Learning the number of particles in nested filtering

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

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State-space model

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

$$\mathbf{x}_t = \mathbf{f}(\mathbf{x}_{t-1}, \boldsymbol{\theta}) + \mathbf{v}_t,$$

 $\mathbf{y}_t = \mathbf{g}(\mathbf{x}_t, \boldsymbol{\theta}) + \mathbf{r}_t,$

- f, g: state transition function and observation function
- v_t, r_t: state and observation noises

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

- Prior pdfs: $\theta \sim p(\theta)$ and $x_0 \sim p(x_0)$
- Transition pdf of the state: $x_t \sim p(x_t|x_{t-1}, \theta)$
- Conditional pdf of the observation: $y_t \sim p(y_t|x_t,\theta)$

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Classical filtering methods:

Bayesian estimation of the state variables, $p(x_t|y_{1:t},\theta^*)$, assuming θ^* is known.

$$p(x_t|y_{1:t-1}, \theta^*) = \int p(x_t|x_{t-1}, \theta^*) p(x_{t-1}|y_{1:t-1}, \theta^*) dx_t$$
 (1)

- 2. Likelihood: $p(y_t|x_t, \theta^*)$

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

estimate both θ and x_t , i.e., $p(x_t, \theta | y_{1:t}) = \dots = 1$



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Every time step *t*:

1. Predictive distribution:

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- 3. Posterior/filtering distribution:

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

In practice, θ^* is not known. It is needed to estimate both θ and x_t , i.e., $p(x_t, \theta|y_{1:t})$.

State-of-the-art methods

Methods for Bayesian inference of both θ and x_t :

- particle Markov chain Monte Carlo (PMCMC)¹
- sequential Monte Carlo square (SMC²)²
- nested particle filters (NPFs)³

¹Andrieu, Doucet, and Holenstein 2010.

²Chopin, Jacob, and Papaspiliopoulos 2013.

³Crisan and Míguez 2018.

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 - → They can be applied to a broad class of models.
 - → They provide theoretical guarantees.

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 - --> 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 SMC² are batch techniques, while the NPF is a recursive method.

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Nested filters

Model inference

Algorithms: Nested particle filter (NPF) and others

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

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

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

At every time step *t*:

```
1<sup>st</sup> layer
p(\boldsymbol{\theta}|\boldsymbol{y}_{1:t-1})
Pred. pdf of \theta
                                           p(\mathbf{x}_t|\boldsymbol{\theta},\mathbf{y}_{1:t})
p(\mathbf{y}_t|\boldsymbol{\theta},\mathbf{y}_{1:t-1})
  p(\theta|\mathbf{y}_{1:t}) \propto p(\mathbf{y}_t|\theta,\mathbf{y}_{1:t-1})p(\theta|\mathbf{y}_{1:t-1})
Post. pdf of 	heta
```

At every time step *t*:

```
1<sup>st</sup> layer
p(\boldsymbol{\theta}|\boldsymbol{y}_{1:t-1})
Pred. pdf of \theta
                                              p(\mathbf{x}_t|\boldsymbol{\theta},\mathbf{y}_{1:t})
p(\mathbf{y}_t|\boldsymbol{\theta},\mathbf{y}_{1:t-1}) = \int p(\mathbf{y}_t|\mathbf{x}_t,\boldsymbol{\theta})p(\mathbf{x}_t|\boldsymbol{\theta},\mathbf{y}_{1:t-1})d\mathbf{x}_t
  p(\theta|\mathbf{y}_{1:t}) \propto p(\mathbf{y}_t|\theta,\mathbf{y}_{1:t-1})p(\theta|\mathbf{y}_{1:t-1})
Post. pdf of \theta
```

At every time step *t*:

```
1<sup>st</sup> layer
p(\boldsymbol{\theta}|\boldsymbol{y}_{1:t-1})
Pred. pdf of \theta
                                            Filtering (given \theta)
                                            p(\boldsymbol{x}_t|\boldsymbol{\theta},\boldsymbol{y}_{1:t-1})
                                                 Pred. pdf of x
                                            p(\mathbf{y}_t|\mathbf{x}_t,\boldsymbol{\theta})
                                           p(\boldsymbol{x}_t|\boldsymbol{\theta},\boldsymbol{y}_{1:t})
                                                                                                                                                                               2<sup>nd</sup> layer
                                              Post. pdf of x
p(\mathbf{y}_t|\boldsymbol{\theta},\mathbf{y}_{1:t-1}) = \int p(\mathbf{y}_t|\mathbf{x}_t,\boldsymbol{\theta})p(\mathbf{x}_t|\boldsymbol{\theta},\mathbf{y}_{1:t-1})d\mathbf{x}_t
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Post. pdf of \theta
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At every time step *t*:

1st layer $p(\boldsymbol{\theta}|\boldsymbol{y}_{1:t-1})$ Pred. pdf of θ Filtering (given θ) $p(x_t|\theta, y_{1:t-1}) = \int p(x_t|x_{t-1}, \theta) p(x_{t-1}|\theta, y_{1:t-1}) dx_{t-1}$ Pred. pdf of x $p(\mathbf{y}_t|\mathbf{x}_t,\boldsymbol{\theta})$ $p(\mathbf{x}_t|\boldsymbol{\theta},\mathbf{y}_{1:t}) \propto p(\mathbf{y}_t|\mathbf{x}_t,\boldsymbol{\theta})p(\mathbf{x}_t|\boldsymbol{\theta},\mathbf{y}_{1:t-1})$ 2nd layer Post. pdf of x $p(\mathbf{y}_t|\boldsymbol{\theta},\mathbf{y}_{1:t-1}) = \int p(\mathbf{y}_t|\mathbf{x}_t,\boldsymbol{\theta})p(\mathbf{x}_t|\boldsymbol{\theta},\mathbf{y}_{1:t-1})d\mathbf{x}_t$ $p(\theta|\mathbf{y}_{1:t}) \propto p(\mathbf{y}_t|\theta,\mathbf{y}_{1:t-1})p(\theta|\mathbf{y}_{1:t-1})$ Post. pdf of θ

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

At $t \ge 1$ and for every θ^i , $i = 1, ..., N_{\theta}$:

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

- Draw $\bar{\boldsymbol{x}}_t^{i,j} \sim p(\boldsymbol{x}_t|\boldsymbol{\theta}^i, \boldsymbol{v}_{1:t-1})$

- Weights: $\tilde{u}_{t}^{i,j} \propto p(\mathbf{v}_{t}|\bar{\mathbf{x}}_{t}^{i,j},\boldsymbol{\theta}^{i})$
- Resampling: for $m = 1, ..., N_x$, $\tilde{\boldsymbol{x}}_{+}^{i,j} = \bar{\boldsymbol{x}}_{+}^{i,m}$
- Then, $p(\theta|\mathbf{y}_{1:t}) = \sum_{i=1}^{N_{\theta}} w_t^i \delta_{\theta^i}(d\theta)$, with $w_t^i = \frac{\tilde{w}_t^i}{\sum_{\theta \in \mathcal{R}^i} \tilde{v}_t^i}$

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

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- Weights: $\tilde{u}_{t}^{i,j} \propto p(\mathbf{v}_{t}|\bar{\mathbf{x}}_{t}^{i,j},\boldsymbol{\theta}^{i})$
- Resampling: for $m=1,\ldots,N_{\mathbf{x}},\ \widetilde{\mathbf{x}}_{+}^{i,j}=\overline{\mathbf{x}}_{+}^{i,m}$
- Then, $p(\theta|\mathbf{y}_{1:t}) = \sum_{i=1}^{N_{\theta}} w_t^i \delta_{\theta^i}(d\theta)$, with $w_t^i = \frac{\tilde{w}_t^i}{\sum_{N_{\theta} = i}^{N_{\theta}}}$

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to approximate $p(\mathbf{y}_t|\mathbf{y}_{1:t-1}, \boldsymbol{\theta}^i)$

- Weights: $\tilde{u}_t^{i,j} \propto p(\mathbf{y}_t | \bar{\mathbf{x}}_t^{i,j}, \boldsymbol{\theta}^i)$
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At $t \ge 1$ and for every θ^i , $i = 1, ..., N_{\theta}$:

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

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

- Draw
$$\bar{\boldsymbol{x}}_t^{i,j} \sim p(\boldsymbol{x}_t | \boldsymbol{\theta}^i, \boldsymbol{y}_{1:t-1})$$

SMC (N_x samples)

to approximate $p(\mathbf{y}_t|\mathbf{y}_{1:t-1}, \boldsymbol{\theta}^i)$

- Weights: $\tilde{u}_{t}^{i,j} \propto p(\mathbf{v}_{t}|\bar{\mathbf{x}}_{t}^{i,j},\boldsymbol{\theta}^{i})$
- Resampling: for $m = 1, ..., N_x$, $\tilde{\mathbf{x}}_t^{i,j} = \bar{\mathbf{x}}_t^{i,m}$ with prob. $u_t^{i,m} = \frac{\tilde{u}_t^{i,m}}{\sum_{t=1}^{N_x} \tilde{u}_t^{i,j}}$
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$$1,\ldots,N_{x}$$
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- Likelihood of θ^i : $\tilde{w}_t^i = w_{t-1}^i \left(\frac{1}{N_t} \sum_{i=1}^{N_x} \tilde{u}_t^{i,j} \right)$
- Then, $p(\theta|\mathbf{y}_{1:t}) = \sum_{i=1}^{N_{\theta}} w_t^i \delta_{\theta^i}(d\theta)$, with $w_t^i = \frac{\tilde{w}_t^i}{\sum_{N_{\theta} = i}^{N_{\theta}}}$

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

- Draw $\bar{\boldsymbol{x}}_t^{i,j} \sim p(\boldsymbol{x}_t | \boldsymbol{\theta}^i, \boldsymbol{y}_{1:t-1})$

SMC (N_x samples)

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- Then, $p(\theta|\mathbf{y}_{1:t}) = \sum_{i=1}^{N_{\theta}} w_t^i \delta_{\theta^i}(d\theta)$, with $w_t^i = \frac{\tilde{w}_t^i}{\sum_{\theta \in \tilde{w}_t^i}}$.

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

• NPF \longrightarrow iittering: $\bar{\theta}_{t}^{i} \sim \kappa_{N_{\theta}}(d\theta|\theta')$, where

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

- $0 < \epsilon_{N_{\theta}} \le \frac{1}{\sqrt{N_{\theta}}}$
- $\kappa(d\theta|\theta')$ is an arbitrary Markov kernel with mean θ' and finite

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

Nested particle filter (NPF)⁴

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

- Jittering: Draw $\bar{\theta}_{t}^{i} \sim \kappa_{N_0}(d\theta|\theta_{t-1}^{i})$

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

Given $\bar{\boldsymbol{\theta}}_t'$, for $j = 1, \dots, N_r$:

Siven
$$\boldsymbol{\theta}_t^i$$
, for $j = 1, ..., N_x$:

- Draw $\bar{\boldsymbol{x}}_t^{i,j} \sim p(\boldsymbol{x}_t | \bar{\boldsymbol{\theta}}_t^i, \boldsymbol{y}_{1:t-1})$

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

- Weights: $\tilde{u}_{\star}^{i,j} \propto p(\mathbf{v}_{\star}|\bar{\mathbf{x}}_{\star}^{i,j},\bar{\boldsymbol{\theta}}_{\star}^{i})$
- Resampling: for $m = 1, ..., N_x$, $\tilde{\boldsymbol{x}}_{t}^{i,j} = \bar{\boldsymbol{x}}_{t}^{i,m}$ with prob. $u_t^{i,m} = \frac{\tilde{u}_t^{i,m}}{\sum_{t=1}^{N_x} \tilde{u}_t^{i,j}}$
- Likelihood of $\vec{\theta}_t'$: $\tilde{w}_t^i = \frac{1}{N} \sum_{i=1}^{N_x} \tilde{u}_t^{i,j}$
- Resampling: for $l = 1, ..., N_{\theta}$, $\{\theta_t^i, \{\mathbf{x}_t^{i,j}\}_{1 \le i \le N_{\bullet}}\} = \{\bar{\theta}_t^l, \{\tilde{\mathbf{x}}_t^{l,j}\}_{1 \le i \le N_{\bullet}}\}$ with prob. w_t^l , so that $p(\theta|\mathbf{y}_{1:t}) = \frac{1}{N_o} \sum_{i=1}^{N_\theta} \delta_{\theta_i^l}(d\theta)$

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 \longrightarrow 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 \longrightarrow Deterministic sampling methods (e.g., UKF).
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Efficient exploration of the parameter space

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

• Quadrature Kalman filter (QKF) in the θ -layer, with

Efficient exploration of the parameter space

Problem: Great amount of samples $(N_{\theta} \times N_x)$ 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.

• Quadrature Kalman filter (QKF) in the θ -layer, with

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Efficient exploration of the parameter space

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

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

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

Adaptive reduction rule

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

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

The statistic takes

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

• If $\frac{\rho_t}{N_{0,t}} > 1 - \epsilon$ (ρ_t is close to its maximum value),

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

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



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The adaptive reduction rule:

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Numerical results - Lorenz 63

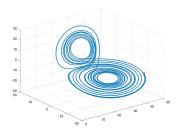
We consider a stochastic Lorenz 63 model, whose dynamics are described by

- the state variables x_t with dimension $d_x = 3$,
- the static parameters $\boldsymbol{\theta} = [\boldsymbol{S}, \boldsymbol{R}, \boldsymbol{B}]^{\mathsf{T}}$ and
- the following SDEs

$$dx_1 = [-S(x_1 - x_2)]d\tau + \sigma dv_1,$$

$$dx_2 = [Rx_1 - x_2 - x_1x_3]d\tau + \sigma dv_2,$$

$$dx_3 = [x_1x_2 - Bx_3]d\tau + \sigma dv_3,$$





• Applying a discretization method with step Δ , we obtain

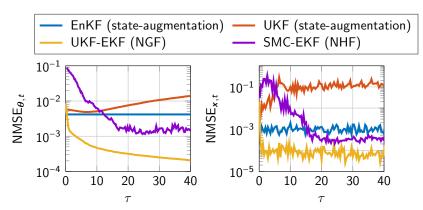
$$\begin{split} x_{1,t+1} &= x_{1,t} - \Delta S(x_{1,t} - x_{2,t}) + \sqrt{\Delta} \sigma v_{1,t}, \\ x_{2,t+1} &= x_{2,t} + \Delta \big[(R - x_{3,t}) x_{1,t} - x_{2,t} \big] + \sqrt{\Delta} \sigma v_{2,t}, \\ x_{3,t+1} &= x_{3,t} + \Delta (x_{1,t} x_{2,t} - B x_{3,t}) + \sqrt{\Delta} \sigma v_{3,t}, \end{split}$$

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 $\mathbf{r}_t \sim \mathcal{N}(\mathbf{r}_t | \mathbf{0}, \sigma_v^2 \mathbf{I}_2)$.

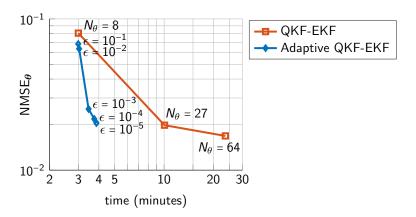
Numerical results⁸



- → The nested schemes outperform the augmented-state methods.
- → The UKF-EKF is three times faster than SMC-EKF.



Numerical results⁹



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



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.

- 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.

Thank you!

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