Learning the number of particles in nested filtering

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Joint work with Joaquín Míguez (Universidad Carlos III de Madrid) and Víctor Elvira (University of Edinburgh).

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State-space model

We are interested in systems can be represented by **Markov state-space dynamical models**:

$$\begin{aligned} \boldsymbol{x}_t &= \boldsymbol{f}(\boldsymbol{x}_{t-1}, \boldsymbol{\theta}) + \boldsymbol{v}_t, \\ \boldsymbol{y}_t &= \boldsymbol{g}(\boldsymbol{x}_t, \boldsymbol{\theta}) + \boldsymbol{r}_t, \end{aligned}$$

- $\boldsymbol{f}$, $\boldsymbol{g}$: state transition function and observation function
- $\boldsymbol{v}_t$, $\boldsymbol{r}_t$: state and observation noises

In terms of a set of **relevant probability density functions (pdfs)**:

- Prior pdfs: $\boldsymbol{\theta} \sim p(\boldsymbol{\theta})$ and $\boldsymbol{x}_0 \sim p(\boldsymbol{x}_0)$
- Transition pdf of the state: $\boldsymbol{x}_t \sim p(\boldsymbol{x}_t | \boldsymbol{x}_{t-1}, \boldsymbol{\theta})$
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State estimation

Classical filtering methods:

Bayesian estimation of the state variables, $p(\boldsymbol{x}_t|\boldsymbol{y}_{1:t}, \theta^\star)$, assuming $\boldsymbol{\theta}^\star$ is known.

Every time step t:

1. Predictive distribution:

$$p(\boldsymbol{x}_t|\boldsymbol{y}_{1:t-1}, \theta^\star) = \int p(\boldsymbol{x}_t|\boldsymbol{x}_{t-1}, \theta^\star)p(\boldsymbol{x}_{t-1}|\boldsymbol{y}_{1:t-1}, \theta^\star)d\boldsymbol{x}_t \quad (1)$$

2. Likelihood: $p(\boldsymbol{y}_t|\boldsymbol{x}_t, \theta^\star)$
3. Posterior/filtering distribution:

$$p(\boldsymbol{x}_t|\boldsymbol{y}_{1:t}, \theta^\star) \propto (\boldsymbol{y}_t|\boldsymbol{x}_t, \theta^\star)p(\boldsymbol{x}_t|\boldsymbol{y}_{1:t-1}, \theta^\star) \quad (2)$$

In practice, $\theta^\star$ is not known. It is needed to **estimate both θ and $\boldsymbol{x}_t$**, i.e., $p(\boldsymbol{x}_t, \theta|\boldsymbol{y}_{1:t})$.

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State-of-the-art methods

Methods for Bayesian inference of both $\boldsymbol{\theta}$ and $\boldsymbol{x}_t$:

- **particle Markov chain Monte Carlo (PMCMC)**[1]
- **sequential Monte Carlo square (SMC^2)**[2]
- **nested particle filters (NPFs)**[3]

⟶ They can quantify the uncertainty or estimation error.
⟶ They can be applied to a broad class of models.
⟶ They provide theoretical guarantees.
⟶ Both PMCMC and SMC^2 are batch techniques, while the NPF is a recursive method.

[1] Andrieu, Doucet, and Holenstein 2010.
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Model inference

We aim at computing the joint posterior pdf $p(\boldsymbol{\theta}, \mathbf{x}_t | \mathbf{y}_{1:t})$, that can be written as

$$p(\mathbf{x}_t, \theta | \mathbf{y}_{1:t}) = \underbrace{p(\mathbf{x}_t | \boldsymbol{\theta}, \mathbf{y}_{1:t})}_{2^{nd} \text{ layer}} \underbrace{p(\boldsymbol{\theta} | \mathbf{y}_{1:t})}_{1^{st} \text{ layer}}$$

⟶ The **key difficulty** in this class of models is the Bayesian estimation of the parameter vector $\boldsymbol{\theta}$.

Model inference

At every time step t:

1st layer

$\underbrace{p(\boldsymbol{\theta}|\boldsymbol{y}_{1:t-1})}_{\text{Pred. pdf of } \boldsymbol{\theta}}$

Filtering (given θ)

$\underbrace{p(\boldsymbol{x}_t|\theta, \boldsymbol{y}_{1:t-1})}_{\text{Pred. pdf of } \boldsymbol{x}}$

$p(\boldsymbol{y}_t|\boldsymbol{x}_t, \theta)$

$\underbrace{p(\boldsymbol{x}_t|\theta, \boldsymbol{y}_{1:t})}_{\text{Post. pdf of } \boldsymbol{x}}$

2nd layer

$p(\boldsymbol{y}_t|\boldsymbol{\theta}, \boldsymbol{y}_{1:t-1})$

$$\underbrace{p(\boldsymbol{\theta}|\boldsymbol{y}_{1:t})}_{\text{Post. pdf of } \boldsymbol{\theta}} \propto p(\boldsymbol{y}_t|\boldsymbol{\theta}, \boldsymbol{y}_{1:t-1})p(\boldsymbol{\theta}|\boldsymbol{y}_{1:t-1})$$

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Naive importance sampling approximation

Initialisation: Draw $\{\boldsymbol{\theta}^i\}_{i=1}^{N_\theta}$ from $p(\boldsymbol{\theta})$

At $t \geq 1$ and for every $\boldsymbol{\theta}^i$, $i = 1, \ldots, N_{\boldsymbol{\theta}}$:

SMC ($N_{\boldsymbol{\theta}}$ samples) to approximate $p(\boldsymbol{\theta}|\boldsymbol{y}_{1:t})$

For $j = 1, \ldots, N_{\boldsymbol{x}}$:

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- Draw $\bar{\boldsymbol{x}}_t^{i,j} \sim p(\boldsymbol{x}_t|\theta^i, \boldsymbol{y}_{1:t-1})$
- Weights: $\tilde{u}_t^{i,j} \propto p(\boldsymbol{y}_t|\bar{\boldsymbol{x}}_t^{i,j}, \boldsymbol{\theta}^i)$
- Resampling: for $m = 1, \ldots, N_{\boldsymbol{x}}$, $\tilde{\boldsymbol{x}}_t^{i,j} = \bar{\boldsymbol{x}}_t^{i,m}$ with prob. $u_t^{i,m} = \frac{\tilde{u}_t^{i,m}}{\sum_{j=1}^{N_{\boldsymbol{x}}} \tilde{u}_t^{i,j}}$

- Likelihood of $\boldsymbol{\theta}^i$: $\tilde{w}_t^i = w_{t-1}^i \left(\frac{1}{N_x} \sum_{j=1}^{N_x} \tilde{u}_t^{i,j} \right)$
- Then, $p(\boldsymbol{\theta}|\boldsymbol{y}_{1:t}) = \sum_{i=1}^{N_\theta} w_t^i \delta_{\boldsymbol{\theta}^i}(d\boldsymbol{\theta})$, with $w_t^i = \frac{\tilde{w}_t^i}{\sum_{i=1}^{N_\theta} \tilde{w}_t^i}$.

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Naive importance sampling approximation

- Careful with $p(\boldsymbol{\theta})$: after several time steps the filter degenerates
- Possible solution: drawing $\{\boldsymbol{\theta}_t^i\} \sim p(\boldsymbol{\theta}|\boldsymbol{y}_{1:t-1})$ at each time step $\longrightarrow$ re-running from scratch the filter for $\boldsymbol{x}$ (i.e., not recursive anymore)

- NPF $\longrightarrow$ jittering: $\bar{\boldsymbol{\theta}}_t^i \sim \kappa_{N_\theta}(d\boldsymbol{\theta}|\boldsymbol{\theta}')$, where

$$\kappa_{N_\theta}(d\boldsymbol{\theta}|\boldsymbol{\theta}') = (1 - \epsilon_{N_\theta})\delta_{\boldsymbol{\theta}'}(\boldsymbol{\theta}) + \epsilon_{N_\theta}\kappa(d\boldsymbol{\theta}|\boldsymbol{\theta}')$$

  - $0 < \epsilon_{N_\theta} \leq \frac{1}{\sqrt{N_\theta}}$
  - $\kappa(d\boldsymbol{\theta}|\boldsymbol{\theta}')$ is an arbitrary Markov kernel with mean $\boldsymbol{\theta}'$ and finite variance, e.g., $\kappa(d\boldsymbol{\theta}|\boldsymbol{\theta}') = \mathcal{N}(\boldsymbol{\theta}|\boldsymbol{\theta}', \tilde{\sigma}^2\boldsymbol{I})$, with $\tilde{\sigma}^2 < \infty$.
- Guarantees convergence to the true posterior when $N \longrightarrow \infty$

Naive importance sampling approximation

- Careful with $p(\boldsymbol{\theta})$: after several time steps the filter degenerates
- Possible solution: drawing $\{\boldsymbol{\theta}_t^i\} \sim p(\boldsymbol{\theta}|\boldsymbol{y}_{1:t-1})$ at each time step $\longrightarrow$ re-running from scratch the filter for $\boldsymbol{x}$ (i.e., not recursive anymore)

- NPF $\longrightarrow$ jittering: $\bar{\boldsymbol{\theta}}_t^i \sim \kappa_{N_\theta}(d\boldsymbol{\theta}|\boldsymbol{\theta}')$, where

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Nested particle filter (NPF)[4]

For $i = 1, \ldots, N_{\boldsymbol{\theta}}$:

- Jittering: Draw $\bar{\boldsymbol{\theta}}_t^i \sim \kappa_{N_\theta}(d\boldsymbol{\theta}|\boldsymbol{\theta}_{t-1}^i)$

SMC ($N_{\boldsymbol{\theta}}$ samples) to approximate $p(\boldsymbol{\theta}|\boldsymbol{y}_{1:t})$

Given $\bar{\boldsymbol{\theta}}_t^i$, for $j = 1, \ldots, N_{\boldsymbol{x}}$:

SMC ($N_{\boldsymbol{x}}$ samples) to approximate $p(\boldsymbol{y}_t|\boldsymbol{y}_{1:t-1}, \bar{\boldsymbol{\theta}}_t^i)$

- Draw $\bar{\boldsymbol{x}}_t^{i,j} \sim p(\boldsymbol{x}_t|\bar{\boldsymbol{\theta}}_t^i, \boldsymbol{y}_{1:t-1})$
- Weights: $\tilde{u}_t^{i,j} \propto p(\boldsymbol{y}_t|\bar{\boldsymbol{x}}_t^{i,j}, \bar{\boldsymbol{\theta}}_t^i)$
- Resampling: for $m = 1, \ldots, N_{\boldsymbol{x}}$, $\tilde{\boldsymbol{x}}_t^{i,j} = \bar{\boldsymbol{x}}_t^{i,m}$ with prob. $u_t^{i,m} = \frac{\tilde{u}_t^{i,m}}{\sum_{j=1}^{N_x} \tilde{u}_t^{i,j}}$

- Likelihood of $\bar{\boldsymbol{\theta}}_t^i$: $\tilde{w}_t^i = \frac{1}{N_x} \sum_{j=1}^{N_x} \tilde{u}_t^{i,j}$
- Resampling: for $l = 1, \ldots, N_{\boldsymbol{\theta}}$, $\{\boldsymbol{\theta}_t^i, \{\boldsymbol{x}_t^{i,j}\}_{1 \le j \le N_{\boldsymbol{x}}}\} = \{\bar{\boldsymbol{\theta}}_t^l, \{\tilde{\boldsymbol{x}}_t^{l,j}\}_{1 \le j \le N_{\boldsymbol{x}}}\}$ with prob. w_t^l, so that $p(\boldsymbol{\theta}|\boldsymbol{y}_{1:t}) = \frac{1}{N_{\boldsymbol{\theta}}} \sum_{i=1}^{N_{\boldsymbol{\theta}}} \delta_{\boldsymbol{\theta}_t^i}(d\boldsymbol{\theta})$

[4] Crisan and Miguez 2017.

Family of nested filters

1. **Nested particle filters (NPFs)**[5].
   - Both layers ⟶ Sequential Monte Carlo (SMC) methods
     High computational complexity: $N_\theta \times N_x$
2. **Nested hybrid filters (NHFs)**[6].
   - θ-layer ⟶ Monte Carlo-based methods (e.g., SMC or SQMC)
   - x-layer ⟶ Gaussian techniques (e.g., EKFs or EnKFs)
3. **Nested Gaussian filters (NGFs)**[7].
   - θ-layer ⟶ Deterministic sampling methods (e.g., UKF).
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[5] Crisan and Míguez 2018.
[6] Pérez-Vieites, Mariño, and Míguez 2017.
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Reducing number of particles online

Problem: Great amount of samples ($N_{\boldsymbol{\theta}} \times N_{\boldsymbol{x}}$) and **waste of computational effort** when they are not well chosen.

Possible approach: reducing automatically the number of samples, N_θ, when the performance is no longer compromised.

We studied the case for a nested Gaussian filter that implements:

- **Quadrature Kalman filter (QKF) in the θ-layer**, with $N_{\boldsymbol{\theta}} = \alpha^{d_\theta}, \alpha > 1$.

The hyperparameter α will depend on t, so the number of samples is now defined as $N_{\boldsymbol{\theta},t} = \alpha_t^{d_{\boldsymbol{\theta}}}$.

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Adaptive reduction rule

New statistic to decide when to reduce $N_{\theta,t}$:

$$\rho_t = \frac{1}{\sum_{n=1}^{N_{\theta,t}} (\bar{s}_t^n)^2} \qquad \text{with} \qquad \bar{s}_t^n = \frac{p(\mathbf{y}_t|\mathbf{y}_{1:t-1}, \theta_t^n)}{\sum_{n=1}^{N_{\theta,t}} p(\mathbf{y}_t|\mathbf{y}_{1:t-1}, \theta_t^n)}$$

The statistic takes

- its **minimum value in** $\rho_t = 1$, which occurs when only one $p(\mathbf{y}_t|\mathbf{y}_{1:t-1}, \theta_t^n)$, for $n = 1, \ldots, N_{\theta,t}$, is different from zero; and
- its **maximum value in** $\rho_t = N_{\theta,t}$, when for all $n = 1, \ldots, N_{\theta,t}$, the evaluations $p(\mathbf{y}_t|\mathbf{y}_{1:t-1}, \theta_t^n)$ are equal.

The adaptive reduction rule:

- If $\frac{\rho_t}{N_{\theta,t}} > 1 - \epsilon$ (ρ_t is close to its maximum value),

$$N_{\theta,t+1} = (\alpha_t - 1)^{d_\theta} < N_{\theta,t}, \text{ with } N_{\theta,t+1} > N_{\min}.$$

- Otherwise, $N_{\theta,t+1} = N_{\theta,t}$.

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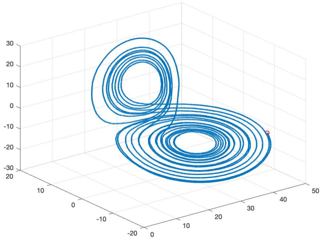
Numerical results - Lorenz 63

We consider a stochastic Lorenz 63 model, whose dynamics are described by

- the **state variables** $\boldsymbol{x}_t$ with dimension $d_x = 3$,
- the **static parameters** $\boldsymbol{\theta} = [S, R, B]^\top$ and
- the following **SDEs**

$$dx_1 = [-S(x_1 - x_2)]d\tau + \sigma dv_1,$$
$$dx_2 = [Rx_1 - x_2 - x_1 x_3]d\tau + \sigma dv_2,$$
$$dx_3 = [x_1 x_2 - Bx_3]d\tau + \sigma dv_3,$$



Numerical results

- Applying a discretization method with step Δ, we obtain

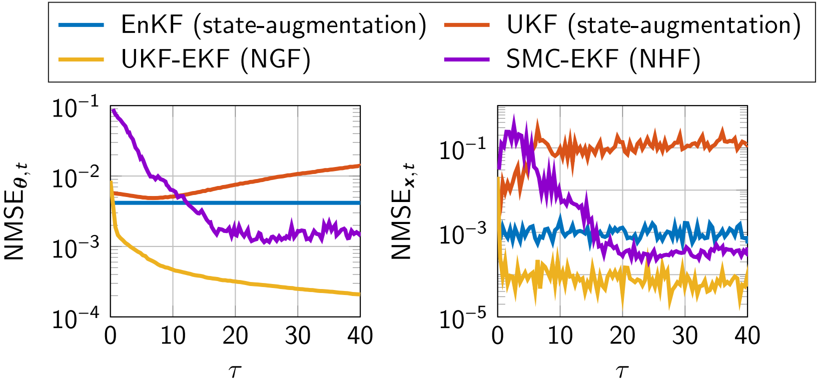
$$
\begin{aligned}
x_{1,t+1} &= x_{1,t} - \Delta S(x_{1,t} - x_{2,t}) + \sqrt{\Delta}\sigma v_{1,t},\\
x_{2,t+1} &= x_{2,t} + \Delta\left[(R - x_{3,t})x_{1,t} - x_{2,t}\right] + \sqrt{\Delta}\sigma v_{2,t},\\
x_{3,t+1} &= x_{3,t} + \Delta(x_{1,t}x_{2,t} - Bx_{3,t}) + \sqrt{\Delta}\sigma v_{3,t},
\end{aligned}
$$

- We assume linear observations of the form

$$
\boldsymbol{y}_t = k_o \begin{bmatrix} x_{1,t} \\ x_{3,t} \end{bmatrix} + \boldsymbol{r}_t,
$$

where k_o is a fixed known parameter and $\boldsymbol{r}_t \sim \mathcal{N}(\boldsymbol{r}_t | \mathbf{0}, \sigma_y^2 \boldsymbol{I}_2)$.

Numerical results[8]

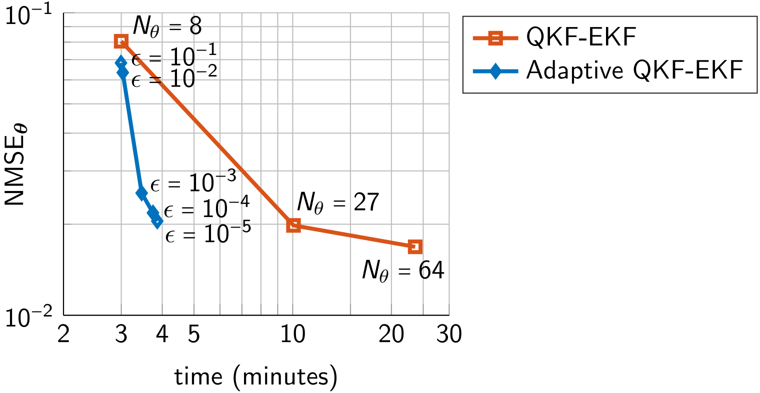


⟶ The nested schemes outperform the augmented-state methods.

⟶ The UKF-EKF is three times faster than SMC-EKF.

[8] Pérez-Vieites and Míguez 2021.

Numerical results[9]



1. QKF-EKF for different fixed $N_{\boldsymbol{\theta}} = \{8, 27, 64\}$.
2. Adaptive QKF-EKF with $N_{\boldsymbol{\theta},1} = 64$.

[9] Pérez-Vieites and Elvira 2023.

Conclusions

1. The nested methodology is online and flexible. It admits different types of filtering techniques in each layer, leading to a **set of algorithms**.

2. For a further reduction of the computational complexity. Automatic reduction of N_θ when points become less informative $\longrightarrow$ reduction of cost for a given performance.

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Thank you!

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