EnKF and filter divergence

David Kelly Andrew Stuart Kody Law

Courant Institute
New York University
New York, NY

dtbkelly.com

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Talk outline

1. What is EnKF?

2. What is known about EnKF?

3. How can we use stochastic analysis to better understand EnKF?

The filtering problem

We have a **deterministic model**

$$\frac{dv}{dt} = F(v) \quad \text{with } v_0 \sim N(m_0, C_0)\ .$$

We will denote $v(t) = \Psi_t(v_0)$. Think of this as **very high dimensional** and **nonlinear**.

We want to **estimate** $v_j = v(jh)$ for some $h > 0$ and $j = 0, 1, \ldots, J$ given the **observations**

$$y_j = Hv_j + \xi_j \quad \text{for } \xi_j \text{ iid } N(0, \Gamma).$$

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Bayes' formula filtering update

Let $Y_j = \{y_0, y_1, \dots, y_j\}$. We want to compute the conditional density $\mathbf{P}(v_{j+1}|Y_{j+1})$, using $\mathbf{P}(v_j|Y_j)$ and y_{j+1}.

By Bayes' formula, we have

$$\mathbf{P}(v_{j+1}|Y_{j+1}) = \mathbf{P}(v_{j+1}|Y_j, y_{j+1}) \propto \mathbf{P}(y_{j+1}|v_{j+1})\mathbf{P}(v_{j+1}|Y_j)$$

But we need to compute the integral

$$\mathbf{P}(v_{j+1}|Y_j) = \int \mathbf{P}(v_{j+1}|Y_j, v_j)\mathbf{P}(v_j|Y_j)dv_j \; .$$

For high dimensional nonlinear systems, this is computationally infeasible.

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For linear models, one can draw samples, using the **Randomized Maximum Likelihood** method.

RML method

Let $u \sim N(\widehat{m}, \widehat{C})$ and $\eta \sim N(0, \Gamma)$. We make an observation

$$y = Hu + \eta \ .$$

We want the conditional distribution of $u|y$. This is called an **inverse problem**.

RML takes a sample

$$\{\widehat{u}^{(1)}, \ldots, \widehat{u}^{(K)}\} \sim N(\widehat{m}, \widehat{C})$$

and turns them into a sample

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RML method: How does it work?

Along with the prior sample $\{\widehat{u}^{(1)}, \ldots, \widehat{u}^{(K)}\}$, we create **artificial observations** $\{y^{(1)}, \ldots, y^{(K)}\}$ where

$$y^{(k)} = y + \eta^{(k)} \qquad \text{where } \eta^{(k)} \sim N(0, \Gamma) \text{ i.i.d}$$

Then define $u^{(k)}$ using the **Bayes formula** update, with $(\widehat{u}^{(k)}, y^{(k)})$

$$u^{(k)} = \widehat{u}^{(k)} + G(\widehat{u})(y^{(k)} - H\widehat{u}^{(k)}) .$$

Where the "Kalman Gain" $G(\widehat{u})$ is computing using the covariance of the prior $\widehat{u}$.

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EnKF uses the same method, but with an **approximation** of the covariance in the Kalman gain.

The set-up for EnKF

Suppose we are given the ensemble $\{u_j^{(1)}, \dots, u_j^{(K)}\}$ at time j. For each ensemble member, we create an **artificial observation**

$$y_{j+1}^{(k)} = y_{j+1} + \xi_{j+1}^{(k)} \quad , \quad \xi_{j+1}^{(k)} \text{ iid } N(0,\Gamma).$$

We update each particle using the **Kalman update**

$$u_{j+1}^{(k)} = \Psi_h(u_j^{(k)}) + G(u_j)\left(y_{j+1}^{(k)} - H\Psi_h(u_j^{(k)})\right) \,,$$

where $G(u_j)$ is the **Kalman gain** computed using the **forecasted ensemble covariance**

$$\widehat{C}_{j+1} = \frac{1}{K}\sum_{k=1}^{K}(\Psi_h(u_j^{(k)}) - \overline{\Psi_h(u_j)})^T(\Psi_h(u_j^{(k)}) - \overline{\Psi_h(u_j)}) \,.$$

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What do we know about EnKF?

Not much.

Theorem : For linear forecast models,
ENKF $\rightarrow$ KF as $N \rightarrow \infty$

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Ideally, we would like a theorem about **long time behaviour** of the filter for a finite ensemble size.

Filter divergence

In certain situations, it has been observed (⋆) that the ensemble can **blow-up** (ie. reach machine-infinity) in **finite time**, even when the model has nice bounded solutions.

This is known as **catastrophic filter divergence**.

We would like to investigate whether this has a **dynamical justification** or if it is simply a **numerical artefact**.

⋆ Harlim, Majda (2010), Gottwald (2011), Gottwald, Majda (2013).

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Assumptions on the dynamics

We make a **dissipativity** assumption on the model. Namely that

$$\frac{dv}{dt} + Av + B(v, v) = f$$

with A linear elliptic and B bilinear, satisfying certain estimates and symmetries.

This guarantees **uniformly bounded** solutions.

Eg. 2d-Navier-Stokes, Lorenz-63, Lorenz-96.

Discrete time results

For a fixed observation frequency $h > 0$ we can prove

Theorem (AS,DK,KL)

If $H = \Gamma = Id$ then there exists constant $\beta > 0$ such that

$$\mathbf{E}|u_j^{(k)}|^2 \leq e^{2\beta jh}\mathbf{E}|u_0^{(k)}|^2 + 2K\gamma^2 \left(\frac{e^{2\beta jh} - 1}{e^{2\beta h} - 1}\right)$$

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Discrete time results with variance inflation

Suppose we replace

$$\widehat{C}_{j+1} \mapsto \alpha^2 I + \widehat{C}_{j+1}$$

at each update step. This is known as **additive variance inflation**.

Theorem (AS,DK,KL)

If $H = Id$ and $\Gamma = \gamma^2 Id$ then there exists constant $\beta > 0$ such that

$$\mathbf{E}|e_j^{(k)}|^2 \leq \theta^j \mathbf{E}|e_0^{(k)}|^2 + 2K\gamma^2 \left(\frac{1-\theta^j}{1-\theta} \right)$$

where $\theta = \frac{\gamma^2 e^{2\beta h}}{\alpha^2 + \gamma^2}$. In particular, if we pick α large enough (so that $\theta < 1$) then

$$\lim_{j \to \infty} \mathbf{E}|e_j^{(k)}|^2 \leq \frac{2K\gamma^2}{1-\theta}$$

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For observations with $h \ll 1$, we need another approach.

The EnKF equations look like a discretization

Recall the ensemble update equation

$$u_{j+1}^{(k)} = \Psi_h(u_j^{(k)}) + G(u_j)\left(y_{j+1}^{(k)} - H\Psi_h(u_j^{(k)})\right)$$
$$= \Psi_h(u_j^{(k)}) + \widehat{C}_{j+1}H^T(H^T\widehat{C}_{j+1}H + \Gamma)^{-1}\left(y_{j+1}^{(k)} - H\Psi_h(u_j^{(k)})\right)$$

Subtract $u_j^{(k)}$ from both sides and divide by h

$$\frac{u_{j+1}^{(k)} - u_j^{(k)}}{h} = \frac{\Psi_h(u_j^{(k)}) - u_j^{(k)}}{h} + \widehat{C}_{j+1}H^T(hH^T\widehat{C}_{j+1}H + h\Gamma)^{-1}\left(y_{j+1}^{(k)} - H\Psi_h(u_j^{(k)})\right)$$

Clearly we need to rescale the noise (ie. Γ).

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Continuous-time limit

If we set $\Gamma = h^{-1}\Gamma_0$ and substitute $y_{j+1}^{(k)}$, we obtain

$$\frac{u_{j+1}^{(k)} - u_j^{(k)}}{h} = \frac{\Psi_h(u_j^{(k)}) - u_j^{(k)}}{h} + \widehat{C}_{j+1} H^T (h H^T \widehat{C}_{j+1} H + \Gamma_0)^{-1}$$
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But we know that

$$\Psi_h(u_j^{(k)}) = u_j^{(k)} + O(h)$$

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We end up with

$$\frac{u_{j+1}^{(k)} - u_j^{(k)}}{h} = \frac{\Psi_h(u_j^{(k)}) - u_j^{(k)}}{h} - C(u_j)H^T\Gamma_0^{-1}H(u_j^{(k)} - v_j) + C(u_j)H^T\Gamma_0^{-1}\left(h^{-1/2}\xi_{j+1} + h^{-1/2}\xi_{j+1}^{(k)}\right) + O(h)$$

This looks like a **numerical scheme** for **Itô S(P)DE**

$$\frac{du^{(k)}}{dt} = F(u^{(k)}) - C(u)H^T\Gamma_0^{-1}H(u^{(k)} - v) + C(u)H^T\Gamma_0^{-1/2}\left(\frac{dB}{dt} + \frac{dW^{(k)}}{dt}\right). \qquad (\bullet)$$

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Kalman-Bucy limit

If F were **linear** and we write $m(t) = \frac{1}{K}\sum_{k=1}^{K} u^{(k)}(t)$ then

$$\frac{dm}{dt} = F(m) - C(u)H^T\Gamma_0^{-1}H(m - v) + C(u)H^T\Gamma_0^{-1/2}\frac{dB}{dt} + O(K^{-1/2}) \,.$$

This is the equation for the **Kalman-Bucy** filter, with empirical covariance $C(u)$. The remainder $O(K^{-1/2})$ can be thought of as a **sampling error**.

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Continuous-time results

Theorem (AS,DK)

Suppose that $\{u^{(k)}\}_{k=1}^{K}$ *satisfy* ($\bullet$) *with* $H = \Gamma = Id$. *Let*

$$e^{(k)} = u^{(k)} - v \ .$$

Then there exists constant $\beta > 0$ *such that*

$$\frac{1}{K}\sum_{k=1}^{K}\mathbf{E}|e^{(k)}(t)|^2 \leq \left(\frac{1}{K}\sum_{k=1}^{K}\mathbf{E}|e^{(k)}(0)|^2\right)\exp\left(\beta t\right) \ .$$

Why do we need $H = \Gamma = Id$?

In the equation

$$\frac{du^{(k)}}{dt} = F(u^{(k)}) - C(u)H^T\Gamma_0^{-1}H(u^{(k)} - v) + C(u)H^T\Gamma_0^{-1/2}\left(\frac{dW^{(k)}}{dt} + \frac{dB}{dt}\right) .$$

The **energy** pumped in by the noise must be balanced by **contraction** of $(u^{(k)} - v)$. So the operator

$$C(u)H^T\Gamma_0^{-1}H$$

must be **positive-definite**.

Both $C(u)$ and $H^T\Gamma_0^{-1}H$ are pos-def, but this doesn't guarantee the same for the **product**!

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Testing stability on the fly

Suppose we can actually measure the spectrum of the operator

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whilst the algorithm is running. If we know that it is pos-def, then the filter must not be blowing up.

If we knew that

$$C(u)H^T\Gamma_0^{-1}H \geq \lambda(t) > 0 \ .$$

Then we can say even more (eg. stability).

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Summary + Future Work

(1) Writing down an SDE/SPDE allows us to see the **important quantities** in the algorithm.

(2) Does not "prove" that catastrophic filter divergence is a numerical phenomenon, but is a decent starting point.

(1) Improve the condition on H.

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(3) Make use of **controllability** and **observability**.

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Thank you!

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D. Kelly, K.Law, A. Stuart.

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