Applied Math Reading Seminar

Data Assimilation II

Columbia University
in the City of New York

March 27, 2023

Notation

- $\mathbb{Z}^+ = \mathbb{N}_0 = \{0, 1, 2, \dots\}$
- $|\cdot|$ **Euclidean**
- For symmetric, positive definite A
  - $\langle \cdot, \cdot \rangle_A := \langle \cdot, A^{-1} \cdot \rangle$
  - $|\cdot|_A^2 := \langle \cdot, \cdot \rangle_A$

Recap

State Space Model

$$
\begin{aligned}
\text{Dynamics models:} \quad & v_{j+1} = \Psi(v_j) + \xi_j,\ j \in \mathbb{Z}^+ \\
\text{Data Model:} \quad & y_{j+1} = h(v_{j+1}) + \eta_{j+1},\ j \in \mathbb{Z}^+ \\
\text{Probabilistic Structure:} \quad & v_0 \sim \mathcal{N}(m_0, C_0),\ \xi_j \sim \mathcal{N}(0, \Sigma),\ \eta_j \sim \mathcal{N}(0, \Gamma) \text{ i.i.d.} \\
\text{Probabilistic Structure:} \quad & v_0 \perp \{\xi_j\} \perp \{\eta_j\}
\end{aligned}
$$

Assume C_0, Σ, Γ are positive definite, $\Psi \in C(\mathbb{R}^d, \mathbb{R}^d)$,and $h \in C(\mathbb{R}^d, \mathbb{R}^k)$.

$$
V := \{v_0, \ldots, v_J\},\ Y := \{y_1, \ldots, y_J\},\ Y_j := \{y_1, \ldots, y_j\}
$$

$$
\begin{aligned}
\textbf{Smoothing Problem}: \quad & \Pi(V) := \mathbb{P}(V \mid Y) \\
\textbf{Filtering Problem}: \quad & \pi_j(v_j) := \mathbb{P}(v_j \mid Y_j),\ j = 1, 2, \ldots, J
\end{aligned}
$$

Recap - Kalman Filter

$$\pi_j(v_j) := \mathbb{P}(v_j \mid Y_j) \quad j = 1, 2, \ldots, J$$

Prediction Step : $\hat{\pi}_{j+1} = \mathcal{P}\pi_j = \mathbb{P}(v_{j+1} \mid Y_j)$

Analysis Step: $\pi_{j+1} = \mathcal{A}_j \widehat{\pi}_{j+1}$

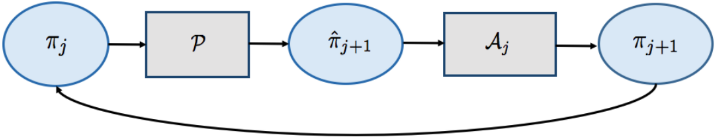

Figure 7.1 Prediction and analysis steps combined.

Summary of Methods

Kalman Filter	$\Psi(\cdot) = M\cdot$	$h(\cdot) = H\ \cdot$	Chapter 8
3DVAR (online)	General Ψ	$h(\cdot) = H\cdot$	Chapter 9
4DVAR (offline)	General Ψ	$h(\cdot) = H\cdot$	Chapter 9
ExKF	General Ψ	$h(\cdot) = H\cdot$	Chapter 10
EnKF	General Ψ	$h(\cdot) = H\cdot$	Chapter 10
EAKF	General Ψ	$h(\cdot) = H\cdot$	Anderson (2001)

Summary of Methods

Kalman Filter	**3DVAR**	**EnKF**
$m_{j+1} = \arg\min_v J(v)$	$m_{j+1} = \arg\min_v J(v)$	$v_{j+1}^{(n)} = \arg\min_v J_n(v)$
$J(v) = \frac{1}{2}\left\|y_{j+1} - Hv\right\|_\Gamma^2 + \frac{1}{2}\left\|v - \widehat{m}_{j+1}\right\|_{\widehat{C}_{j+1}}^2$	$J(v) = \frac{1}{2}\left\|y_{j+1} - Hv\right\|_\Gamma^2 + \frac{1}{2}\left\|v - \widehat{m}_{j+1}\right\|_{\widehat{C}}^2$	$J_n(v) = \frac{1}{2}\left\|y_{j+1}^{(n)} - Hv\right\|_\Gamma^2 + \frac{1}{2}\left\|v - \widehat{v}_{j+1}^{(n)}\right\|_{\widehat{C}_{j+1}^2}^2$
$\widehat{m}_{j+1} = Mm_j$	$\widehat{m}_{j+1} = \Psi\left(m_j\right)$	$\widehat{v}_{j+1}^{(n)} = \Psi\left(v_j^{(n)}\right) + \xi_j^{(n)}$
$\widehat{C}_{j+1}$ update exact	$\hat{C}$ no update	$\widehat{C}_{j+1}$ update by ensemble estimate
$m_{j+1} = (I - K_{j+1}H)\,\widehat{m}_{j+1} + K_{j+1}y_{j+1}$	$m_{j+1} = (I - KH)\widehat{m}_{j+1} + Ky_{j+1}$	$v_{j+1}^{(n)} = (I - K_{j+1}H)\,\widehat{v}_{j+1}^{(n)} + K_{j+1}y_{j+1}^{(n)}$

Kalman Filter (Linear-Gaussian Setting)

Linear dynamics and linear observations, $M \in \mathbb{R}^{d \times d}$, $H \in \mathbb{R}^{k \times d}$

State Space Model

Dynamics models: $v_{j+1} = Mv_j + \xi_j, \; j \in \mathbb{Z}^+$

Data Model: $y_{j+1} = Hv_{j+1} + \eta_{j+1}, \; j \in \mathbb{Z}^+$

Probabilistic Structure: $v_0 \sim \mathcal{N}(m_0, C_0), \xi_j \sim \mathcal{N}(0, \Sigma), \eta_j \sim \mathcal{N}(0, \Gamma)$ i.i.d.

Probabilistic Structure: $v_0 \perp \{\xi_j\} \perp \{\eta_j\}$

Kalman Filter

Algorithm 1: Kalman Filter Algorithm

Input: $\{y_j\}_{j=1}^{J}$, $\pi_0 = \mathcal{N}(m_0, C_0)$, Σ, Γ

Result: $\widehat{\pi}_{j+1} = \mathcal{N}\left(\widehat{m}_{j+1}, \widehat{C}_{j+1}\right)$ and $\pi_{j+1} = \mathcal{N}\left(m_{j+1}, C_{j+1}\right)$

for $j \leftarrow 0$ **to** $J-1$ **do**

Prediction:

$$\widehat{m}_{j+1} = Mm_j$$
$$\widehat{C}_{j+1} = MC_jM^\top + \Sigma$$

Analysis:

$$m_{j+1} = \widehat{m}_{j+1} + K_{j+1}d_{j+1}$$
$$C_{j+1} = (I - K_{j+1}H)\,\widehat{C}_{j+1}$$

where

$$d_{j+1} = y_{j+1} - H\widehat{m}_{j+1}$$
$$S_{j+1} = H\widehat{C}_{j+1}H^\top + \Gamma$$
$$K_{j+1} = \widehat{C}_{j+1}H^\top S_{j+1}^{-1}$$

end

3DVAR

State Space Model

Dynamics models:	$v_{j+1} = \Psi(v_j) + \xi_j,\ j \in \mathbb{Z}^+$
Data Model:	$y_{j+1} = H v_{j+1} + \eta_{j+1},\ j \in \mathbb{Z}^+$
Probabilistic Structure:	$v_0 \sim \mathcal{N}(m_0, C_0),\ \xi_j \sim \mathcal{N}(0, \Sigma),\ \eta_j \sim \mathcal{N}(0, \Gamma)$ i.i.d.
Probabilistic Structure:	$v_0 \perp \{\xi_j\} \perp \{\eta_j\}$

Uses a fixed predicted covariance $\hat{C}$ (independent of j). So the Kalman gain K is also fixed.

$$K = H\hat{C}H^\top S^{-1}$$

where

$$S = H\hat{C}H^\top + \Gamma.$$

EnKF

- $v_j \in \mathbb{R}^k$, $y_j \in \mathbb{R}^d$. $k, d \gg 1$
- Hard to store and invert $\hat{C}_{j+1}$
- Solve this by approximating posterior with ensemble

$$\pi_j^N(v_j) \approx \frac{1}{N} \sum_{n=1}^{N} \delta\left(v_j - v_j^{(n)}\right)$$

- Usually $N \ll k$
- Uses the empirical sample covariance for Kalman gain update

EnKF

Algorithm 2: EnKF

Input: Ensemble Size N. $\{y_j\}_{j=1}^{J}$. Initial ensemble $\{v_0^{(n)}\}$. Σ, Γ. $s \in \{0,1\}$.

Result: Ensembles $\{v_j^{(n)}\}_{n=1}^{N}, \quad j = 0, 1, \ldots, J$

for $j \leftarrow 0$ **to** $J-1$ **do**

Prediction:

$$\xi_j^{(n)} \sim \mathcal{N}(0, \Sigma), \quad \text{i.i.d.}, \quad n = 1, \ldots, N,$$
$$\widehat{v}_{j+1}^{(n)} = \Psi\left(v_j^{(n)}\right) + \xi_j^{(n)}, \quad n = 1, \ldots, N,$$
$$\widehat{m}_{j+1} = \frac{1}{N}\sum_{n=1}^{N} \widehat{v}_{j+1}^{(n)},$$
$$\widehat{C}_{j+1} = \frac{1}{N}\sum_{n=1}^{N} \left(\widehat{v}_{j+1}^{(n)} - \widehat{m}_{j+1}\right) \otimes \left(\widehat{v}_{j+1}^{(n)} - \widehat{m}_{j+1}\right).$$

Analysis:

$$\eta_{j+1}^{(n)} \sim \mathcal{N}(0, \Gamma), \quad n = 1, \ldots, N$$
$$y_{j+1}^{(n)} = y_{j+1} + s\eta_{j+1}^{(n)}, \quad n = 1, \ldots, N$$
$$v_{j+1}^{(n)} = (I - K_{j+1}H)\,\widehat{v}_{j+1}^{(n)} + K_{j+1}y_{j+1}^{(n)}, \quad n = 1, \ldots, N.$$

end

EnKF

Theorem 10.3 (Perturbed Observation EnKF — Randomized Likelihood Viewpoint)

Suppose that $\widehat{v}_{j+1}^{(n)} \sim \mathcal{N}\left(\widehat{m}_{j+1}, \widehat{C}_{j+1}\right)$ with $\widehat{C}_{j+1}$ positive definite. Let $v_{j+1}^{(n)}$ be the minimizer of

$$\mathrm{J}_n(v) := \frac{1}{2}\left|y_{j+1} + \eta_{j+1}^{(n)} - Hv\right|_{\Gamma}^{2} + \frac{1}{2}\left|v - \widehat{v}_{j+1}^{(n)}\right|_{\widehat{C}_{j+1}}^{2}, \quad \eta_{j+1}^{(n)} \sim \mathcal{N}(0, \Gamma)$$

where $\widehat{v}_{j+1}^{(n)}$ and $\eta_{j+1}^{(n)}$ are independent. Then $v_{j+1}^{(n)} \sim \mathcal{N}\left(m_{j+1}, C_{j+1}\right)$, where m_{j+1} and C_{j+1} are defined by

$$\begin{aligned} m_{j+1} &= \widehat{m}_{j+1} + K_{j+1}\left(y_{j+1} - H\widehat{m}_{j+1}\right) \\ C_{j+1} &= \left(I - K_{j+1}H\right)\widehat{C}_{j+1} \end{aligned}$$

and

$$K_{j+1} := \widehat{C}_{j+1}H^{\top}\left(H\widehat{C}_{j+1}H^{\top} + \Gamma\right)^{-1}$$

EnKF

Theorem 10.4 (Implementation of EnKF in N-Dimensional Subspace)

Given the prediction defined by,

$$\widehat{v}_{j+1}^{(n)} = \Psi\left(v_j^{(n)}\right) + \xi_j^{(n)}, \quad \widehat{m}_{j+1} = \frac{1}{N}\sum_{n=1}^{N} \widehat{v}_{j+1}^{(n)}, \quad \widehat{C}_{j+1} = \frac{1}{N}\sum_{n=1}^{N}\left(\widehat{v}_{j+1}^{(n)} - \widehat{m}_{j+1}\right) \otimes \left(\widehat{v}_{j+1}^{(n)} - \widehat{m}_{j+1}\right).$$

the Kalman update formula may be found by minimizing

$$\mathrm{F}_n(b) := \frac{1}{2}\left| y_{j+1}^{(n)} - H\widehat{v}_{j+1}^{(n)} - \frac{1}{N}\sum_{m=1}^{N} b_m H\left(\widehat{v}_{j+1}^{(n)} - \widehat{m}_{j+1}\right)\right|_\Gamma^2 + \frac{1}{2N}\sum_{m=1}^{N} b_m^2$$

with respect to b and substituting into $v = \widehat{v}_{j+1}^{(n)} + \frac{1}{N}\sum_{m=1}^{N} b_m \left(\widehat{v}_{j+1}^{(m)} - \widehat{m}_{j+1}\right)$.