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Nested filtering methods for Bayesian inference in state space models

Sara Pérez Vieites

CERI Systèmes Numériques, IMT Nord Europe (Lille, France).

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

February, 2023

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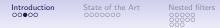
Introduction

We aim at **estimating the time evolution** of **dynamical systems** of different fields of science, such as:

- **Geophysics**. Prediction of the weather, ice sea changes, climate (i.e. fluid dynamics).
- **Biochemistry**. Prediction of the interactions and population of certain molecules.
- **Ecology**. Prediction of the population of prey and predator species in certain region.
- Quantitative finance. Evaluation/estimation of price options and risk.
- **Engineering**. Object/target tracking for applications such as surveillance or air traffic control.

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 \rightarrow There are plenty of applications where the estimation of a dynamical system is needed.



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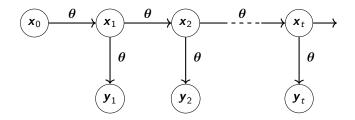
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State-space model

These systems can be represented by **Markov state-space dynamical models**:



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State-space model

The state (\mathbf{x}_t) , the observations (\mathbf{y}_t) and the parameters $(\boldsymbol{\theta})$ of these state-space systems are related following the **equations**

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

- **f** and **g** are the state transition function and the observation function

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v_t and *r_t* are 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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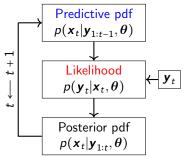
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State estimation

 \rightarrow Goal: Bayesian estimation of the state variables, $p(\mathbf{x}_t | \mathbf{y}_{1:t}, \theta)$.

Classical filtering methods assume θ is known, and compute



Both $p(\mathbf{x}_t | \mathbf{x}_{t-1}, \theta)$ and $p(\mathbf{y}_t | \mathbf{x}_t, \theta)$ are described by the model.

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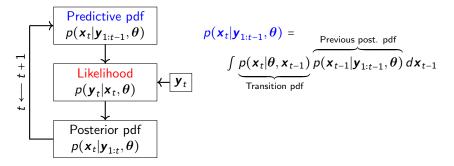
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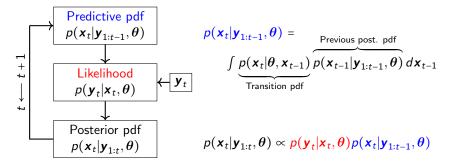
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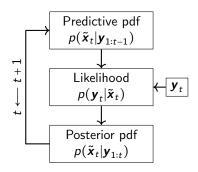
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State-of-the-art methods for parameter and state estimation

1. State augmentation methods with artificial dynamics



- Use of an extended state vector $\tilde{\boldsymbol{x}}_t = [\boldsymbol{x}_t, \boldsymbol{\theta}_t]^{\mathsf{T}}$.
- Artificial dynamics are introduced in θ to avoid degeneracy.
- Easy to apply but the artifical dynamics might introduce bias and the method lacks theoretical guarantees.

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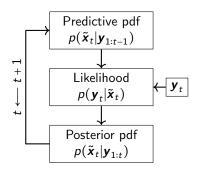
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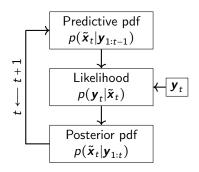
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2. Particle learning (PL) techniques

- It is a sampling-resampling scheme.
- It depends only on a set of finite-dimensional statistics. In a Monte Carlo setting this means that the static parameters can be efficiently represented by sampling.
- The posterior probability distribution of θ conditional on the states x₀,..., x_t can be computed in closed form.
- However, this approach is restricted to very specific models.

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3. Recursive maximum likelihood (RML) methods

- They enable the sequential processing of the observed data as they are collected.
- They are well-principled.
- They can be applied to a broad class of models.
- However, they do not yield full posterior distributions of the unknowns and therefore, they only output point estimates instead.

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- 4. There have been advances leading to methods that
 - aim at calculating the **posterior probability distribution of the unknown variables and parameters** of the models and they can quantify the uncertainty or estimation error.
 - can be applied to a broad class of models.
 - are well-principled probabilistic methods with theoretical guarantees.

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State-of-the-art methods for parameter and state estimation

Some examples are:

- particle Markov chain Monte Carlo (PMCMC)¹
- sequential Monte Carlo square (SMC²)²

→ they are batch techniques: the whole sequence of observations has to to be re-processed from scratch.

 The computational cost becomes prohibitive in high-dimensional problems.

¹Andrieu, Doucet, and Holenstein, "Particle Markov chain Monte Carlo methods".

²Chopin, Jacob, and Papaspiliopoulos, "SMC²: A sequential Monte Carlo algorithm with particle Markov chain Monte Carlo updates" $\mathbb{P} \mapsto \mathbb{P} = \mathbb{P} \setminus \mathbb{P} = \mathbb{P} \setminus \mathbb{P}$

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Summary and Motivation

The state-of-the-art methods have one or more of the following issues:

- Lack of theoretical guarantees.
- Restricted to very specific models.
- Estimation error not quantified (it only provides point estimates).
- Batch technique (the whole sequence of observations have to be re-processed from scratch every time step).
- Prohibitive computational cost for high-dimensional problems.

 \rightarrow We propose a **set of algorithms** that estimate the **joint posterior probability distribution of the parameters and the state**, while solving all the issues.

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Model inference

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

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

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

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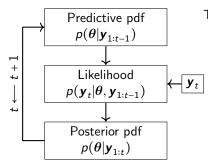


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1st layer of inference



The **posterior pdf** can be written as $p(\theta|\mathbf{y}_{1:t}) \propto p(\mathbf{y}_t|\theta, \mathbf{y}_{1:t-1})p(\theta|\mathbf{y}_{1:t-1})$

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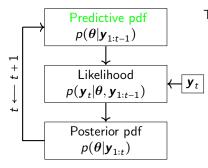


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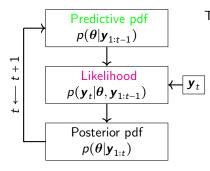


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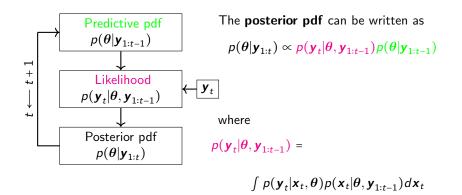


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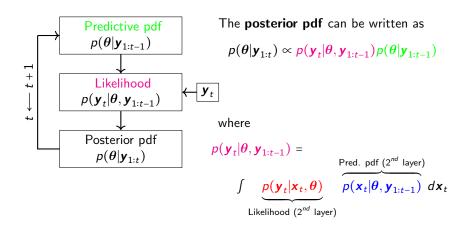


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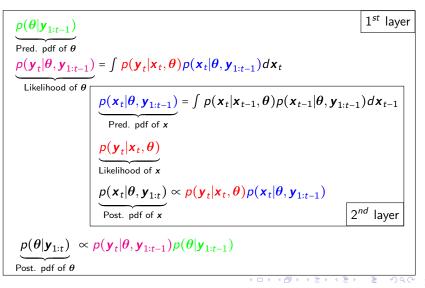


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Family of nested filters

- 1. Nested particle filters (NPFs)³.
 - Both layers → Sequential Monte Carlo (SMC) methods
- 2. Nested hybrid filters (NHFs)⁴.
 - 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)⁵.
 - θ -layer \longrightarrow Deterministic sampling methods (e.g., UKF).
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⁴Pérez-Vieites, Mariño, and Míguez, "Probabilistic scheme for joint parameter estimation and state prediction in complex dynamical systems".

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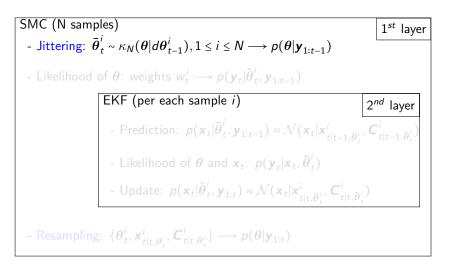


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SMC (N samples) - Jittering: $\bar{\boldsymbol{\theta}}_{t}^{i} \sim \kappa_{N}(\boldsymbol{\theta} \boldsymbol{d}\boldsymbol{\theta}_{t-1}^{i}), 1 \leq i \leq N \longrightarrow p(\boldsymbol{\theta} \boldsymbol{y}_{1:t-1})$	1 st layer
- Likelihood of $m{ heta}$: weights $w_t^i \longrightarrow p(m{y}_t m{ar{ heta}}_t^i, m{y}_{1:t-1})$	
EKF (per each sample <i>i</i>)	2 nd layer
- Prediction: $p(\mathbf{x}_t \overline{\theta}_t^i, \mathbf{y}_{1:t-1}) \approx \mathcal{N}(\mathbf{x}_t \mathbf{x}_{t t-1,\overline{\theta}}^i)$	$({m h}_t^i, {m C}^i_{t t-1,ar {m heta}^i_t})$
- Likelihood of $m{ heta}$ and $m{x}_t$: $p(m{y}_t m{x}_t,ar{m{ heta}}_t^i)$	
- Update: $p(\boldsymbol{x}_t \bar{\boldsymbol{\theta}}_t^i, \boldsymbol{y}_{1:t}) \approx \mathcal{N}(\boldsymbol{x}_t \boldsymbol{x}_{t t, \bar{\boldsymbol{\theta}}_t^i}^i, \boldsymbol{C}_{t t, i}^i)$	\bar{p}_t^i)
- Resampling: $\{\boldsymbol{\theta}_t^i, \boldsymbol{x}_{t t, \boldsymbol{\theta}_t^i}^i, \boldsymbol{C}_{t t, \boldsymbol{\theta}_t^i}^i\} \longrightarrow p(\boldsymbol{\theta} \boldsymbol{y}_{1:t})$	

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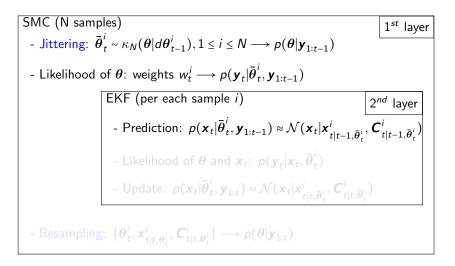


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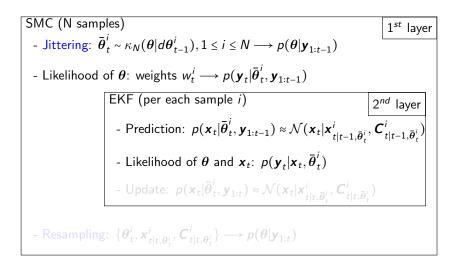


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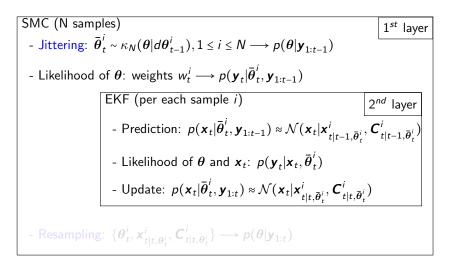


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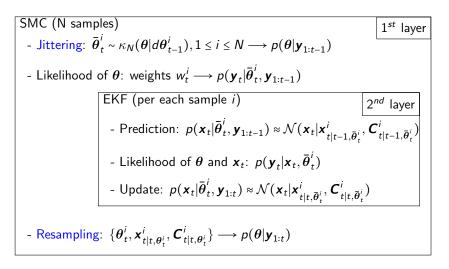


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Recursivity of NPF and NHF

- θ is static and samples θ_{t-1}^i do not evolve. After several resampling steps the filter would degenerate.
- It is convenient to have a procedure to generate a new set $\{\bar{\boldsymbol{\theta}}_t^i\}_{1 \leq i \leq N}$ which yields an approximation of $p(\boldsymbol{\theta}|\boldsymbol{y}_{1:t-1})$.
- → The jittering step allows these filters to run **recursively**: We mutate the particles $\theta_{t-1}^1, \ldots, \theta_{t-1}^N$ independently using ittering kernel $r_{W}(\theta|d\theta)$ and obtain $\bar{\theta}^1 = \bar{\theta}^N$





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Conclusions

Recursivity of NPF and NHF

- θ is static and samples θ_{t-1}^i do not evolve. After several resampling steps the filter would degenerate.
- It is convenient to have a procedure to generate a new set $\{\bar{\boldsymbol{\theta}}_t^i\}_{1 \leq i \leq N}$ which yields an approximation of $p(\boldsymbol{\theta}|\boldsymbol{y}_{1:t-1})$.
- \rightarrow The jittering step allows these filters to run recursively:

We mutate the particles $\theta_{t-1}^1, \ldots, \theta_{t-1}^N$ independently using a jittering kernel $\kappa_N(\theta|d\theta)$ and obtain $\bar{\theta}_t^1, \ldots, \bar{\theta}_t^N$.





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Convergence Theorem (NHF)

The sequence of posterior probability measures of the unknown parameters, $p(\theta|\mathbf{y}_{1:t})$, $t \ge 1$, can be constructed recursively starting from a prior $p(\theta)$ as

 $p(\theta|\mathbf{y}_{1:t}) \propto u_t(\theta) \star p(\theta|\mathbf{y}_{1:t-1})$

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

A.1. The estimator $\hat{u}_t(\theta)$ is random and can be written as

$$\hat{u}_t(\boldsymbol{\theta}) = u_t(\boldsymbol{\theta}) + b_t(\boldsymbol{\theta}) + m_t(\boldsymbol{\theta}),$$

where $u_t(\theta) \coloneqq p(\mathbf{y}_t | \theta, \mathbf{y}_{1:t-1})$ is the **true likelihood**, $m_t(\theta)$ is a zero-mean **random variable** with finite variance and $b_t(\theta)$ is a deterministic and bounded **bias function**.





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Convergence Theorem (NHF)

Theorem 1

Let the sequence of observations $y_{1:t_o}$ be arbitrary but fixed, with $t_o < \infty$, and choose an arbitrary function $h \in B(D)$. Let $p^N(d\theta|\mathbf{y}_{1:t}) = \frac{1}{N} \sum_{i=1}^N \delta_{\theta_t^i}(d\theta)$ be the random probability measure in the parameter space generated by the nested filter. If A.1 holds and under regularity conditions, then

$$\|\int h(\boldsymbol{\theta})p^{N}(d\boldsymbol{\theta}|\boldsymbol{y}_{1:t}) - \int h(\boldsymbol{\theta})\bar{p}(\boldsymbol{\theta}|\boldsymbol{y}_{1:t})d\boldsymbol{\theta}\|_{p} \leq \frac{c_{t}\|h\|_{\infty}}{\sqrt{N}},$$

for $t = 0, 1, ..., t_o$, where $\{c_t\}_{0 \le t \le t_o}$ is a sequence of constants independent of N. \Box

If, instead of the true likelihood $u_t(\theta)$, we use another biased function $\bar{u}_t(\theta) \neq u_t(\theta)$ to update the posterior probability measure $p(\theta|\mathbf{y}_{1:t})$, then we obtain the new sequence of measures

$$\bar{\boldsymbol{p}}(\boldsymbol{\theta}|\boldsymbol{y}_{1:t}) \propto \bar{u}_t(\boldsymbol{\theta}) \star \bar{\boldsymbol{p}}(\boldsymbol{\theta}|\boldsymbol{y}_{1:t-1}), \quad t = 1, 2, \dots$$





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Convergence Theorem (NHF)

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Nested Gaussian filter (NGF)

UKF (M sigma-points)	1 st layer
- Generate sigma-points: $\{\boldsymbol{\theta}_t^i, w_t^i\}, 0 \le i \le M - 1 \longrightarrow p(\boldsymbol{\theta} \boldsymbol{y}_{1:})$)
- Likelihood of $ heta \longrightarrow p(oldsymbol{y}_t oldsymbol{ heta}_t^i, oldsymbol{y}_{1:t-1})$	
EKF (per each sample sigma-point <i>i</i>)	2 nd layer
- Prediction: $p(\mathbf{x}_t \boldsymbol{\theta}_t^i, \mathbf{y}_{1:t-1}) \approx \mathcal{N}(\mathbf{x}_t \mathbf{x}_{t t-1,\bar{\boldsymbol{\theta}}}^i)$	$m{C}_{t t-1,ar{m{ heta}}_t^i}^i)$
- Likelihood of $ heta$ and $m{x}_t$: $p(m{y}_t m{x}_t, m{ heta}_t^i)$	
- Update: $\rho(\boldsymbol{x}_t \boldsymbol{\theta}_t^i, \boldsymbol{y}_{1:t}) \approx \mathcal{N}(\boldsymbol{x}_t \boldsymbol{x}_{t t, \boldsymbol{\theta}_t^i}^i, \boldsymbol{C}_{t t, \boldsymbol{\theta}_t^i}^i)$	$\binom{i}{t}$
- Compute $\hat{\boldsymbol{\theta}}_t^i$ and $\hat{\boldsymbol{C}}_t^{\boldsymbol{\theta}} \longrightarrow p(\boldsymbol{\theta} \boldsymbol{y}_{1:t}) \approx \mathcal{N}(\boldsymbol{\theta}_t \hat{\boldsymbol{\theta}}_t^i, \hat{\boldsymbol{C}}_t^{\boldsymbol{\theta}})$	

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Nested Gaussian filter (NGF)

UKF (M sigma-points) 1st layer - Generate sigma-points: $\{\boldsymbol{\theta}_t^i, \boldsymbol{w}_t^i\}, 0 \le i \le M - 1 \longrightarrow p(\boldsymbol{\theta}|\boldsymbol{y}_{1:t-1})$ - Likelihood of $\theta \longrightarrow p(\mathbf{y}_t | \boldsymbol{\theta}_t^i, \mathbf{y}_{1:t-1})$ EKF (per each sample sigma-point *i*) 2nd layer - Prediction: $p(\mathbf{x}_t | \boldsymbol{\theta}_t^i, \mathbf{y}_{1:t-1}) \approx \mathcal{N}(\mathbf{x}_t | \mathbf{x}_{t|t-1, \bar{\boldsymbol{\theta}}_t^i}^i, \mathbf{C}_{t|t-1, \bar{\boldsymbol{\theta}}_t^i}^i)$ - Likelihood of $\boldsymbol{\theta}$ and \boldsymbol{x}_t : $p(\boldsymbol{y}_t | \boldsymbol{x}_t, \boldsymbol{\theta}_t^i)$ - Update: $p(\mathbf{x}_t | \boldsymbol{\theta}_t^i, \mathbf{y}_{1:t}) \approx \mathcal{N}(\mathbf{x}_t | \mathbf{x}_{t|t, \boldsymbol{\theta}_t^i}^i, \boldsymbol{C}_{t|t, \boldsymbol{\theta}_t^i}^i)$





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Conclusions

Recursivity of NGF

- \rightarrow This filter is **not recursive**.
 - As every time step t the sigma-points θⁱ_t are recalculated, the computations of the second layer need to start from scratch.
 - In order to make it recursive we approximate

$$p(\boldsymbol{x}_{t-1}|\boldsymbol{y}_{1:t-1},\boldsymbol{\theta}_t^i) \approx p(\boldsymbol{x}_{t-1}|\boldsymbol{y}_{1:t-1},\boldsymbol{\theta}_{t-1}^i).$$





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Conclusions

Recursive NGF

Every time step the norm $\| \boldsymbol{\theta}_t^i - \boldsymbol{\theta}_{t-1}^i \|_p$ is computed and compared against a prescribed relative **threshold** $\lambda > 0$.

- If $\| \boldsymbol{\theta}_t^i \boldsymbol{\theta}_{t-1}^i \|_{p} < \lambda \| \boldsymbol{\theta}_{t-1}^i \|_{p}$, we assume $p(\boldsymbol{x}_{t-1} | \boldsymbol{y}_{1:t-1}, \boldsymbol{\theta}_t^i) \approx p(\boldsymbol{x}_{t-1} | \boldsymbol{y}_{1:t-1}, \boldsymbol{\theta}_{t-1}^i)$.
- If $\| \boldsymbol{\theta}_{t}^{i} \boldsymbol{\theta}_{t-1}^{i} \|_{p} \ge \lambda \| \boldsymbol{\theta}_{t-1}^{i} \|_{p}$, we need to compute the pdf $p(\boldsymbol{x}_{t-1} | \boldsymbol{y}_{1:t-1}, \boldsymbol{\theta}_{t}^{i})$ from the prior $p(\boldsymbol{x}_{0})$.

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Focusing on an efficient use of the available computational resources.

- Reduction of the number of θ -samples when the filter converges [Accepted paper, ICASSP 2023]⁶.
- Adapting the number of samples of each layer online

 \longrightarrow Further study of $p(\mathbf{y}_t | \mathbf{y}_{1:t-1}, \boldsymbol{\theta})$.

⁶Pérez-Vieites and Elvira, "Adaptive Gaussian nested filter for parameter estimation and state tracking in dynamical systems": ロトイクトイモトイモト モーシュクヘア 29/37

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The Lorenz 63 model

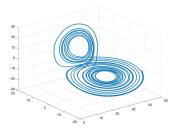
We consider a stochastic Lorenz 63 model, whose dynamics are described by

- 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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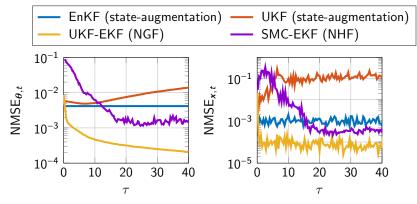


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Numerical results [Signal Processing 2021]⁷



 \longrightarrow The nested schemes outperform the augmented-state methods.

 \rightarrow The UKF-EKF is three times faster than SMC-EKF.



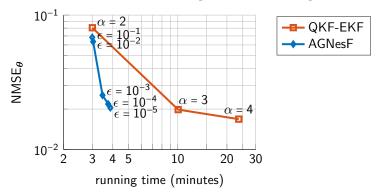
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Numerical results [ICASSP 2023]⁸



- 1. NGF: QKF-EKF with different number of points/samples, N_{θ} (the greater α , the greater N_{θ} .
- 2. Adaptive Gaussian nested filter (AGNesF).

⁸Pérez-Vieites and Elvira, "Adaptive Gaussian nested filter for parameter estimation and state tracking in dynamical systems": $\Box \rightarrow \langle \Box \rangle + \langle \Box \rangle +$

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Conclusions

We have introduced a generalized nested methodology

- 1. that is flexible. It admits different types of filtering techniques in each layer, leading to a **set of algorithms**.
- 2. that works recursively.
- 3. with theoretical guarantees (under general assumptions).

Open to collaborate and discuss possible applications !

- Time-series problems with availability of relatively frequent observations / data
- e.g., remote sensing, energy, ecology, but not only



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Thank you!

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