N(h(v_{j+1}), \Gamma)$$

the analysis step of Kalman filtering was derived throught the posterior

$$\begin{aligned} \pi(v_{j+1}|y_{1:j+1}) &\propto \pi(y_{j+1}|v_{j+1})\pi(v_{j+1}|y_{1:j}) \\ &\propto \exp\Big(-\frac{1}{2}|y_{j+1} - Hv_{j+1}|_{\Gamma}^2 - \frac{1}{2}|v_{j+1} - \hat{m}_{j+1}|_{\hat{C}_{j+1}}^2\Big). \end{aligned} \tag{3}$$

Viewing the minus log-posterior as a cost/objective function,

$$\mathsf{J}(u) := \frac{1}{2}|y_{j+1} - Hu|_{\Gamma}^2 + \frac{1}{2}|u - \hat{m}_{j+1}|_{\hat{C}_{j+1}}^2$$

the analysis mean can be derived through variational principles:

$$m_{j+1} = \arg\min_{u \in \mathbb{R}^d} \mathsf{J}(u).$$

Kalman filter evolution of mean

In other words, the evolution of $m_j \mapsto m_{j+1}$ in Kalman filtering can be described by

$$\begin{aligned}
\hat{m}_{j+1} &= \Psi(m_j) \\
\mathsf{J}(u) &:= \frac{1}{2}|y_{j+1} - Hu|_\Gamma^2 + \frac{1}{2}|u - \hat{m}_{j+1}|_{\hat{C}_{j+1}}^2 \\
m_{n+1} &= \arg\min_{u \in \mathbb{R}^d} \mathsf{J}(u).
\end{aligned} \tag{4}$$

implicitly depending on $\hat{C}_{j+1}$ and y_{j+1}.

Equation (4) will be the basis for motivating three approximate Gaussian filtering algorithms.

Overview

1. 3DVAR
2. Extended Kalman filtering
3. Ensemble Kalman filtering

Filtering setting

Dynamics: Initial condition $V_0 \sim N(m_0, C_0)$ and for $j = 0, 1, \ldots$

$$\begin{aligned} V_{j+1} &= \Psi(V_j) + \xi_j, \\ Y_{j+1} &= HV_{j+1} + \eta_{j+1}, \quad j = 0, 1, \ldots \end{aligned} \tag{5}$$

with

$$\xi_j \overset{iid}{\sim} N(0, \Sigma), \quad \eta_j \overset{iid}{\sim} N(0, \Gamma) \quad \text{and} \quad \{\eta_j\} \perp \{\xi_j\} \perp \{V_0\}.$$

3DVAR: Fix the prediction covariance $\hat{C}_{j+1} := \hat{C}$ for all $j \geq 0$, and apply variational principle

$$\begin{aligned} \hat{m}_{j+1} &= \Psi(m_j) \\ \mathsf{J}(u) &:= \frac{1}{2}|y_{j+1} - Hu|_{\Gamma}^2 + \frac{1}{2}|u - \hat{m}_{j+1}|_{\hat{C}}^2 \\ m_{j+1} &= \arg\min_{u \in \mathbb{R}^d} \mathsf{J}(u). \end{aligned} \tag{6}$$

3DVAR

Alternatively, we may write,

$$\begin{aligned} \hat{m}_{j+1} &= \Psi(m_j) \\ K &= \hat{C}H^T(H\hat{C}H^T + \Gamma)^{-1} \\ m_{j+1} &= (I - KH)\hat{m}_{j+1} + Ky_{j+1} \end{aligned} \tag{7}$$

Properties:

- The gain K is time-independent!
- 3D – model physical space is typically three dimensional (v_n being a discretized representation of the state over 3D physical space, e.g. pressure, temperature, wind direction).
- VAR – method is derived from variational principle over 3D physical space.
- In numerical weather prediction, typcially $d \geq 10^6$, and "sparsification" from the true $\hat{C}_j$ to $\hat{C}$ is needed to construct a feasible filtering method.
- Gaussian approximation: $V_{j+1}|Y_{1:j} = y_{1:j} \sim N(\hat{m}_{j+1}, \hat{C})$ and $V_{j+1}|Y_{1:j+1} = y_{1:j+1} \sim N(m_{j+1}, (I - KH)\hat{C})$, with poor tracking of the covariance.

Example

Dynamics:

$$\begin{aligned} V_{j+1} &= 2.5\sin(V_j) + \xi_j \\ V_0 &\sim N(0,1) \end{aligned} \tag{8}$$

where $\xi_j \sim N(0, 0.09)$

Observations:

$$Y_j = V_j + \eta_j, \quad j = 1, 2, \ldots,$$

with $\eta_j \sim N(0,1)$.

3DVAR: We have that $\Psi(v) = 2.5\sin(v)$, $H = 1$ and $\Gamma = 1$.

1. Fix $\hat{C} = 2$, for example, and off-line/pre compute

$$K = \hat{C}H^T(H\hat{C}H^T + \Gamma)^{-1} = \frac{2}{3}.$$

2. iterate $m_j \mapsto m_{j+1}$.

A guess for $\hat{C}$ may be motivated from Kalman filtering:

$$\hat{C}_{j+1} = A^T C_j A + \Sigma = A^T(I - KH)\hat{C}_j A + \Sigma, \quad AA^T \approx |\Psi'(v)|^2 \approx 1.25?$$

Test

for one observation sequence $y_{1:J} = v^{\dagger}_{1:J} + \eta_{1:J}$ generated from synthetic data $v^{\dagger}_{1:J}$.

Error measure: MSE approximating the "truth" for different values of $\hat{C}$.

$$\frac{1}{J+1}\sum_{k=0}^{J} |v_k^{\dagger} - m_k|^2$$

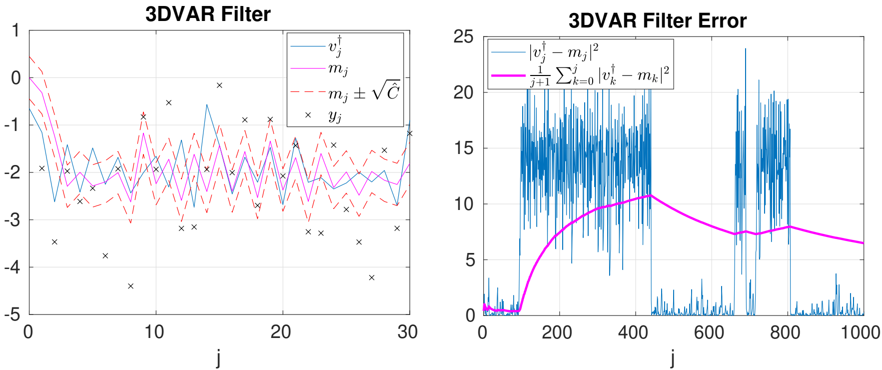
Implementation: The 3DVAR iteration

$$\begin{aligned} K &= \hat{C}H^T(H\hat{C}H^T + \Gamma)^{-1} \\ \hat{m}_{j+1} &= \Psi(m_j) \\ m_{j+1} &= (I - KH)\hat{m}_{j+1} + Ky_{j+1} \end{aligned} \tag{9}$$

becomes

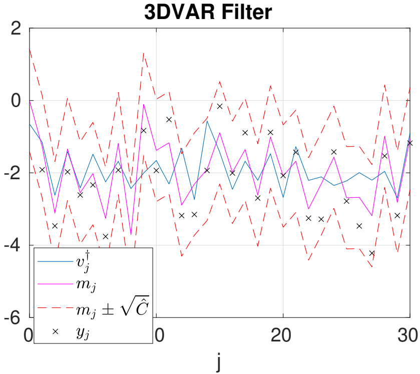
```
K=(cHat*H')/(H*cHat*H'+gamma^2);
for j=1:J
    mHat=2.5*sin(m(j));   m(j+1)=(1 - K*H)*mHat+K*y(j+1);
end
```

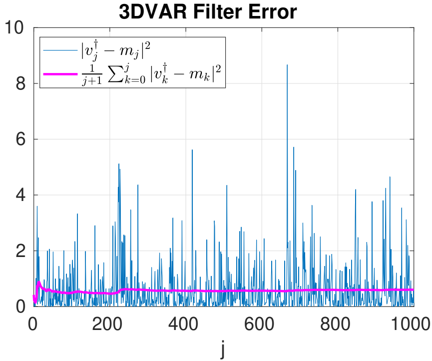
Test with $\hat{C} = 0.2$



$$\frac{1}{J+1}\sum_{k=0}^{J}|v_k^\dagger - m_k|^2 \approx 6.4866$$

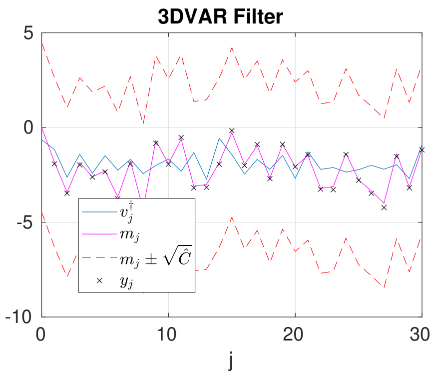
Numerical test, $\hat{C} = 2$

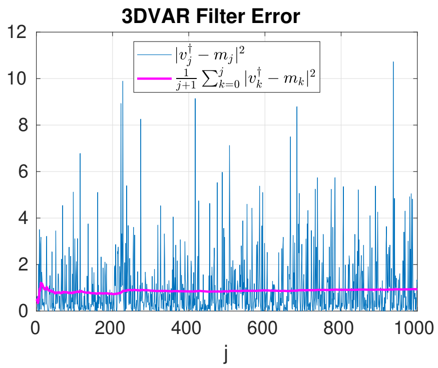




$$\frac{1}{J+1}\sum_{k=0}^{J}|v_k^\dagger - m_k|^2 \approx 0.6023$$

Test with $\hat{C} = 20$





$$\frac{1}{J+1}\sum_{k=0}^{J} |v_k^\dagger - m_k|^2 \approx 0.9373$$

Illustration of high dimensional filtering problem

Weather prediction[1]: for $(t, x) \in [0, T] \times \mathbb{R}^3$,

$$\frac{d\mathbf{v}}{dt} = -\alpha\nabla p - \nabla\phi + \mathbf{F} - 2\Omega \times \mathbf{v} \qquad \text{Cons. momentum}$$

$$\frac{\partial \rho}{\partial t} = -\nabla \cdot (\rho\mathbf{v}) \qquad \text{Cons. mass}$$

$$p/\rho = RT \qquad \text{Eq. of state}$$

$$Q = C_p \frac{dT}{dt} - \rho^{-1}\frac{dp}{dt} \qquad \text{Cons. energy}$$

$$\frac{\partial \rho q}{\partial t} = -\nabla \cdot (\rho\mathbf{v}q) + \rho(E - C) \qquad \text{Cons. water vapor mixing ratio}$$

$\mathbf{v}(t, x)$ - wind velocity field, $\rho(t, x)$ - air density, p - pressure, T - temperature, q - vapor mixing ratio.

Observations:

$$Y(t_{n+1}) = h(v, \rho, p, T, q)(t_{n+1}) + \eta_{n+1}.$$

[1] E. Kalnay, Atmospheric data assimilation and applications.

Rough idea of numerical weather prediction

Introduce a mesh

$\mathcal{I} = \{(x_i, x_j, x_k) \in \mathbb{R}^3 \mid (x_i, x_j, x_k) \text{ is a point in (a subset of) the atmosphere}\}$

3DVAR prediction: Numerical solution of the weather model with filtering **conditional mean** $m_j \approx \mathbb{E}\left[\{(v, \rho, p, T, q)(t_j, x)\}_{x\in\mathcal{I}} \mid Y_{1:j} = y_{1:j}\right]$ as initial condition. That is,

$$m_j \overset{\bar{\Psi}(m_n)}{\mapsto} \hat{m}_{j+1} \approx \mathbb{E}\left[\{(v, \rho, p, T, q)(t_{j+1}, x)\}_{x\in\mathcal{I}} \mid Y_{1:j} = y_{1:j}\right].$$

Note: State-space dimension $d = |\mathcal{I}| \times 7$.

Analysis: Apply 3DVAR principle with a typically low-bandwith, fixed $\hat{C} \approx \mathrm{Cov}[\{(v, \rho, p, T, q)(t_{j+1}, x)\}_{\mathbf{x}\in\mathcal{I}} | Y_{1:j} = y_{1:j}]$,

$$m_{j+1} = (I - KH)\hat{m}_{j+1} + Ky_{j+1}.$$

Recovery of true signal by 3DVAR

Theorem 1 (LSZ 4.10)

Assume the true signal is given by

$$v_{j+1}^{\dagger} = \Psi(v_j^{\dagger})$$

and observations by

$$y_{j+1} = Hv_{j+1}^{\dagger} + \epsilon_{j+1}, \quad \textit{with} \sup_{j\geq 0} \|\epsilon_j\| \leq \epsilon.$$

If, for 3DVAR with any value of $m_0 \in \mathbb{R}^d$ and $\hat{C}$ is chosen such that it holds for all $u, v \in \mathbb{R}^d$ and some $a < 1$ that

$$\|(I - KH)\Psi(u) - (I - KH)\Psi(v)\| \leq a\|u - v\|,$$

then

$$\limsup_{j\geq 0} \|v_j^{\dagger} - m_j\| \leq \frac{\|K\|}{1 - a}\epsilon.$$

Proof idea:

Write

$$m_{j+1} = (I - KH)\Psi(m_j) + K\underbrace{\left(H\Psi(v_j^\dagger) + \epsilon_{j+1}\right)}_{y_{j+1}}$$

$$v_{j+1}^\dagger = (I - KH)\Psi(v_j^\dagger) + KH\Psi(v_j^\dagger).$$

Then for

$$\begin{aligned}
\|m_{j+1} - v_{j+1}^\dagger\| &\le \|(I - KH)\Psi(m_j) - (I - KH)\Psi(v_j^\dagger)\| + \|K\epsilon_{j+1}\| \\
&\le a\|m_j - v_j^\dagger\| + \|K\|\|\epsilon_{j+1}\| \\
&\le a\|m_j - v_j^\dagger\| + \|K\|\epsilon \\
&\le \ldots \le a^{j+1}\|m_0 - v_0^\dagger\| + \|K\|\epsilon\sum_{k=0}^{j} a^k
\end{aligned}$$

and $a^{j+1}\|m_0 - v_0^\dagger\| \to 0$ as $j \to \infty$.

Remarks on Theorem 1

- Note that the asymptotic tracking ability holds **regardless of the magnitude of** $\|m_0 - v_0^\dagger\|$ as long as $a < 1$.
- Not that interesting result if $H = I$, since if one were to choose the filtering approach of total reliance on observations: $m_j = y_j$, then one would anyway achieve

$$\|v_j^\dagger - m_j\| = \|\epsilon_j\| \leq \epsilon.$$

- Relevant in **partial observation** settings $H \in \mathbb{R}^{k \times d}$ with $k < d$. Then it shows that accurate observations of unstable components may lead to good tracking of the state of all components.
- (SST Theorem 9.2) extends result from deterministic upper bound on noise error $|\epsilon_j| < \epsilon$ to Gaussian random noise setting $y_j = Hv_j^\dagger + \epsilon_j$ with $\epsilon_j \sim N(0, \gamma^2 I)$, and

$$\limsup_{j \to \infty} \mathbb{E}\left[\, \|m_j - v_j^\dagger\| \right] \leq \frac{\|K\|}{1-a}\, \gamma,$$

Choice of $\hat{C}$ guided by the preceding result.

- 3DVAR applied to a filtering problem with fixed $H = I$ and $\Gamma = \gamma^2 I$, and $\hat{C} = \sigma^2 I$ with adjustable parameter σ^2 yields

$$K = \frac{\gamma^2}{\sigma^2 + \gamma^2} I \quad \text{and} \quad (I - KH)\Psi(v) = \frac{(\gamma/\sigma)^2}{1 + (\gamma/\sigma)^2} \Psi(v)$$

- Choosing σ^2 so large that

$$\frac{(\gamma/\sigma)^2}{1 + (\gamma/\sigma)^2} \|D\Psi(v)\| < 1 \quad \forall v \in \mathbb{R}^d$$

  will lead stability in the form Theorem 1 (when other assumptions hold).

- In the example with $\Psi(v) = 2.5 \sin(v)$ and $\gamma^2 = 1$,

$$\frac{(\gamma/\sigma)^2}{1 + (\gamma/\sigma)^2} \|D\Psi\|_\infty < 1 \iff \frac{2.5}{\sigma^2 + 1} < 1 \iff \sigma^2 > 1.5.$$

- Interpretation: model variance inflation of σ^2 may help ensure stability of tracking (effectively it means putting more trust on observations).

Tracking of truth under partial observations

Consider now **partial** observations $H = (I_k, 0)^T \in \mathbb{R}^{k\times d}$, fixed $\Gamma = \gamma^2 I_k$ and $\hat{C} = \sigma^2 I_d$. Then

$$I_d - KH = \begin{bmatrix} \frac{\eta^2}{1+\eta^2} I_k & 0 \\ 0 & I_{d-k} \end{bmatrix}$$

with $\eta = \gamma/\sigma$.

For a linear dynamics mapping $\Psi(u) = Lu$ with

$$D\Psi = L = \begin{bmatrix} b_1 I_k & 0 \\ 0 & b_2 I_{d-k} \end{bmatrix}$$

we obtain

$$(I_d - KH)D\Psi = \begin{bmatrix} \frac{b_1\eta^2}{1+\eta^2} I_k & 0 \\ 0 & b_2 I_{d-k} \end{bmatrix}$$

Conclusion: $\|(I_d - KH)D\Psi\| < 1$ is only possible to achieve when $|b_2| < 1$. (This is a stability condition in dynamics of unobserved components.) Whatever the magnitude of $|b_1|$, on the other hand, this can be controlled by appropriately inflating σ^2.

4DVAR

Is an extension of 3DVAR in the analyisis step applying the variational principle over both 3D space and **time** (i.e., allowing for measurements scattered also over a time window)

Given dynamics:

$$V_{j+1} = \Psi(V_j) + \xi_j,$$

with $\xi_j \overset{iid}{\sim} N(0, \Sigma)$ and observations $y_{1:J}$ as before,

w4DVAR weak constraint 4DVAR is for stochastic dynamics $\Sigma > 0$. Then assimilation is done over the time window $0 : J$ in one step:

$$m_{0:J} = \arg \min_{v_{0:J} \in \mathbb{R}^{d(J+1)}} \frac{1}{2}|v_0 - m_0|^2_{C_0} + \frac{1}{2}\sum_{j=0}^{J-1} |v_{j+1} - \Psi(v_j)|^2_{\Sigma} + \frac{1}{2}\sum_{j=1}^{J} |y_j - Hv_j|^2_{\Gamma}$$

If Ψ is bounded and continuous, then a minimizer $m_{0:J}$ exists and corresponds to a MAP estimator for the very same smoothing problem over the same time-window [SST 9.3].

4DVAR is for settings with deterministic dynamics, i.e., $\Sigma = 0$, when w4DVAR turns into a minimization problem

$$m_{0:J} = \arg\min_{v_{0:J}} \frac{1}{2}|v_0 - m_0|^2_{C_0} + \frac{1}{2}\sum_{j=1}^{J} |y_j - Hv_j|^2_{\Gamma}$$

subject to the strong constraint

$$v_{j+1} = \Psi(v_j), \quad j = 0, 1, \ldots, J-1.$$

Comparisons 4DVAR vs 3DVAR

- 4DVAR is a minimization problem in typically higher-dimensional space than 3DVAR
- Both methods originally developed for numerical weather prediction, with emphasis on an efficient method for high-dimensional state space analysis/update.
- We focus here on one, but there exist many hybrid versions of 3D/4DVAR combined with other filtering techniques for the prediction step, cf., E. Kalnay "Atmospheric modeling, data assimilation and predictability".

Overview

Filtering setting

Initial condition $V_0 \sim N(m_0, C_0)$ and for $j = 0, 1, \ldots$

$$\begin{aligned} V_{j+1} &= \Psi(V_j) + \xi_j, \\ Y_{j+1} &= HV_{j+1} + \eta_{j+1}, \end{aligned} \tag{10}$$

and Gaussian noise assumptions as before.

Extened Kalman filtering (ExKF): At time j and given state (m_j, C_j), linearize dynamics around m_j:

$$\Psi_L(v; m_j) := \Psi(m_j) + D\Psi(m_j)(v - m_j).$$

And apply Kalman filtering one prediction-update step to the linearized dynamics

$$V_{j+1} = \Psi(m_j) + D\Psi(m_j)(V_j - m_j) + \xi_j,$$

Extended Kalman filtering algorithm

Given any sequence $y_1, y_2, \dots$ and $V_j | Y_{1:j} = y_{1:j} \sim N(m_j, C_j)$,

Prediction step

$$\begin{aligned}\hat{m}_{j+1} &= \mathbb{E}\left[\, \Psi(m_j) + D\Psi(m_j)(V_j - m_j) + \xi_j | Y_{1:j} = y_{1:j}\right] \\ &= \Psi(m_j)\end{aligned}$$

$$\begin{aligned}\hat{C}_{j+1} &= \mathrm{Cov}[\Psi(m_j) + D\Psi(m_j)(V_j - m_j) + \xi_j | Y_{1:j} = y_{1:j}] \\ &= D\Psi(m_j) C_j D\Psi(m_j)^T + \Sigma\end{aligned}$$

Analysis step

$$\begin{aligned}K_{j+1} &= \hat{C}_{j+1} H^T (H \hat{C}_{j+1} H^T + \Gamma)^{-1} \\ m_{j+1} &= (I - K_{j+1} H)\hat{m}_{j+1} + K_{j+1} y_{j+1} \\ C_{j+1} &= (I - K_{j+1} H)\hat{C}_{j+1}\end{aligned}$$

Example

Dynamics:

$$
\begin{aligned}
V_{j+1} &= 2.5\sin(V_j) + \xi_j \\
V_0 &\sim N(0,1)
\end{aligned}
\tag{11}
$$

where $\xi_j \sim N(0, 0.09)$ **Observations:**

$$
Y_j = V_j + \eta_j, \quad j = 1, 2, \ldots,
$$

with $\eta_j \sim N(0, 1)$.

ExKF: linearized dynamics mapping becomes

$$
\Psi_L(v; m_j) = 2.5\sin(m_j) + 2.5\cos(m_j)(v - m_j),
$$

Starting with $(m_0, C_0) = (0, 1)$ apply linearized mapping $\Psi_L(v; 0)$ and Kalman filtering to transition $(m_0, C_0) \mapsto (m_1, C_1)$, apply linearized mapping $\Psi_L(v; m_1)$ to and KF to transition $(m_1, C_1) \mapsto (m_2, C_2)$ ...

Test

for one observation sequence $y_{1:J} = v^{\dagger}_{1:J} + \eta_{1:J}$ generated from synthetic data $v^{\dagger}_{1:J}$.

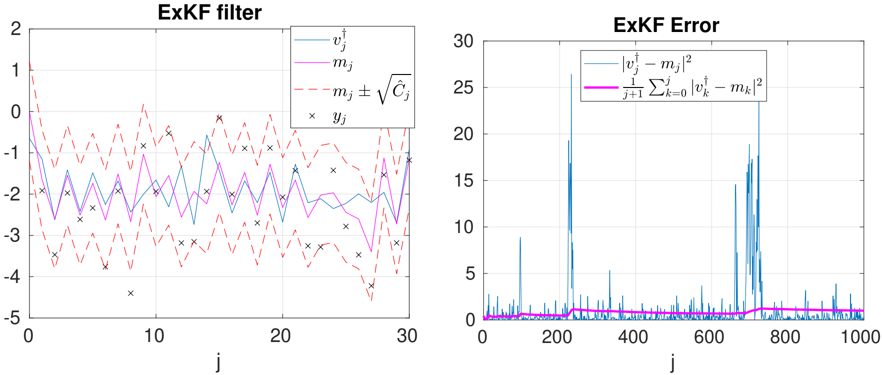
Implementation: The ExKF given m_j and C_j:

```
Psi  = @(v) 2.5*sin(v); %Dynamics mapping
DPsi = @(v) 2.5*cos(v); %Jacobian

for j=1:J

    %ExKF filtering
    mHat = Psi(m(j));
    cHat = DPsi(m(j))*C(j)*DPsi(m(j))' + Sigma;
    K      = (cHat*H')/(H*cHat*H'+Gamma);
    m(j+1) = (1-K*H)*mHat+K*y(j);
    C(j+1) = (1-K*H)*cHat;

end
```

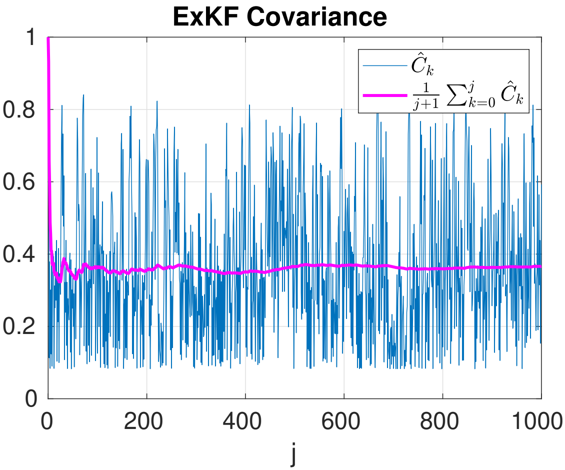


$$\frac{1}{1001}\sum_{k=0}^{1000}|v_k^\dagger - m_k|^2 \approx 0.9969 \quad \text{and} \quad \frac{1}{10001}\sum_{k=0}^{10000}|v_k^\dagger - m_k|^2 \approx 0.6169.$$

(MSE ≈ 0.9969 is not very impressive, this is roughly same error as one would get for

$$\frac{1}{J}\sum_{k=1}^{J}|v_k^\dagger - y_k|^2, \quad \text{since} \quad y_k = v_k^\dagger + \eta_k \text{ and } \eta_k \sim N(0,1).)$$

For comparison with the 3DVAR fixed prediction covariance $\hat{C}$, plot of evolution of $\hat{C}_j$ for ExKF:



Remarks on errors of ExKF and 3DVAR

- It generally does hold that

$$\mathbb{E}\left[\Psi(V)+\xi\right] = \Psi(\mathbb{E}\left[V\right]) \implies \hat{m}_j = \Psi(m_j) \overset{\text{in general}}{\neq} \mathbb{E}\left[\Psi(V_j) | Y_{1:j} = y_{1:j}\right].$$

- Nor does it generally hold that $V_j | Y_{1:j} = y_{1:j}$ is Gaussian when Ψ is nonlinear, and the analysis step, being derived under the assumption of Gaussian posterior

$$\pi(v_j|y_{1:j}) \propto \exp\Big(-\frac{1}{2}|y_{j+1} - Hv_{j+1}|_\Gamma^2 - \frac{1}{2}|v_{j+1} - \hat{m}_{j+1}|^2_{\hat{C}_{j+1}}\Big).$$

which, may only approximately hold, and the consecutive variational principle

$$m_{j+1} = \arg\min_{u\in\mathbb{R}^d} \frac{1}{2}|y_{j+1} - Hu|_\Gamma^2 + \frac{1}{2}|u - \hat{m}_{j+1}|^2_{\hat{C}_{j+1}}$$

is thus also only an approximation.

Overview

Ensemble Kalman filtering

We again consider the problem with $V_0 \sim N(m_0, C_0)$ and for $j = 0, 1, \ldots$

$$\begin{aligned} V_{j+1} &= \Psi(V_j) + \xi_j, \\ Y_{j+1} &= HV_{j+1} + \eta_{j+1}, \end{aligned} \tag{12}$$

and Gaussian noise assumptions as before.

EnKF initial condition is ensemble of iid "particles" $v_0^{(i)} \overset{iid}{\sim} \mathbb{P}_{V_0}$ for $i = 1, 2, \ldots, M$ and whose empirical measure approximates the true initial distribution:

$$\mathbb{P}_{V_0}(dv) \approx \frac{1}{M} \sum_{i=1}^{M} \delta_{v_0^{(i)}}(dv)$$

EnKF Prediction at time $j = 1$

To approximate the prediction $\mathbb{P}_{V_1}$, all particles are simulated one step ahead:

$$\hat{v}_1^{(i)} = \Psi(v_0^{(i)}) + \xi_1^{(i)}, \quad i = 1, 2, \ldots, M$$

where $\{\xi_j^{(i)}\}$ are iid $N(0, \Sigma)$-distributed and

$$\mathbb{P}_{V_1}(dv) \approx \frac{1}{M} \sum_{i=1}^{M} \delta_{\hat{v}_1^{(i)}}(dv).$$

Sample prediction mean and covariance

$$\hat{m}_1 := \frac{1}{M} \sum_{i=1}^{M} \hat{v}_1^{(i)}, \qquad \hat{C}_1 := \frac{1}{M-1} \sum_{i=1}^{M} (\hat{v}_1^{(i)} - \hat{m}_1)(\hat{v}_1^{(i)} - \hat{m}_1)^T.$$

EnKF analysis at time $j = 1$

- The Kalman gain is computed using the $\hat{C}_1$:

$$K_1 = \hat{C}_1 H^T (H \hat{C}_1 H^T + \Gamma)^{-1}$$

- and the observation y_1 is assimilated into each particle by

$$\left.\begin{aligned} y_1^{(i)} &= y_1 + \eta_1^{(i)} && \textbf{perturbed observations} \\ v_1^{(i)} &= (I - K_1 H)\hat{v}_1^{(i)} + K_1 y_1^{(i)} && \end{aligned}\right\} \quad \text{for } i = 1, 2, \ldots, M,$$

  with $\eta_j^{(i)} \overset{iid}{\sim} N(0, \Gamma)$.

- As before, the empirical measure of $\{v_1^{(i)}\}$ approximates $V_1 | Y_1 = y_1$:

$$\mathbb{P}_{V_1 | Y_1 = y_1}(dv) \approx \frac{1}{M} \sum_{i=1}^{M} \delta_{v_1^{(i)}}(dv)$$

Iterated EnKF formulas

Given any sequence $y_1, y_2, \ldots$ and the EnKF updated ensemble at time $\{v_j^{(i)}\}_{i=1}^M$ the transition $\{v_j^{(i)}\}_{i=1}^M \mapsto \{v_{j+1}^{(i)}\}_{i=1}^M$ is described by

Prediction step

$$\hat{v}_{j+1}^{(i)} = \Psi(v_j^{(i)}) + \xi_j^{(i)}, \quad i = 1, 2, \ldots, M$$

$$\hat{C}_{j+1} = \frac{1}{M-1} \sum_{i=1}^{M} (\hat{v}_{j+1}^{(i)} - \hat{m}_{j+1})(\hat{v}_{j+1}^{(i)} - \hat{m}_{j+1})^T \qquad \hat{m}_{j+1} = \frac{1}{M} \sum_{i=1}^{M} \hat{v}_{j+1}^{(i)}$$

Analysis step

$$K_{j+1} = \hat{C}_{j+1} H^T (H \hat{C}_{j+1} H^T + \Gamma)^{-1}$$

and

$$\left.\begin{aligned} y_{j+1}^{(i)} &= y_{j+1} + \eta_{j+1}^{(i)} \\ v_{j+1}^{(i)} &= (I - K_{j+1} H) \hat{v}_{j+1}^{(i)} + K_{j+1} y_{j+1}^{(i)} \end{aligned}\right\} \quad \text{for } i = 1, 2, \ldots, M,$$

Comments

- In settings when $\hat{C}_j$ is non-singular, the analysis step can be viewed as the variational principle

$$v_j^{(i)} := \arg\min_{u \in \mathbb{R}^d} \frac{1}{2}|y_j^{(i)} - Hu|_\Gamma^2 + \frac{1}{2}|u - \hat{m}_j|_{\hat{C}_j}^2$$

  (see [SST Chp 9] for an extension of this argument when $\hat{C}_j$ is singular).

- A random perturbation $\eta_j^{(i)}$ is added to the observation in the analysis step for each particle for the purpose of consistency: in the setting with linear dynamics $\Psi(v) = Av$,

$$\lim_{M\to\infty} \mathbb{E}\left[\hat{C}_j^{EnKF}\right] \begin{cases} < \hat{C}_j^{Kalman} & \text{without perturbed obs} \\ = \hat{C}_j^{Kalman} & \text{with perturbed obs} \end{cases}$$

- It can be shown that $v_{j+1}^{(i)} \in \mathrm{Span}(\{\hat{v}_{j+1}^{(i)}\}_{i=1}^M)$.

Comments

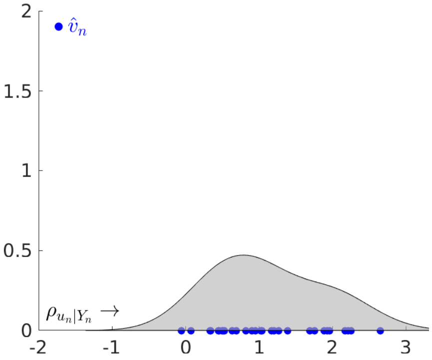
- The EnKF empirical measure is of course an approximation of but the method has obvious advantages over other in terms of feasibility and storage.

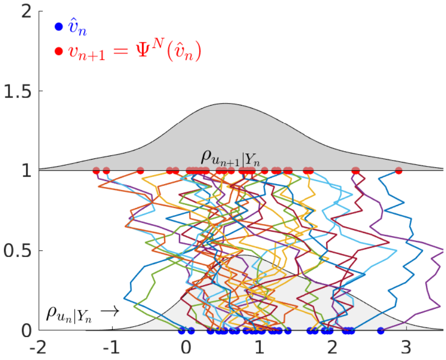
- Storage: EnKF needs to store $\mathcal{O}(M \times d)$ values, while for the Kalman filter it is $\mathcal{O}(d \times d)$ values. If "true" dimension of problem is much smaller than d, then EnKF is often successful in tracking the truth at a lower cost.

- It is more directly applicable to nonlinear problems than ExKF, and better at handling nonlinearities than both ExKF and 3DVAR.

Animated idea of EnKF

(With, at odds with the notation used in this lecture $\hat{v}_j$ here is the analysis/updated state and v_j the prediction state at time j, and Y_j is shorthand for $Y_{1:j} = y_{1:j}$.)





Animated idea of EnKF

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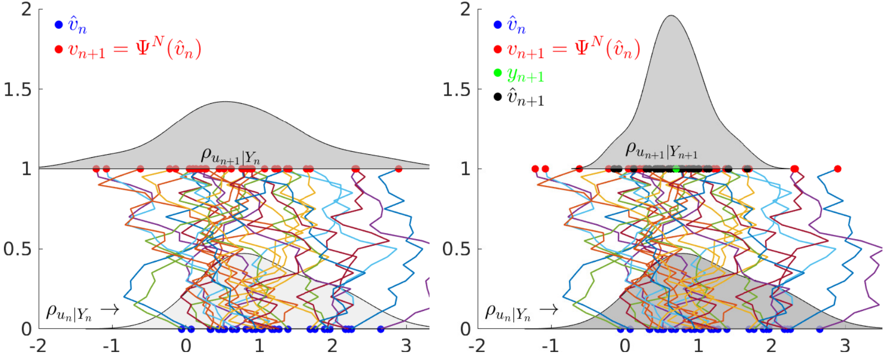
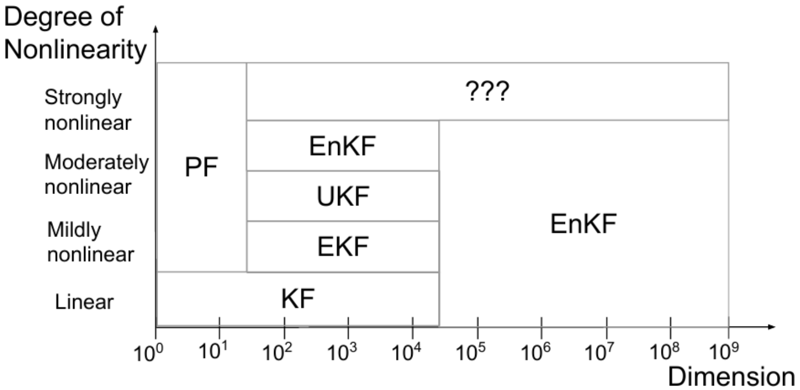


Best filtering method measured in terms of accuracy and efficiency



KF = Kalman filter; PF = particle filter; EKF = extended KF;
UKF = unscented KF; EnKF = ensemble KF

Figure from talk by Mattias Katzfuss on "Extended ensemble Kalman filters for high-dimensional hierarchical state-space models".

Plan for next lecture

- Implementation and convergence properties of EnKF in large ensemble limit.
- Particle filtering.