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Adaptive Gaussian nested filter for joint parameter and state estimation in state-space models

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State-space model

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

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

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

- Prior pdfs: $\theta \sim p(\theta)$ and $x_0 \sim p(x_0)$
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State estimation

Classical filtering methods:

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

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

2. Likelihood: $p(\mathbf{y}_t | \mathbf{x}_t, \boldsymbol{\theta}^*)$

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

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

State estimation

Classical filtering methods:

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

Every time step t:

1. Predictive distribution:

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

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

$$p(\boldsymbol{x}_t | \boldsymbol{y}_{1:t}, \boldsymbol{\theta}^*) \propto (\boldsymbol{y}_t | \boldsymbol{x}_t, \boldsymbol{\theta}^*) p(\boldsymbol{x}_t | \boldsymbol{y}_{1:t-1}, \boldsymbol{\theta}^*)$$
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estimate both θ and x_t , i.e., $p(x_t, \theta | y_1, t) = 1 = 0$

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State estimation

Classical filtering methods:

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

Every time step *t*:

1. Predictive distribution:

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

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(2)

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

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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
 - \longrightarrow They can quantify the uncertainty or estimation error,
 - → they can be applied to a broad class of models,
 - \longrightarrow they provide theoretical guarantees,
 - \rightarrow they are batch techniques.
 - → The computational cost becomes prohibitive in high-dimensional problems.

¹Andrieu, Doucet, and Holenstein 2010.

²Chopin, Jacob, and Papaspiliopoulos 2011.



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Conclusions

Model inference

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

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

 \rightarrow The **key difficulty** in this class of models is the Bayesian estimation of the parameter vector θ .

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Model inference

At every time step t:



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Model inference

At every time step t:



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

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

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Model inference

At every time step t:



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

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Model inference

At every time step t:



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

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Post. pdf of θ

Naive importance sampling approximation

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

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

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

For $j = 1, \dots, N_x$: SMC (N_x samples)

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

- Weights:
$$\tilde{u}_t^{i,j} \propto p(\boldsymbol{y}_t | \bar{\boldsymbol{x}}_t^{i,j}, \boldsymbol{\theta}^i)$$

- Resampling: for
$$m = 1, ..., N_x$$
, $\tilde{\mathbf{x}}_t^{i,j} = \bar{\mathbf{x}}_t^{i,m}$
with prob. $u_t^{i,m} = \frac{\tilde{u}_t^{i,m}}{\sum_{t=1}^{N_x} \tilde{u}_t^{i,j}}$

- Likelihood of
$$oldsymbol{ heta}^i$$
: $ilde{w}^i_t = w^i_{t-1} \Big(rac{1}{N_x} \sum_{j=1}^{N_x} ilde{u}^{i,j}_t \Big)$

- Then, $p(\theta|\mathbf{y}_{1:t}) = \sum_{i=1}^{N_{\theta}} w_t^i \delta_{\theta_t^i}(d\theta)$, 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

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

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

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

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

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

- Weights:
$$\tilde{u}_t^{\prime,j} \propto p(\mathbf{y}_t | \bar{\mathbf{x}}_t^{\prime,j}, \boldsymbol{\theta}^{\prime})$$

- Resampling: for $m = 1, ..., N_x$, $\tilde{\mathbf{x}}_t^{i,j} = \bar{\mathbf{x}}_t^{i,m}$ with prob. $u_t^{i,m} = \frac{\tilde{u}_t^{i,m}}{\sum_{i=1}^{N_x} \tilde{u}_t^{i,j}}$

- Likelihood of
$$\theta^i$$
: $\widetilde{w}_t^i = w_{t-1}^i \left(\frac{1}{N_x} \sum_{j=1}^{N_x} \widetilde{u}_t^{i,j} \right)$

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

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- Likelihood of θ^i : $\tilde{w}_t^i = w_{t-1}^i \left(\frac{1}{N_x} \sum_{j=1}^{N_x} \tilde{u}_t^{i,j} \right)$

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

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

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- 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, $p(\boldsymbol{\theta} | \boldsymbol{y}_{1:t}) = \sum_{i=1}^{N_{\theta}} w_{t}^{i} \delta_{\boldsymbol{\theta}_{t}^{i}}(d\boldsymbol{\theta})$, with $w_{t}^{i} = \frac{\tilde{w}_{t}^{i}}{\sum_{i=1}^{N_{\theta}} \tilde{w}_{t}^{i,j}}$.

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

At $t \ge 1$ and for every θ^i , $i = 1, ..., N_{\theta}$: to approximate $p(\theta|\mathbf{y}_{1:t})$

For
$$j = 1, ..., N_x$$
:
- Draw $\bar{\mathbf{x}}_t^{i,j} \sim p(\mathbf{x}_t | \boldsymbol{\theta}^i, \mathbf{y}_{1:t-1})$
SMC (N_x samples)
to approximate $p(\mathbf{y}_t | \mathbf{y}_{1:t-1}, \boldsymbol{\theta}^i)$

- Weights:
$$\tilde{u}_t^{i,j} \propto p(\boldsymbol{y}_t | \boldsymbol{\bar{x}}_t^{i,j}, \boldsymbol{\theta}^i)$$

- Resampling: for
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, $\tilde{\mathbf{x}}_t^{i,j} = \bar{\mathbf{x}}_t^{i,m}$
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- Likelihood of
$$\theta^i$$
: $\tilde{w}_t^i = w_{t-1}^i \left(\frac{1}{N_x} \sum_{j=1}^{N_x} \tilde{u}_t^{i,j} \right)$

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

After several time steps the filter degenerates.

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Nested particle filter $(NPF)^3$

For $i = 1, \ldots, N_{\theta}$:		SMC (N_{θ} samples)
- Jittering: Draw $ar{m{ heta}}_t^i \sim \kappa_{N_{m{ heta}}}(m{ heta} dm{ heta}_{t-1}^i)$)	to approximate $p(\boldsymbol{\theta} \boldsymbol{y}_{1:t})$
Given $\bar{\boldsymbol{\theta}}_{t}^{i}$, for $j = 1, \ldots, N_{\mathbf{x}}$:	SMC (N_x samples)	
- Draw $\bar{\boldsymbol{x}}_{t}^{i,j} \sim p(\boldsymbol{x}_{t} \bar{\boldsymbol{\theta}}_{t}^{i}, \boldsymbol{y}_{1:t-1})$ to approximate $p(\boldsymbol{y}_{t} \boldsymbol{y}_{1:t-1}, \bar{\boldsymbol{\theta}}_{t}^{i})$		
- Weights: $ ilde{u}_t^{i,j} \propto p(oldsymbol{y}_t oldsymbol{ar{x}}_t^{i,j}, oldsymbol{ar{ heta}}_t^i)$		
- Resampling: for $m = 1,, N_x$, $\tilde{\mathbf{x}}_t^{i,j} = \bar{\mathbf{x}}_t^{i,m}$		
with prob. $u_t^{i,m} = \frac{\widetilde{u}_t^{i,m}}{\sum_{j=1}^{N_x} \widetilde{u}_t^{i,j}}$		
- Likelihood of $\bar{\theta}_t^i$: $\tilde{w}_t^i = \frac{1}{N_x} \sum_{j=1}^{N_x} \tilde{u}_t^{i,j}$		
- Resampling: for $l = 1, \dots, N_{\theta}$, $\{\theta_t^i, \{\mathbf{x}_t^{i,j}\}_{1 \le j \le N_x}\} = \{\bar{\theta}_t^l, \{\tilde{\mathbf{x}}_t^{l,j}\}_{1 \le j \le N_x}\}$		
with prob. w'_t , so that $p(\theta \mathbf{y}_{1:t}) = \frac{1}{N_{\theta}} \sum_{i=1}^{N_{\theta}} \delta_{\theta'_t}(d\theta)$		

³Crisan and Miguez 2017.

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Nested particle filter $(NPF)^3$

For
$$i = 1, ..., N_{\theta}$$
:
- Jittering: Draw $\overline{\theta}_{t}^{i} \sim \kappa_{N_{\theta}}(\theta | d\theta_{t-1}^{i})$
Given $\overline{\theta}_{t}^{i}$, for $j = 1, ..., N_{x}$:
- Draw $\overline{x}_{t}^{i,j} \sim p(x_{t} | \overline{\theta}_{t}^{i}, y_{1:t-1})$
- Weights: $\widetilde{u}_{t}^{i,j} \propto p(y_{t} | \overline{x}_{t}^{i,j}, \overline{\theta}_{t}^{i})$
- Resampling: for $m = 1, ..., N_{x}$, $\widetilde{x}_{t}^{i,j} = \overline{x}_{t}^{i,m}$
with prob. $u_{t}^{i,m} = \frac{\widetilde{u}_{t}^{i,m}}{\sum_{j=1}^{N_{x}} \widetilde{u}_{t}^{i,j}} = \{\overline{\theta}_{t}^{i}, \{\overline{x}_{t}^{i,j}\}_{1 \le j \le N_{x}}\}$
with prob. w_{t}^{i} , so that $p(\theta | y_{1:t}) = \frac{1}{N_{\theta}} \sum_{i=1}^{N_{\theta}} \delta_{\theta_{t}^{i}}(d\theta)$

High computational complexity: $N_{\theta} \times N_x$ samples.

³Crisan and Miguez 2017.



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Conclusions

Family of nested filters

1. Nested particle filters (NPFs)⁴.

• Both layers → Sequential Monte Carlo (SMC) methods

2. Nested hybrid filters (NHFs)⁵.

- θ -layer \longrightarrow Monte Carlo-based methods (e.g., SMC or SQMC)
- x-layer \longrightarrow Gaussian techniques (e.g., EKFs or EnKFs)
- 3. Nested Gaussian filters (NGFs)⁶.
 - θ -layer \longrightarrow Deterministic sampling methods (e.g., UKF).
 - x-layer \rightarrow Gaussian techniques (e.g., EKFs or EnKFs).

⁴Crisan and Míguez 2018.

⁵Pérez-Vieites, Mariño, and Míguez 2017. ⁶Pérez-Vieites and Míguez 2021.



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Adapting N_{θ}

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

Objective: efficient allocation of computational resources

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 $N_{\theta} = \alpha^{d_{\theta}}, \alpha > 1.$
- Extended Kalman filters (EKFs) in the x-layer.

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

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Adaptive reduction rule

In order to decide when to reduce $N_{\theta,t}$, we use

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

The statistic takes

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

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

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

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The Lorenz 63 model

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 $\theta = [S, R, B]^{\mathsf{T}}$ and
- the following **SDEs**

$$dx_{1} = [-S(x_{1} - x_{2})]d\tau + \sigma dv_{1},$$

$$dx_{2} = [Rx_{1} - x_{2} - x_{1}x_{3}]d\tau + \sigma dv_{2},$$

$$dx_{3} = [x_{1}x_{2} - Bx_{3}]d\tau + \sigma dv_{3},$$



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The Lorenz 63 model

• Applying a discretization method with step Δ , we obtain

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

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

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

⁷Pérez-Vieites and Elvira 2023.

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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. When two learning tasks take place, it is important to have a good allocation of computational resources so that performance is improved.
- 3. First adaptive rule for N_{θ} , that provides an automatic reduction of the computational complexity for any given performance.

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Thank you!

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