Nested filtering methods for Bayesian inference in state space models

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Joint work with
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Introduction

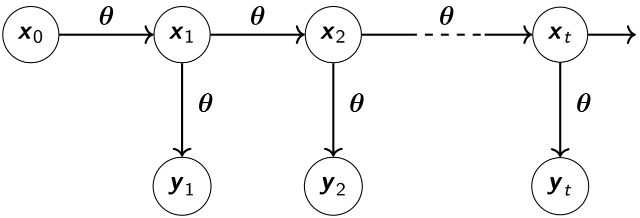
We aim at **estimating the time evolution** of **dynamical systems** of different fields of science, such as:

- **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.
- ...

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

State-space model

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



State-space model

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

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

- $\boldsymbol{f}$ and $\boldsymbol{g}$ are the state transition function and the observation function
- $\boldsymbol{v}_t$ and $\boldsymbol{r}_t$ are 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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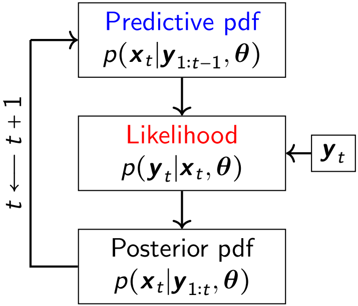
State estimation

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

Classical filtering methods assume $\boldsymbol{\theta}$ is known, and compute



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

$\longrightarrow$ Usually $\boldsymbol{\theta}$ is not given and it needs to be estimated as well.
Therefore, we are interested in both parameter and state estimation.

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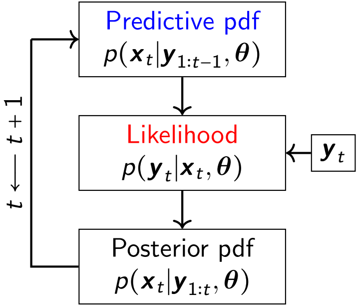

$$p(\boldsymbol{x}_t|\boldsymbol{y}_{1:t-1},\boldsymbol{\theta}) = \int \underbrace{p(\boldsymbol{x}_t|\boldsymbol{\theta},\boldsymbol{x}_{t-1})}_{\text{Transition pdf}} \overbrace{p(\boldsymbol{x}_{t-1}|\boldsymbol{y}_{1:t-1},\boldsymbol{\theta})}^{\text{Previous post. pdf}} d\boldsymbol{x}_{t-1}$$

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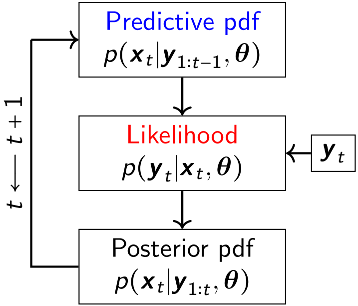

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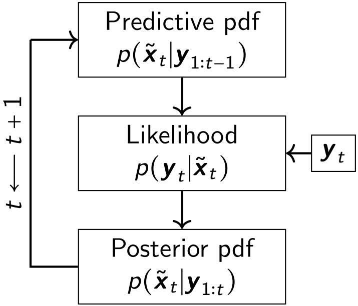
State-of-the-art methods for parameter and state estimation

1. **State augmentation methods with artificial dynamics**



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

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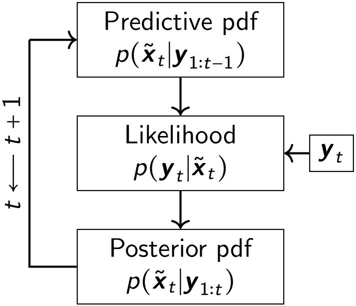

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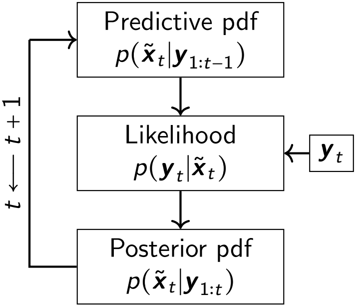

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State-of-the-art methods for parameter and state estimation

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 $\boldsymbol{\theta}$ conditional on the states $\boldsymbol{x}_0, \ldots, \boldsymbol{x}_t$ can be computed in closed form.
- However, this approach is restricted to very specific models.

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

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 (SMC^2)**[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.

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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.

$\longrightarrow$ 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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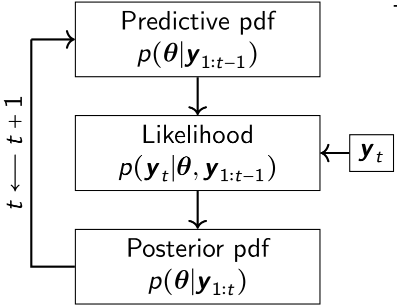
Model inference

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

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

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

1^{st} layer of inference



The **posterior pdf** can be written as

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

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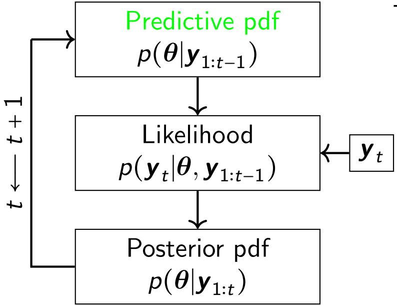

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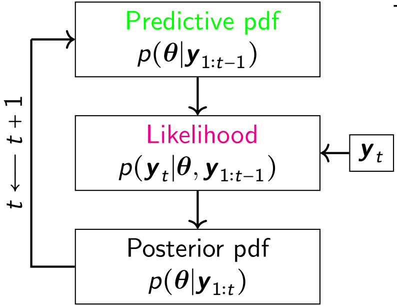

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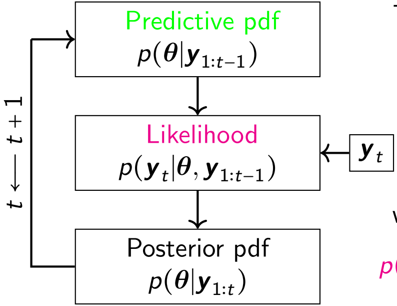

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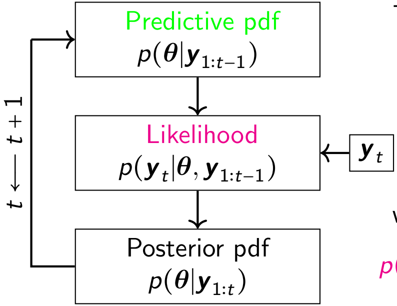
where

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

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

1^{st} layer of inference



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

where

$$p(\boldsymbol{y}_t|\boldsymbol{\theta}, \boldsymbol{y}_{1:t-1}) = \int \underbrace{p(\boldsymbol{y}_t|\boldsymbol{x}_t, \boldsymbol{\theta})}_{\text{Likelihood } (2^{nd} \text{ layer})} \overbrace{p(\boldsymbol{x}_t|\boldsymbol{\theta}, \boldsymbol{y}_{1:t-1})}^{\text{Pred. pdf } (2^{nd} \text{ layer})} d\boldsymbol{x}_t$$

Model inference

1st layer

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

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

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

$$\underbrace{p(\mathbf{y}_t|\mathbf{x}_t,\boldsymbol{\theta})}_{\text{Likelihood of } \mathbf{x}}$$

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

2nd layer

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

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 ⟶ Monte Carlo-based methods (e.g., SMC or SQMC)
   - x-layer ⟶ Gaussian techniques (e.g., EKFs or EnKFs)
3. **Nested Gaussian filters (NGFs)**[5].
   - θ-layer ⟶ Deterministic sampling methods (e.g., UKF).
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Nested hybrid filter (NHF)

SMC (N samples)

1st layer

- Jittering: $\bar{\boldsymbol{\theta}}_t^i \sim \kappa_N(\boldsymbol{\theta}|d\boldsymbol{\theta}_{t-1}^i), 1 \leq i \leq N \longrightarrow p(\boldsymbol{\theta}|\boldsymbol{y}_{1:t-1})$
- Likelihood of θ: weights $w_t^i \longrightarrow p(\boldsymbol{y}_t|\bar{\boldsymbol{\theta}}_t^i, \boldsymbol{y}_{1:t-1})$

EKF (per each sample i)

2nd layer

- Prediction: $p(\boldsymbol{x}_t|\bar{\boldsymbol{\theta}}_t^i, \boldsymbol{y}_{1:t-1}) \approx \mathcal{N}(\boldsymbol{x}_t|\boldsymbol{x}^i_{t|t-1,\bar{\boldsymbol{\theta}}_t^i}, \boldsymbol{C}^i_{t|t-1,\bar{\boldsymbol{\theta}}_t^i})$
- Likelihood of $\boldsymbol{\theta}$ and $\boldsymbol{x}_t$: $p(\boldsymbol{y}_t|\boldsymbol{x}_t, \bar{\boldsymbol{\theta}}_t^i)$
- Update: $p(\boldsymbol{x}_t|\bar{\boldsymbol{\theta}}_t^i, \boldsymbol{y}_{1:t}) \approx \mathcal{N}(\boldsymbol{x}_t|\boldsymbol{x}^i_{t|t,\bar{\boldsymbol{\theta}}_t^i}, \boldsymbol{C}^i_{t|t,\bar{\boldsymbol{\theta}}_t^i})$

- Resampling: $\{\boldsymbol{\theta}_t^i, \boldsymbol{x}^i_{t|t,\boldsymbol{\theta}_t^i}, \boldsymbol{C}^i_{t|t,\boldsymbol{\theta}_t^i}\} \longrightarrow p(\boldsymbol{\theta}|\boldsymbol{y}_{1:t})$

Nested hybrid filter (NHF)

SMC (N samples)

1^{st} layer

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- Likelihood of $\boldsymbol{\theta}$: weights $w_t^i \longrightarrow p(\boldsymbol{y}_t|\bar{\boldsymbol{\theta}}_t^i, \boldsymbol{y}_{1:t-1})$

EKF (per each sample i)

2^{nd} layer

- Prediction: $p(\boldsymbol{x}_t|\bar{\boldsymbol{\theta}}_t^i, \boldsymbol{y}_{1:t-1}) \approx \mathcal{N}(\boldsymbol{x}_t|\boldsymbol{x}^i_{t|t-1,\bar{\boldsymbol{\theta}}_t^i}, \boldsymbol{C}^i_{t|t-1,\bar{\boldsymbol{\theta}}_t^i})$

- Likelihood of $\boldsymbol{\theta}$ and $\boldsymbol{x}_t$: $p(\boldsymbol{y}_t|\boldsymbol{x}_t, \bar{\boldsymbol{\theta}}_t^i)$

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EKF (per each sample i) — 2^{nd} layer

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Recursivity of NPF and NHF

- θ is static and **samples θ^i_{t-1} do not evolve**. After several resampling steps the filter would degenerate.
- It is convenient to have a procedure to generate a new set $\{\bar{\theta}^i_t\}_{1\leq i\leq N}$ which yields an approximation of $p(\theta|\mathbf{y}_{1:t-1})$.

$\longrightarrow$ The jittering step allows these filters to run **recursively**:

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

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Convergence Theorem (NHF)

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

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

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

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

where $u_t(\theta) := p(\boldsymbol{y}_t|\theta, \boldsymbol{y}_{1:t-1})$ 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 $p^N(d\boldsymbol{\theta}|\mathbf{y}_{1:t}) = \frac{1}{N}\sum_{i=1}^{N}\delta_{\boldsymbol{\theta}_t^i}(d\boldsymbol{\theta})$ be the random probability measure in the parameter space generated by the nested filter. If A.1 holds and under regularity conditions, then

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

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

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

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- Generate sigma-points: $\{\boldsymbol{\theta}_t^i, w_t^i\}, 0 \leq i \leq M-1 \longrightarrow p(\boldsymbol{\theta}|\boldsymbol{y}_{1:t-1})$
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Recursivity of NGF

$\longrightarrow$ This filter is **not recursive**.

- As every time step t the **sigma-points θ_t^i are recalculated**, the computations of the second layer need to **start from scratch**.
- In order to make it **recursive** we approximate

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

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 $\| \boldsymbol{\theta}_t^i - \boldsymbol{\theta}_{t-1}^i \|_p > \lambda \| \boldsymbol{\theta}_{t-1}^i \|_p$,
  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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Ongoing work

Focusing on an efficient use of the available computational resources.

- Reduction of the number of $\boldsymbol{\theta}$-samples when the filter converges [Accepted paper, ICASSP 2023][6].
- Adapting the number of samples of each layer online
  $\longrightarrow$ Further study of $p(\boldsymbol{y}_t|\boldsymbol{y}_{1:t-1}, \boldsymbol{\theta})$.

[6] Pérez-Vieites and Elvira, "Adaptive Gaussian nested filter for parameter estimation and state tracking in dynamical systems".

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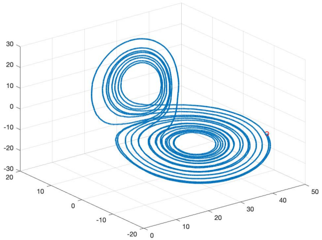
The Lorenz 63 model

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**

$$dx_1 = [-S(x_1 - x_2)]d\tau + \sigma dv_1,$$
$$dx_2 = [Rx_1 - x_2 - x_1x_3]d\tau + \sigma dv_2,$$
$$dx_3 = [x_1x_2 - Bx_3]d\tau + \sigma dv_3,$$



The Lorenz 63 model

- Applying a discretization method with step Δ, we obtain

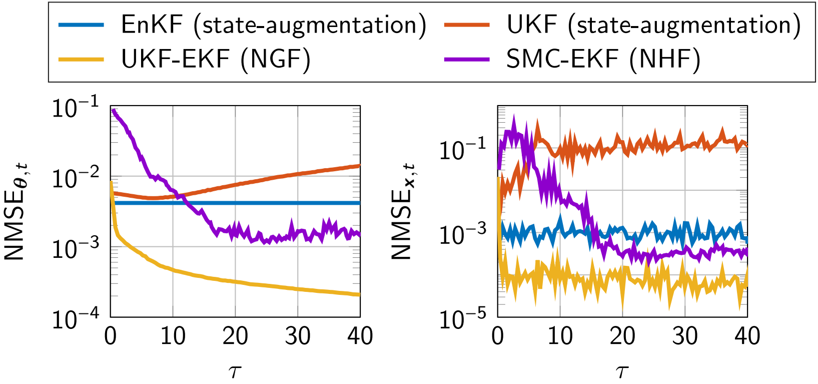
$$x_{1,t+1} = x_{1,t} - \Delta S(x_{1,t} - x_{2,t}) + \sqrt{\Delta}\sigma v_{1,t},$$
$$x_{2,t+1} = x_{2,t} + \Delta[(R - x_{3,t})x_{1,t} - x_{2,t}] + \sqrt{\Delta}\sigma v_{2,t},$$
$$x_{3,t+1} = x_{3,t} + \Delta(x_{1,t}x_{2,t} - Bx_{3,t}) + \sqrt{\Delta}\sigma v_{3,t},$$

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

Numerical results [Signal Processing 2021][7]

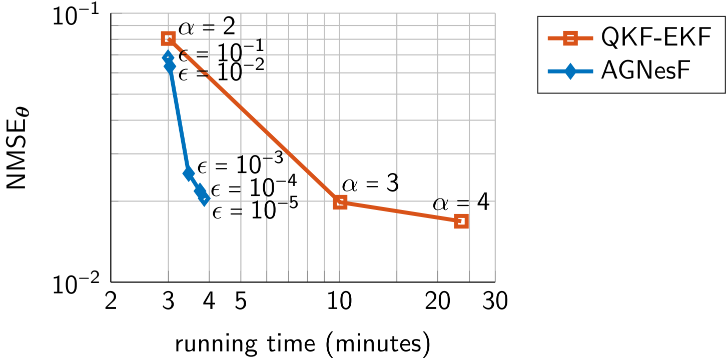


⟶ The nested schemes outperform the augmented-state methods.

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

[7] Pérez-Vieites and Míguez, "Nested Gaussian filters for recursive Bayesian inference and nonlinear tracking in state space models".

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).

[8] Pérez-Vieites and Elvira, "Adaptive Gaussian nested filter for parameter estimation and state tracking in dynamical systems".

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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!

- Pérez-Vieites & Elvira (2023). *Adaptive Gaussian nested filter for parameter estimation and state tracking in dynamical systems*. In ICASSP 2023 [Accepted].
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