Mathematics and numerics for data assimilation and state estimation – Lecture 21

Mathematics for Uncertainty Quantification

RWTH AACHEN UNIVERSITY

Summer semester 2020

Overview

1. Model error and model fitting
2. Kalman–Bucy filter
3. Continuous-time limit of discrete-time filtering
4. The Kushner–Stratonovich equation
5. Filtering in high/infinite-dimensional state space

Summary lecture 20

- Fokker-Planck equation, numerical integration of SDE and applications in filtering problems. Filtering methods for continuous-time dynamics and discrete-time observations.

- Plan for today: Model error and fitting. Filtering in continuous-time dynamics and observations, and filtering in high-dimensional state-space.

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Model uncertainty

Assume that we are given a sequence of observations $y_{1:J}$, or a collection of such sampled from

$$Y_j = h(V_j) + \eta_j.$$

The exact dynamics for V_j, which we denote Ψ, is unknown, but we can sample from a set of approximate dynamics $\{\Psi_\alpha\}_{\alpha \in \mathcal{M}o}$. That is

Unknown dyn: $V_{j+1} = \Psi(V_j)$, **known approx dyn** $V^\alpha_{j+1} = \Psi_\alpha(V^\alpha_j)$.

Question: given a collection $y_{1:J}$ and the true observation model, how can we estimate model errors to compare different models?

Strategy: Estimate error in the data space rather than in the state space.

Non-Bayesian approach

Assume the setting of exact observations

$$Y_j = h(V_j).$$

Given a collection of M_0 observation sequences $\{y_{1:J}^{(i)}\}_{i=1}^{M_O}$, we associate it to an empirical measure $\pi_{Y_{1:J}}(y_{1:J})$.

Computing the error for Ψ_α:

- Generate M_D path realizations of the dynamics $\{v_{1:J}^{\alpha,(i)}\}_{i=1}^{M_D}$.
- Associate each of these paths to observation sequences $y_{1:J}^{\alpha,(i)} = h(v_{1:J}^{\alpha,(i)})$.
- Approximate the error/divergence etc with the relevant error measure in the data space. For instance, root-mean-square error,

$$RMSE(\alpha) = \| Y_{1:J}^{\alpha} - \mathbb{E}[\, Y_{1:J}] \|_{L^2(\Omega)} \approx \sqrt{\frac{1}{M_D} \sum_{i=1}^{M_D} |y_{1:J}^{\alpha,(i)} - E_{M_O}[y_{1:J}^{(\cdot)}]|^2}$$

- Best model: $\alpha^* = \arg\min_{\alpha \in \mathcal{M}_O} RMSE(\alpha)$.

[See RC 4.4] for more on scoring rules.

Bayesian approach to model selection

Assume we are given one observation sequence $Y_{1:J} = y_{1:J}$ from the noisy observation model

$$Y_{1:J} = h(V_{1:J}) + \eta_{1:J}$$

where we assume the "truth" $v^\dagger_{1:J}$ that produced the observation was generated from a model Ψ_α for some $\alpha \in \mathcal{M}o$.

Bayesian framework:

1. Assign a prior pdf π_α to the model space.
2. and Bayesian inversion yields

$$\pi_{\alpha|Y_{1:J}}(\alpha|y_{1:J}) \propto \pi_{Y_{1:J}|\alpha}(y_{1:J}|\alpha)\pi_\alpha(\alpha)$$

3. Select model for instance by

$$\alpha^* = MAP(\pi_{\alpha|Y_{1:J}}(\cdot|y_{1:J}).$$

Problem: evaluating $\pi_{Y_{1:J}|\alpha}(y_{1:J}|\alpha)$ may not be straightforward.

Approximating the likelihood

Note that

$$\begin{aligned}
\pi_{Y_{1:J}|\alpha}(y_{1:J}|\alpha) &= \int \pi_{Y_{1:J},V_{1:J}|\alpha}(y_{1:J}, v_{1:J}|\alpha) dv_{1:J} \\
&= \int \pi_{Y_{1:J}|V_{1:J},\alpha}(y_{1:J}|v_{1:J}, \alpha) \pi_{V_{1:J}|\alpha}(v_{1:J}|\alpha) dv_{1:J} \\
&= \int \pi_{Y_{1:J}|V_{1:J}}(y_{1:J}|v_{1:J}) \pi_{V_{1:J}|\alpha}(v_{1:J}|\alpha) dv_{1:J}.
\end{aligned}$$

Hence, the likelihood can be approximated by the Monte Carlo method:

$$\pi_{Y_{1:J}|\alpha}(y_{1:J}|\alpha) \approx \sum_{i=1}^{M} \frac{\pi_{Y_{1:J}|V_{1:J}}(y_{1:J}|V_{1:J}^{\alpha,(i)})}{M}$$

where $V_{1:J}^{\alpha,(i)} \overset{iid}{\sim} \pi_{V_{1:J}|\alpha}(\cdot|\alpha)$.

Toy problem

Dynamics

$$V_{j+1} = \alpha V_j, \qquad V_0 = 1,$$

and with prior $\pi_\alpha(\alpha) = \mathbb{1}_{[-1,1]}(\alpha)$.

Observations

$$Y_{j+1} = V_{j+1} + \eta_{j+1}, \qquad \eta_j \overset{iid}{\sim} N(0,1),$$

and given obs sequence $y_j = (-1)^j$ for $j = 1, 2, \ldots, J$.

Since $V_j = \alpha^j$ (each α leads to a unique dynamics), we derive that

$$\pi_{\alpha|Y_{1:J}}(\alpha|y_{1:J}) \propto \pi_{Y_{1:J}|\alpha}(y_{1:J}|\alpha)\pi_\alpha(\alpha) \propto \mathbb{1}_{[-1,1]}(\alpha)\exp\left(-\frac{1}{2}\sum_{j=1}^{J}\left((-1)^j - \alpha^j\right)^2\right)$$

We conclude that

$$MAP\left(\pi_{\alpha|Y_{1:J}}(\cdot|y_{1:J})\right) = -1.$$

Model parameter estimation/selection through filtering

Consider the parameter dependent dynamics

$$V_{\tau_{j+1}} = \Psi_\alpha(V_{\tau_j})$$

and a sequence of observations

$$Y_{\tau_{j+1}} = h(V_{\tau_{j+1}}) + \eta_{j+1}$$

Filtering strategy to parameter estimation: Augment the state space with α. New dynamics $(V_{\tau_j}, \alpha_{\tau_j})$:

$$V_{\tau_{j+1}} = \Psi_{\alpha_{\tau_j}}(V_{\tau_j})$$
$$\alpha_{\tau_{j+1}} = \alpha_{\tau_j} + \nu_j$$

where ν_j is noise. (Adding noise may improve the exploration of possible α but, unless careful, it may also render the dynamics unstable!)

Can be implemented using for instance EnKF or particle filtering with the goal that $\alpha_{\tau_j} \to \alpha_{true}$. [See ubung 9].

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Continuous-time observations

We now shift to studying filtering problems with dynamics

$$dV_t = b(V_t)dt + \sigma(V_t)dW_t, \qquad t \geq 0$$

and **continuous-time observations**

$$Y_t = h(V_t) + \gamma(V_t)\dot{U}_t, \qquad t \geq 0,$$

where W and U are independent Wiener processes (and $\dot{U}$ is white noise: in this case, the formal derivative of a Wiener process).

For mathematical convenience (to go from white noise to Itô SDE), one rather consider the observation

$$Z_t = \int_0^t Y_s ds = \int_0^t h(V_s)ds + \int_0^t \gamma(V_s)\frac{dU_s}{\cancel{ds}}\cancel{ds}$$

or, equivalently,

$$dZ_t = h(V_t)dt + \gamma(V_t)dU_t, \qquad Z_0 = 0.$$

1D linear filtering problem

Dynamics

$$dV_t = LV_t dt + \sigma dW_t, \quad V_0 \sim N(m_0, C_0)$$

and observations

$$dZ_t = HV_t dt + \gamma dU_t, \quad Z_0 = 0,$$

with scalars H, L, σ, γ and $\gamma > 0$, and $\{W_t\} \perp \{U_t\} \perp V_0$.

Theorem 1 (1D Kalman-Bucy filter)

Both V_t and Z_t are Gaussian processes, and $V_t | Z_{[0,t]} = z_{[0,t]} \sim N(m_t, C_t)$ with

$$dm_t = \left(L - \frac{H^2 C_t}{\gamma^2}\right) m_t dt + \frac{HC_t}{\gamma^2} dz_t, \qquad m_0 = \mathbb{E}\left[V_0 \right],$$

and C_t solving the Riccati equation

$$\dot{C}_t = 2LC_t - \frac{H^2}{\gamma^2} C_t^2 + \sigma^2, \quad C_0 = \mathrm{Var}[V_0],$$

Remark: The result is typically presented as SDE for $\hat{V}_t = \mathbb{E}\left[V_t | Z_{[0,t]} \right]$.

Example [Oksendal 6.2.9]

Noisy observations of a constant process

$$dV_t = 0, \qquad V_0 \sim N(m_0, C_0)$$
$$dZ_t = V_t dt + \gamma dU_t, \quad Z_0 = 0,$$

Equations for moments in $V_t | Z_{[0,t]} = z_{[0,t]} \sim N(m_t, C_t)$:

$$dm_t = -\frac{C_t}{\gamma^2} m_t dt + \frac{HC_t}{\gamma^2} dz_t,$$

and

$$\dot{C}_t = -\frac{1}{\gamma^2} C_t^2 \implies C_t = \frac{C_0 \gamma^2}{\gamma^2 + C_0 t}$$

Plugging C_t into equation for m_t gives

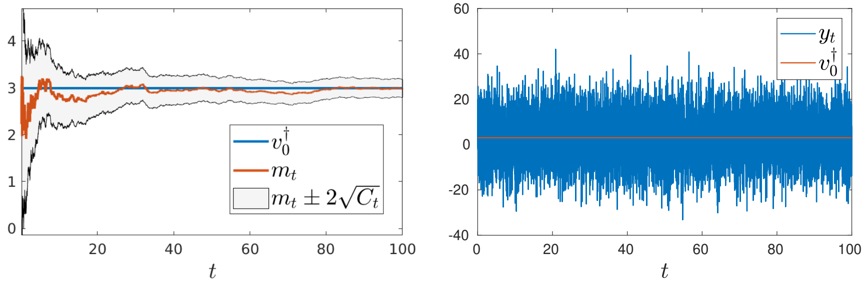
$$m_t = \frac{\gamma^2}{\gamma^2 + C_0 t} m_0 + \frac{C_0}{\gamma^2 + C_0 t} z_t$$

Hence $m_t \approx z_t / t$ for $t \gg 1$.

Illustration

With $\gamma = 1$, $V_0 \sim N(m_0 = 1, C_0 = 4)$ and $v_0^\dagger = 3$ and

$$z_t = v_0^\dagger t + u_t^\dagger, \qquad \text{(and numerical approx of)} \quad y_t = \dot{z}_t$$



Example [Oksendal 6.2.10]

Noisy observation of a Wiener process

$$\begin{aligned} dV_t &= dW_t, \qquad V_0 \sim N(m_0 = 0, C_0 = 0) \\ dZ_t &= V_t dt + dU_t, \qquad Z_0 = 0 \end{aligned}$$

Yields that $V_t | Z_{[0,t]} = z_{[0,t]} \sim N(m_t, C_t)$ where

$$\frac{dC_t}{\sigma^2 - C_t^2} = dt \implies C_t = \frac{\exp(2t) - 1}{\exp(2t) + 1} = \tanh(t),$$

and

$$m_t = \frac{1}{e^t + e^{-t}} \int_0^t \left(e^s - e^{-s} \right) dz_s$$

Observation: the conditional mean weights recent observations more than the distant past:

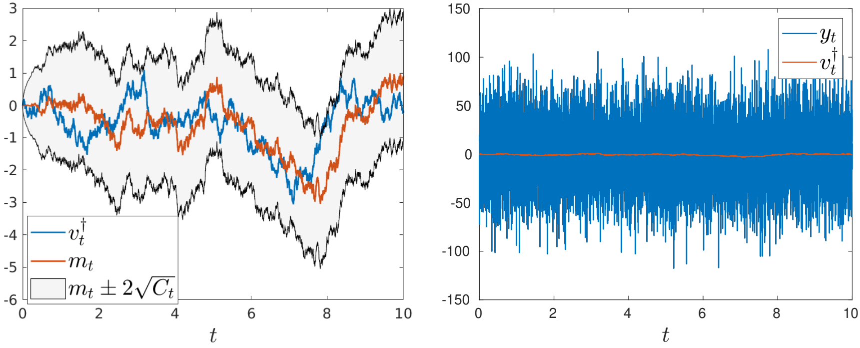
$$m_t \approx \int_0^t \frac{e^s}{e^t} dz_s = \int_0^t \frac{e^s}{e^t} y_s ds$$

for $t \gg 1$, recalling that $z_t = \int_0^t y_s ds$.

Illustration

Numerical approximations of

$$z_t = \int_0^t v_s^\dagger ds + u_t^\dagger, \qquad \text{and} \quad y_t = \dot{z}_t$$



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From discrete to continuous time

The continuous-time filtering problem

$$dV_t = b(V_t)dt + \sqrt{\Sigma_0}dW_t$$
$$dZ_t = h(V_t) + \sqrt{\Gamma_0}dU_t$$

with positive definite Γ_0, Σ_0 can be formally derived as the continuous-time limit of

$$\begin{aligned} V_{\tau_{j+1}} &= V_{\tau_j} + b(V_{\tau_j})\Delta\tau + \sqrt{\Sigma}\xi_j \\ Y_{\tau_{j+1}} &= h(V_{\tau_{j+1}}) + \sqrt{\Gamma}\eta_j \end{aligned} \tag{1}$$

where ξ_j, η_k iid standard Gaussians.

First introduce the discrete primitive

$$\frac{Z_{\tau_{j+1}} - Z_{\tau_j}}{\Delta\tau} = Y_{\tau_{j+1}} \quad \text{(recalling that for continuous problem} \quad \dot{Z}_t = Y_t)$$

and the scaling

$$\Sigma = \Delta\tau\Sigma_0, \quad \Gamma = \frac{1}{\Delta\tau}\Gamma_0$$

Then

$$
\begin{aligned}
V_{\tau_{j+1}} - V_{\tau_j} &= b(V_{\tau_j})\Delta\tau + \sqrt{\Sigma_0 \Delta\tau}\,\xi_j \\
Z_{\tau_{j+1}} - Z_{\tau_j} &= h(V_{\tau_{j+1}})\Delta\tau + \Delta\tau\sqrt{\frac{\Gamma_0}{\Delta\tau}}\,\eta_j
\end{aligned}
$$

Recalling that

$$
W_{\tau_{j+1}} - W_{\tau_j} \sim N(0, \Delta\tau) \quad \text{and} \quad U_{\tau_{j+1}} - U_{\tau_j} \sim N(0, \Delta\tau),
$$

we rewrite

$$
\begin{aligned}
V_{\tau_{j+1}} - V_{\tau_j} &= b(V_{\tau_j})\Delta\tau + \sqrt{\Sigma_0}\,\Delta W_j \\
Z_{\tau_{j+1}} - Z_{\tau_j} &= h(V_{\tau_{j+1}})\Delta\tau + \sqrt{\Gamma_0}\,\Delta U_j
\end{aligned}
$$

and obtain in the limit $\Delta\tau \downarrow 0$,

$$
\begin{aligned}
dV_t &= b(V_t)dt + \sqrt{\Sigma_0}\,dW_t \\
dZ_t &= h(V_t)dt + \sqrt{\Gamma_0}\,dU_t
\end{aligned}
$$

A second look at the Kalman-Bucy filter

Theorem 2 (Multidimensional Kalman-Bucy filter [LSZ Thm 8.1])

Consider

$$dV_t = LV_t dt + \sqrt{\Sigma_0} dW_t, \qquad V_0 \sim N(m_0, C_0)$$
$$dZ_t = HV_t dt + \sqrt{\Gamma_0} dU_t, \qquad Z_0 = 0,$$

with $L, \Sigma_0 \in \mathbb{R}^{d\times d}$, $H \in \mathbb{R}^{k\times d}$ *and* $\Gamma_0 \in \mathbb{R}^{k\times k}$, *positive definite* Γ_0, Σ_0, *and independence* $\{W_t\} \perp \{U_t\} \perp V_0$.
Then V_t *and* Z_t *are Gaussian processes, and* $V_t | Z_{[0,t]} = z_{[0,t]} \sim N(m_t, C_t)$ *with*

$$dm_t = Lm_t dt + C_t H^T \Gamma_0^{-1}(dz_t - Hm_t dt), \qquad m_0 = \mathbb{E}\left[V_0 \right],$$

and (the matrix ODE)

$$\dot{C}_t = LC_t + C_t L + \Sigma_0 - C_t H^T \Gamma_0^{-1} HC_t, \qquad C_0 = \mathrm{Var}[V_0],$$

Sketch of proof

Let us look at the continuous-time limit of the Kalman filter

$$V_{\tau_{j+1}} - V_{\tau_j} = LV_{\tau_j}\Delta\tau + \sqrt{\Sigma_0\Delta\tau}\xi_j$$

$$\frac{Z_{\tau_{j+1}} - Z_{\tau_j}}{\Delta\tau} = HV_{\tau_{j+1}} + \sqrt{\frac{\Gamma_0}{\Delta\tau}}\eta_j$$

i.e., of

$$V_{\tau_{j+1}} = (I + L\Delta\tau)V_{\tau_j} + \sqrt{\Sigma_0\Delta\tau}\xi_j$$

$$Y_{\tau_{j+1}} = HV_{\tau_{j+1}} + \sqrt{\frac{\Gamma_0}{\Delta\tau}}\eta_j$$

With $V_{\tau_j}|Y_{\tau_{1:j}} = y_{\tau_{1:j}} \sim N(m_{\tau_j}, C_{\tau_j})$, Kalman filtering (with $A = (I + L\Delta\tau)$) yields the prediction

$$\hat{m}_{\tau_{j+1}} = (I + L\Delta\tau)m_{\tau_j} = m_{\tau_j} + Lm_{\tau_j}\Delta\tau$$

$$\begin{aligned}\hat{C}_{\tau_{j+1}} &= (I + L\Delta\tau)C_{\tau_j}(I + L\Delta\tau)^T + \Delta\tau\Sigma_0 \\ &= C_{\tau_j} + (LC_{\tau_j} + C_{\tau_j}L^T + \Sigma_0)\Delta\tau + o(\Delta\tau)\end{aligned}$$

And for the analysis

$$K = \hat{C}_{\tau_{j+1}} H^T (H \hat{C}_{\tau_{j+1}} H^T + \frac{\Gamma_0}{\Delta\tau})^{-1} = C_{\tau_j} H^T \Gamma_0^{-1} \Delta\tau + o(\Delta\tau)$$

and

$$y_{\tau_{j+1}} - H \hat{m}_{\tau_{j+1}} = y_{\tau_{j+1}} - H(m_{\tau_j} + L m_{\tau_j} \Delta\tau)$$

so that

$$\begin{aligned} m_{\tau_{j+1}} &= \hat{m}_{\tau_{j+1}} + K(y_{\tau_{j+1}} - H\hat{m}_{\tau_{j+1}}) \\ &= m_{\tau_j} + L m_{\tau_j} \Delta\tau + C_{\tau_j} H^T \Gamma_0^{-1} (y_{\tau_{j+1}} - H m_{\tau_j}) \Delta\tau + o(\Delta\tau). \end{aligned}$$

And, recalling that $\hat{C}_{\tau_{j+1}} = C_{\tau_j} + (L C_{\tau_j} + C_{\tau_j} L^T + \Sigma_0)\Delta\tau + o(\Delta\tau)$,

$$\begin{aligned} C_{\tau_{j+1}} &= (I - KH)\hat{C}_{\tau_{j+1}} \\ &= C_{\tau_j} + (L C_{\tau_j} + C_{\tau_j} L^T + \Sigma_0)\Delta\tau - C_{\tau_j} H^T \Gamma_0^{-1} H C_{\tau_j} \Delta\tau + o(\Delta\tau). \end{aligned}$$

Next, truncate $o(\Delta\tau)$ terms and rewrite as follows

Up to order $\Delta\tau$,

$$
\begin{aligned}
m_{\tau_{j+1}} - m_{\tau_j} &= Lm_{\tau_j}\Delta\tau + C_{\tau_j}H^T\Gamma_0^{-1}(y_{\tau_{j+1}} - Hm_{\tau_j})\Delta\tau \\
&= Lm_{\tau_j}\Delta\tau + C_{\tau_j}H^T\Gamma_0^{-1}(z_{\tau_{j+1}} - z_{\tau_j} - Hm_{\tau_j}\Delta\tau),
\end{aligned}
$$

where we used that $y_{\tau_{j+1}}\Delta\tau = z_{\tau_{j+1}} - z_{\tau_j}$, and

$$
C_{\tau_{j+1}} - C_{\tau_j} = (LC_{\tau_j} + C_{\tau_j}L^T + \Sigma_0)\Delta\tau - C_{\tau_j}H^T\Gamma_0^{-1}HC_{\tau_j}\Delta\tau.
$$

Taking the limit $\Delta\tau \downarrow 0$ leads to Kalman-Bucy equations:

$$
dm = Lmdt + CH^T\Gamma_0^{-1}(dz - Hmdt),
$$

and

$$
dC = \Big(LC + CL^T + \Sigma_0 - CH^T\Gamma_0^{-1}HC\Big)dt.
$$

Nonlinear filtering methods

For the nonlinear filtering problem

$$\begin{aligned} dV_t &= b(V_t)dt + \sqrt{\Sigma_0}dW_t \\ dZ_t &= HV_t + \sqrt{\Gamma_0}dU_t \end{aligned} \tag{2}$$

there exist, as in the discrete-time setting, approximate Gaussian filtering methods: 3DVAR, ExKF, EnKF, and (also non-Gaussian methods, e.g., particle filters) [LSZ Chapter 8.2].

Definition 3 (Continuous-time ExKF)

The distribution of $V_t | Z_{[0,t]} = z_{[0,t]}$ is approximated by $N(m_t, C_t)$ where

$$dm = b(m_t)dt + C_t H^T \Gamma_0^{-1}(dz_t - Hm_t dt), \qquad m_0 = \mathbb{E}\left[V_0 \right],$$

and

$$\dot{C}_t = Db(m_t)C_t + C_t(Db(m_t))^T + \Sigma_0 - C_t H^T \Gamma_0^{-1} H C_t, \qquad C_0 = \mathrm{Var}[V_0],$$

with Db denoting the Jacobian of $b : \mathbb{R}^d \to \mathbb{R}^d$.

Derivation of continuous-time ExKF:

- Apply ExKF on discrete-time approximation of (2),

$$\begin{aligned} V_{\tau_{j+1}} &= V_{\tau_j} + b(V_{\tau_j})\Delta\tau + \sqrt{\Sigma}\xi_j \\ Y_{\tau_{j+1}} &= h(V_{\tau_{j+1}}) + \sqrt{\Gamma}\eta_j \end{aligned} \tag{3}$$

  leading to a system of difference equations for m_{τ_j} and C_{τ_j}.

- Taking the continuous-time limit $\Delta\tau \downarrow 0$ leads to the ExKF system of differential equations for m and C, similarly as for Kalman-Bucy.

Example – Nonlinear filtering

Consider the following stochastic version of Lorenz 63

$$
\begin{aligned}
dv_1 &= \alpha(v_1 - v_2)dt + \sigma dW_1(t) \\
dv_2 &= -\Big(\alpha v_v + v_2 + v_1 v_3\Big)dt + \sigma dW_2(t) \\
dv_3 &= v_1 v_2 - b v_3 + b(r + \alpha) + \sigma dW_3(t)
\end{aligned}
\tag{4}
$$

with $\sigma = 2$ and standard coefficient values $(\alpha, b, r) = (10, 8/3, 28)$.

On compact form, with $v = (v_1, v_2, v_3)^T$ and $W = (W_1, W_2, W_3)$, we rewrite

$$dv = f(v)dt + \sigma dW.$$

Observations:

$$dz = Hvdt + \gamma dU, \qquad z(0) = 0,$$

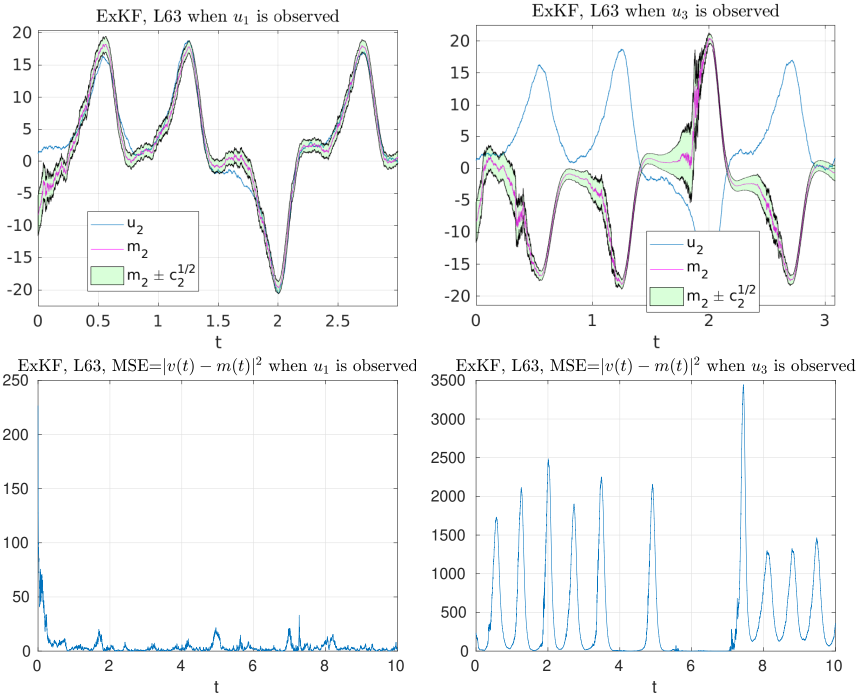
with either $H = (0, 0, 1)$ or $(1, 0, 0)$ and $\gamma = 1/2$.

Objective: "continuous-time" ExKF filtering with estimates of m_0 and C_0 given (in practice, fine-timestep numerical integration of associated discrete-time filtering problem).

Main steps in code (more details in [LSZ p16c.m])

```
%Initial data
m0=zeros(3,1); C0=eye(3);% prior initial condition covariance
v(:,1)=m0+sqrtm(C0)*randn(3,1);% initial truth
m(:,1)=10*randn(3,1);% initial mean/ESTIMATE
c(:,:,1)=10*C0;% initial covariance operator/ESTIMATE
H=[1,0,0];% observation operator
tau=1e-4;% time discretization is tau

%% solution % assimilate!
for j=1:J
    % truth
    v(:,j+1)=v(:,j)+tau*f(v(:,j))+sigma*sqrt(tau)*randn(3,1);
    z(:,j+1)=z(:,j)+tau*H*v(:,j+1) + gamma*sqrt(tau)*randn;% observa
    mhat=m(:,j)+tau*f(m(:,j));% estimator predict
    chat=(I+tau*Df(m(:,j)))*c(:,:,j)* ...
        (I+tau*Df(m(:,j)))'+sigma^2*tau*I;% covariance predict
    d=(z(j+1)-z(j))/tau-H*mhat;% innovation
    K=(tau*chat*H')/(H*chat*H'*tau+gamma^2);% Kalman gain
    m(:,j+1)=mhat+K*d;% estimator update
    c(:,:,j+1)=(I-K*H)*chat;% covariance update
end
```


ExKF, L63 when u_1 is observed
ExKF, L63 when u_3 is observed
ExKF, L63, MSE=$|v(t) - m(t)|^2$ when u_1 is observed
ExKF, L63, MSE=$|v(t) - m(t)|^2$ when u_3 is observed
u_2
m_2
$m_2 \pm c_2^{1/2}$
t

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In linear-Gaussian settings, the continuous-time filtering problem can be solved exactly.

Under sufficient regularity, we have the following extension to nonlinear settings:

Theorem 4 (Kushner–Stratonovich equation)

Consider the filtering problem

$$
\begin{aligned}
dV_t &= b(V_t)dt + \sqrt{\Sigma_0}dW_t, \quad V_0 \sim p(0,x) \\
dZ_t &= h(V_t)dt + \sqrt{\Gamma_0}dU_t, \quad Z_0 = 0.
\end{aligned}
$$

If b and h are sufficiently smooth, then there exists a pdf $p(t,x)$ for $V_t|Z_{[0,t]} = z_{[0,t]}$, and it is the solution of

$$
p_t(t,x) = \mathcal{L}^* p(t,x) + p(t,x)\left(h(x) - \int_{\mathbb{R}^d} h(y)p(t,y)dy\right)\Gamma_0^{-1}\left(\frac{dz}{dt} - \int_{\mathbb{R}^d} h(y)p(t,y)dy\right)
$$

over $(x,t) \in \mathbb{R}^d \times [0,T]$, and (cf. the Fokker-Planck equation)

$$
\mathcal{L}^* p(t,x) = -\nabla_x \cdot (b(x)p(t,x)) + \frac{1}{2}\sum_{i,j=1}^{d} \partial_{x_i x_j}(\Sigma_{0,ij}\, p(t,x)).
$$

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3 Continuous-time limit of discrete-time filtering

4 The Kushner–Stratonovich equation

5 Filtering in high/infinite-dimensional state space

Problem description

Filtering problem

$$\left.\begin{array}{ll} \text{Dynamics} & u_{\tau_{j+1}} = \Psi(u_{\tau_j}) \\ \text{Observations} & Y_{\tau_{j+1}} = Hu_{\tau_{j+1}} + \eta_{j+1} \end{array}\right\} \qquad j = 0, 1, \dots$$

With

- u_{τ_j} almost surely belongs to an infinite-dimensional Hilbert space $\mathcal{H}$, e.g., $u(\tau_j, \cdot) \in L^2(\mathbb{R})$.
- dynamics is possibly non-linear $\Psi : L^2(\Omega, \mathcal{H}) \to L^2(\Omega, \mathcal{H})$,
- linear operator $H : \mathcal{H} \to \mathbb{R}^k$.
- hence **finite-dimensional observations** y_{τ_j}, and $\eta_j \overset{iid}{\sim} N(0, \Gamma)$ with $\eta_j \perp \{u_{\tau_j}\}$, and $\Gamma \in \mathbb{R}^{k \times k}$.

Objective: Approximate pdf of $u_{\tau_j} | Y_{\tau_{1:j}} = y_{\tau_{1:j}}$.

Forward model approximation: $\Psi \approx \Psi^{N_t, N_x}$ with discretization both time and space. Something like $\Delta t = \Delta\tau / N_t$ and $\Delta x = \mathcal{O}(N_x^{-1})$.

Problem description

Filtering problem

$$\left.\begin{array}{ll}\text{Dynamics} & u_{\tau_{j+1}} = \Psi(u_{\tau_j}) \\ \text{Observations} & Y_{\tau_{j+1}} = H u_{\tau_{j+1}} + \eta_{j+1}\end{array}\right\} \qquad j = 0, 1, \ldots$$

With

- u_{τ_j} almost surely belongs to an infinite-dimensional Hilbert space $\mathcal{H}$, e.g., $u(\tau_j, \cdot) \in L^2(\mathbb{R})$.
- dynamics is possibly non-linear $\Psi : L^2(\Omega, \mathcal{H}) \to L^2(\Omega, \mathcal{H})$,
- linear operator $H : \mathcal{H} \to \mathbb{R}^k$.
- hence **finite-dimensional observations** y_{τ_j}, and $\eta_j \overset{iid}{\sim} N(0, \Gamma)$ with $\eta_j \perp \{u_{\tau_j}\}$, and $\Gamma \in \mathbb{R}^{k \times k}$.

Objective: Approximate pdf of $u_{\tau_j} | Y_{\tau_{1:j}} = y_{\tau_{1:j}}$.

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Numerical example, 1D SPDE

1D stochastic reaction-diffusion equation

$$\begin{aligned} \mathrm{d}u &= ((\Delta - I)u + f(u))\,\mathrm{d}t + \mathrm{d}W \qquad (t,x) \in [0,\infty) \times (0,1), \\ u(0,x) &= 4(x-1/2)^2 \\ u(t,0) &= u(t,1), \qquad \forall t \in [0,\infty). \end{aligned}$$

- operator A is spectral decomposition of $\Delta - I$

$$A = \sum_{j=1}^{\infty} \lambda_j \phi_j \otimes \phi_j, \quad \text{with} \quad \lambda_j \eqsim -j^2$$

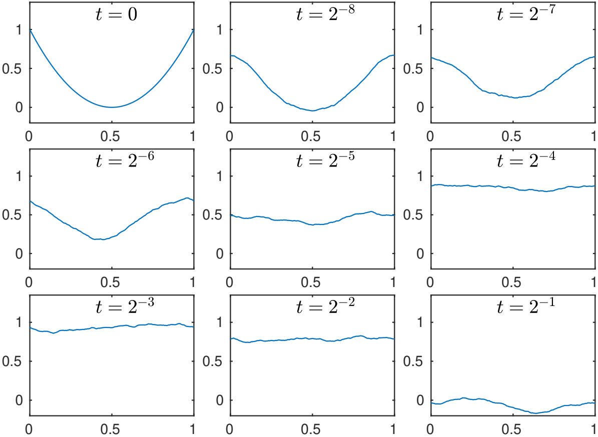
  where $\phi_j(x)$ are Fourier series functions $\{1, \sin(2\pi x), \cos(2\pi x), \ldots\}$.
- With space-time colored noise

$$W(t,x) = \sum_{j \in \mathbb{N}} j^{-1} W^{(j)}(t) \phi_j(x)$$

- consider mild solutions

$$u_{\tau_{j+1}} = \Psi(u_{\tau_j}) := e^{A\Delta\tau} u_{\tau_j} + \int_0^{\Delta\tau} e^{A(T-s)} f(u_{\tau_j+s}) ds + \int_0^{\Delta\tau} e^{A(t-s)} dW_{\tau_j+s}$$

Simulation of SPDE



Simulation of the SPDE with reaction term $f(u) = \sin(\pi u)$ over one observation-time interval $\Delta\tau = 1/2$, by Ψ^{N_t,N_x} with $N_x = N_t = 2^{12}$. See arxiv preprint A. Chernov et al. "Multilevel ensemble Kalman filtering for spatio-temporal processes" for more details.

EnKF filtering in high-dimensions

Approximate $\Psi \approx \Psi^{N_t,N_x}$, with elements $u_j \in \mathcal{H}^{N_x} \subset \mathcal{H}$ (let us here assume $\mathcal{H}^{N_x}$ is an N_x-dimensional state-space).

Sample iid $v_0^{(i)} \sim \text{Projection}_{\mathcal{H}^{N_x}} \mathbb{P}_{u_0}$ for $i = 1, 2, \ldots, M$ and (using the shorthand $v_j^{(i)} := v_{\tau_j}^{(i)}$ below)

Prediction

$$\hat{v}_{j+1}^{(i)} = \Psi^{N_t,N_x}(v_j^{(i)}), \quad i = 1, 2, \ldots, M, \qquad \text{and}$$

$$\hat{C}_{j+1} = \underbrace{\mathrm{Cov}_M[\hat{v}_{j+1}^{(\cdot)}]}_{\in \mathbb{R}^{N_x \times N_x}}, \quad \text{or rather} \quad \hat{C}_{j+1} H^* = \underbrace{\mathrm{Cov}_M[\hat{v}_{j+1}^{(\cdot)}, \hat{v}_{j+1}^{(\cdot)}]}_{\in \mathbb{R}^{N_x \times k}},$$

Analysis

$$v_{j+1}^{(i)} = \hat{v}_{j+1}^{(i)} + K(y_{j+1}^{(i)} - H\hat{v}_{j+1}^{(i)}), \quad \text{where} \quad K = \hat{C}_{j+1} H^* (H \hat{C}_{j+1} H^* + \Gamma)^{-1}.$$

Localization for EnKF

- When state-space dimension $N_x \gg 1$, the sample-covariance

$$\hat{C}_j^M = \mathrm{Cov}_M[\hat{v}_j^{(\cdot)}],$$

  tend to have "spurious correlations", meaning that for some ℓ, m

$$|\hat{C}_{j,\ell,m}^M - \hat{C}_{j,\ell,m}^\infty| \gg \hat{C}_{j,\ell,m}^\infty, \quad \text{with} \quad \hat{C}_j^\infty \text{ denoting the reference cov.}$$

- Not a problem that can be easily solved through increasing M, as there is a cost associated to that.
- Two diametrically opposite approaches for dealing with this (cf. Reich and Cotter chp 8.2-8.3)
  - **Variance inflation:** To increase the magnitude of components of $\hat{C}_{j,\ell,m}^M$ where you expect it to be underestimated, inflate for instance the model uncertainty.
  - **Covariance localization:** To reduce the magnitude of components of $\hat{C}_{j,\ell,m}^M$ where you expect it to be underestimated, do for instance

$$\text{spatial/spectral localiazation: } \textbf{replace} \quad \hat{C}_j^M \quad \textbf{by} \quad \rho \circ \hat{C}_j^M$$

    where $\circ$ is the element-wise product and $\rho_{\ell m} = \mathbb{1}_{|\ell - m| \leq n}$ is a banded filter matrix.

Summary

- Have treated filtering in the continuous-time dynamics and observations setting.
- The Kalman-Bucy filter solves the linear-Gaussian filtering problem, while the Kushner-Stratonovich equation applies more generally.
- Described extension of EnKF to filtering problems with high/infinite-dimensional state-space.
- Still unclear how well particle filtering can perform in high-dimensional filtering. The number of particles required to avoid degeneracy is conjectured to typically scale exponentially with state-space dimension.
- Next time: Presentations by Dmitry Kabanov on Ensemble Kalman Inversion applied to machine learning, and by Luis Espath on Bayesian optimal experimental design (relating to Bayesian inversion, studying what is the best observation model to use when one can chose among many).