

Nested filtering methods for Bayesian inference in state space models

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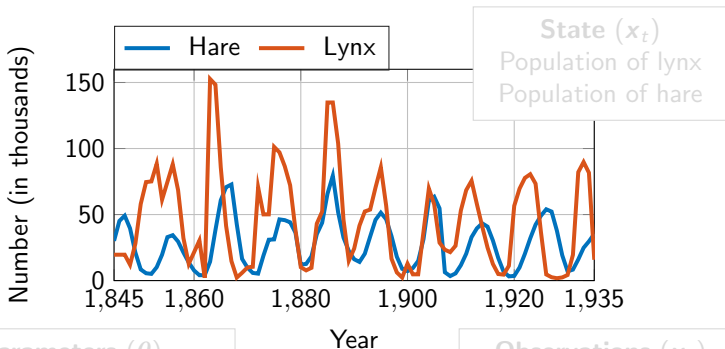
Introduction

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.
- ...

Introduction

Study of hare-lynx interactions in a region of Canada.



Parameters (θ)

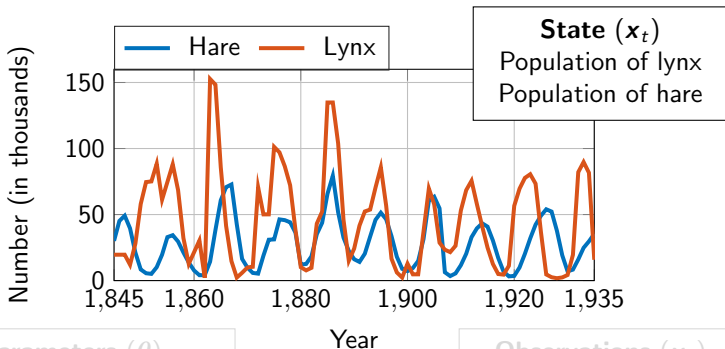
Prey growth rate
Predator-prey encounters
Predator growth rate
Predator mortality rate

Observations (y_t)

Number of pelts sold
Sighting
etc

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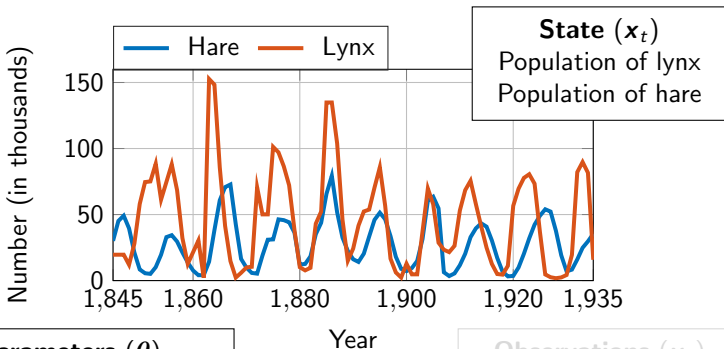
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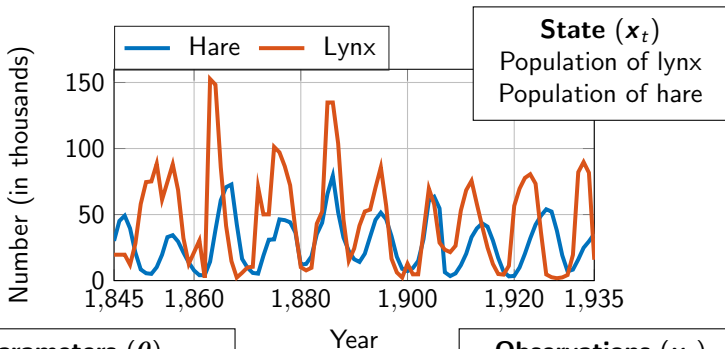


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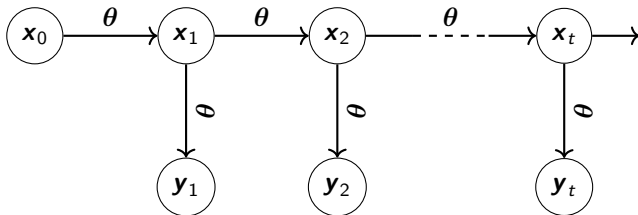
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State-space model

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



State-space model

These state-space systems can be written as

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

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

- \mathbf{f} and \mathbf{g} are the state transition function and the observation function
- \mathbf{v}_t and \mathbf{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 $\mathbf{x}_0 \sim p(\mathbf{x}_0)$
- Transition pdf of the state: $\mathbf{x}_t \sim p(\mathbf{x}_t | \mathbf{x}_{t-1}, \boldsymbol{\theta})$
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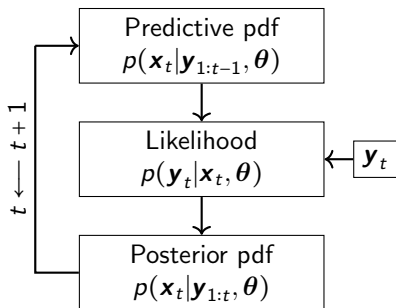
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State estimation

→ We are interested in the **Bayesian estimation of the state variables**, this is the **posterior density function of the state** $p(\mathbf{x}_t | \mathbf{y}_{1:t}, \boldsymbol{\theta})$.

Classical filtering methods:



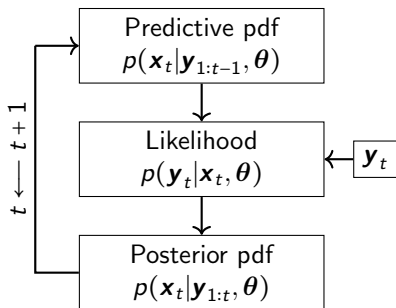
- They assume $\boldsymbol{\theta}$ is known.
- The **predictive pdf** can be computed with the conditional pdf $p(\mathbf{x}_t | \mathbf{x}_{t-1}, \boldsymbol{\theta})$ (given by the state-space model).
- The **likelihood** is given by the state-space model.

→ Usually $\boldsymbol{\theta}$ is not given.

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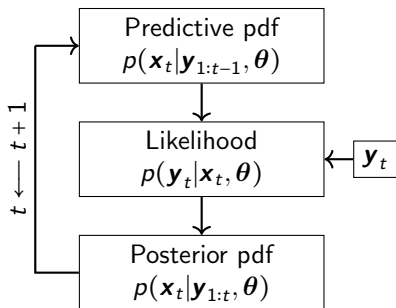
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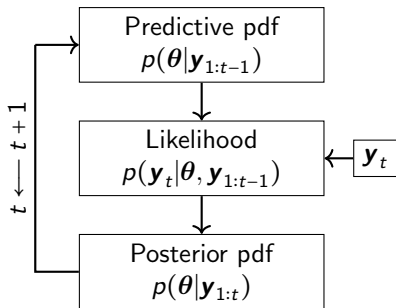


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Parameter estimation

Applying the **same principles** to parameter estimation

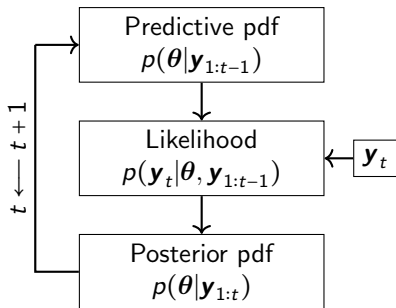


- The **likelihood** is **NOT** described by the state-space model.
- Neither the likelihood nor the posterior distribution of θ can be **computed directly**.

→ Several approaches have been proposed to solve this problem.

Parameter estimation

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→ **Several approaches** have been proposed to solve this problem.

State of the Art Methods

Some **methods for parameter and state estimation** can be classified as

- **State augmentation methods with artificial dynamics.** They use an **extended state vector** $\tilde{\mathbf{x}}_t = [\mathbf{x}_t, \boldsymbol{\theta}_t]^\top$.
- **Particle learning (PL) techniques.** It is a **sampling-resampling scheme** that depends only on a set of **finite-dimensional statistics**.
- **Recursive maximum likelihood (RML) methods.** They are **well-principled** but they provide **only output point estimates**.

State of the Art Methods

During the past years, there have been advances leading to methods that

- aim at calculating the **posterior probability distribution of the unknown variables and parameters** of the models.
- can be applied to a **broad class of models**.
- are **well-principled probabilistic methods** with **theoretical guarantees**.

State of the Art Methods

Some examples are:

- **sequential Monte Carlo square (SMC²)**¹ → batch technique
- **particle Markov chain Monte Carlo (PMCMC)**² → batch
- **nested particle filter (NPF)**³: two intertwined layers of Monte Carlo methods (one for the state tracking and the other for the parameter estimation)
 - it is a recursive technique.
 - The computational cost becomes prohibitive in high-dimensional problems.

¹Chopin, Jacob, and Papaspiliopoulos, “SMC²: A sequential Monte Carlo algorithm with particle Markov chain Monte Carlo updates”.

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Summary

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.
- Batch technique.
- Prohibitive computational cost for high-dimensional problems.

Objectives

We propose a **generalised methodology** that estimate the **joint posterior probability distribution of the parameters and the state** that

- works **recursively**,
- uses the **nested structure** of the NPF and
- reduces the **computational cost**.

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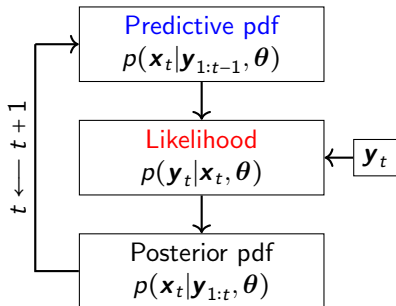
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Optimal filter

We assume θ and the previous post. pdf $p(\mathbf{x}_{t-1}|\mathbf{y}_{1:t-1}, \theta)$ are known.

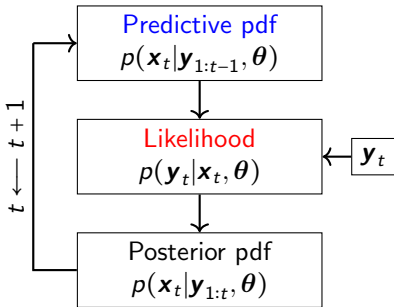


The **posterior pdf** can be written as

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

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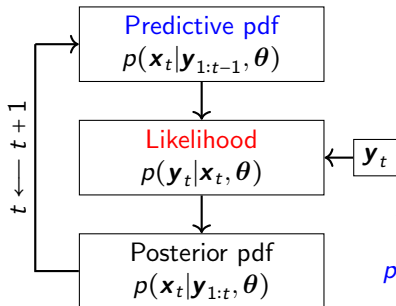


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where

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

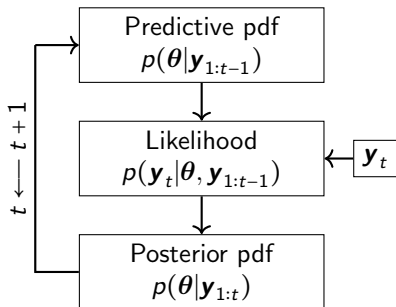
Model inference

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

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

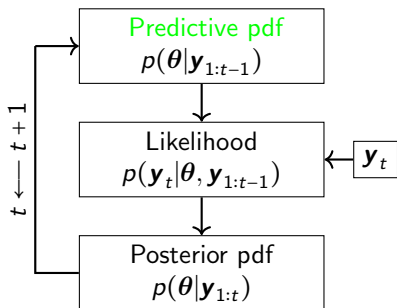
→ The **key difficulty** in this class of models is **the Bayesian estimation of the parameter vector $\boldsymbol{\theta}$** .

1st layer of inference



The **posterior pdf** can be written as

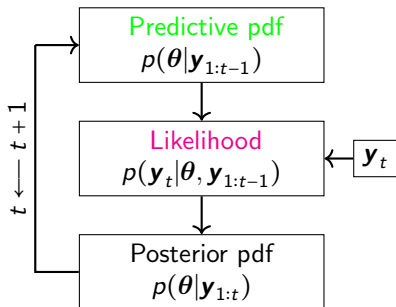
$$p(\theta | \mathbf{y}_{1:t}) \propto p(\mathbf{y}_t | \theta, \mathbf{y}_{1:t-1}) p(\theta | \mathbf{y}_{1:t-1})$$

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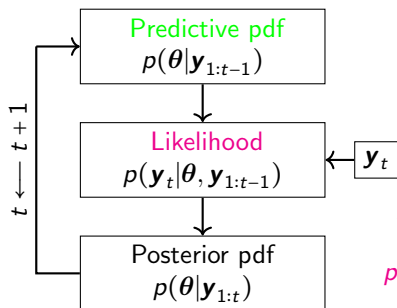
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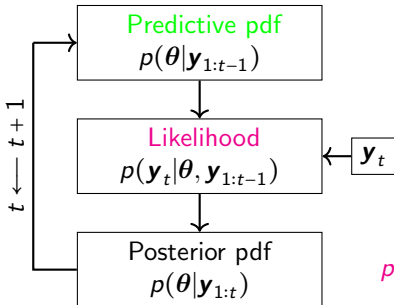
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where

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

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

1st layer of inference



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where

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

Model inference

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

Pred. pdf of θ

$$\underbrace{p(y_t|\theta, y_{1:t-1})}_{\text{Likelihood of } \theta} = \int p(y_t|x_t, \theta)p(x_t|\theta, y_{1:t-1})dx_t$$

Likelihood of θ

$$\underbrace{p(x_t|\theta, y_{1:t-1})}_{\text{Pred. pdf of } x} = \int p(x_t|x_{t-1}, \theta)p(x_{t-1}|\theta, y_{1:t-1})dx_{t-1}$$

Pred. pdf of x

$$\underbrace{p(y_t|x_t, \theta)}_{\text{Likelihood of } x}$$

Likelihood of x

$$\underbrace{p(x_t|\theta, y_{1:t})}_{\text{Post. pdf of } x} \propto p(y_t|x_t, \theta)p(x_t|\theta, y_{1:t-1})$$

Post. pdf of x

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

Post. pdf of θ

1st layer

2nd layer

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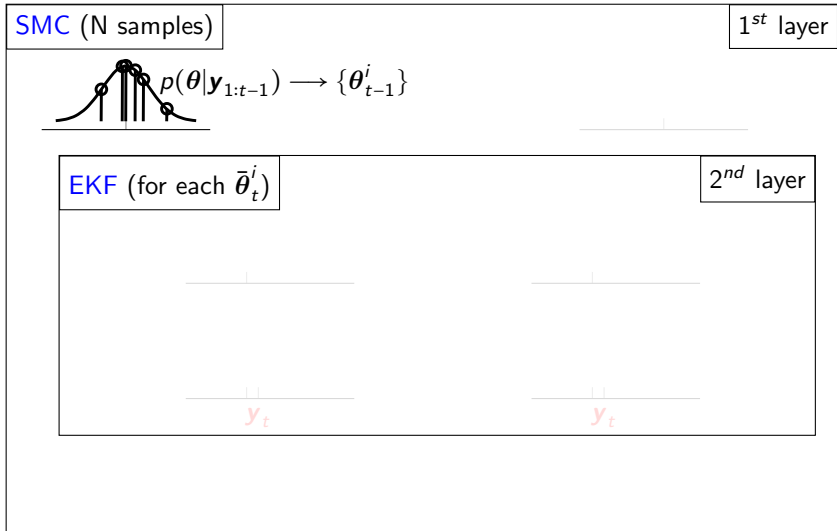
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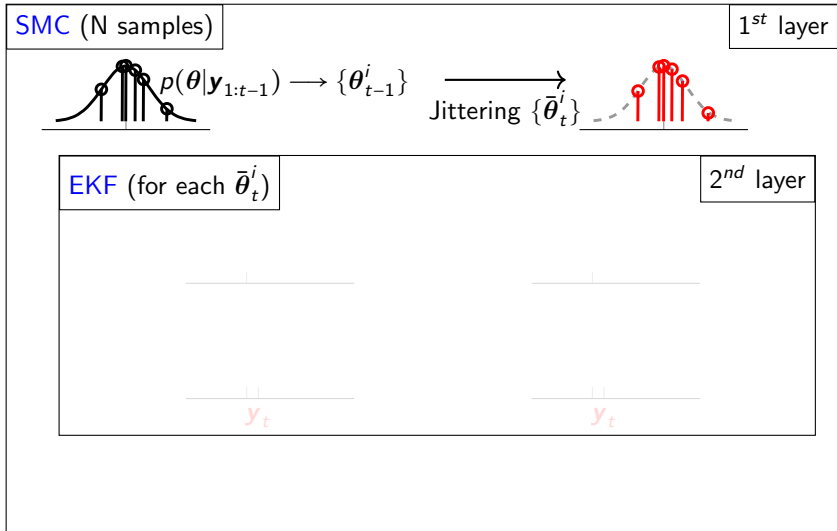
Nested hybrid filter

- We introduce the use of **different types of Monte Carlo methods** in the **first layer** of the algorithm (SMC or SQMC).
- **Gaussian methods** are applied in the **second layer** (EKFs, EnKFs, etc).
- We obtain theoretical guarantees on the **convergence**.

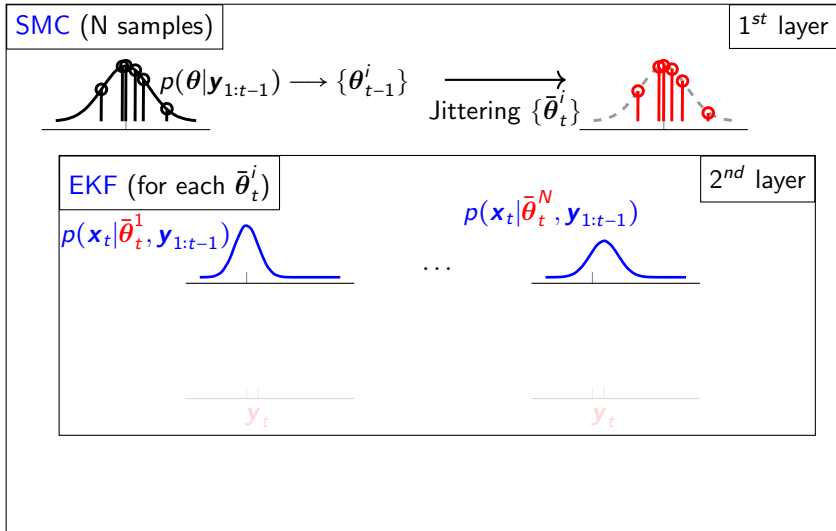
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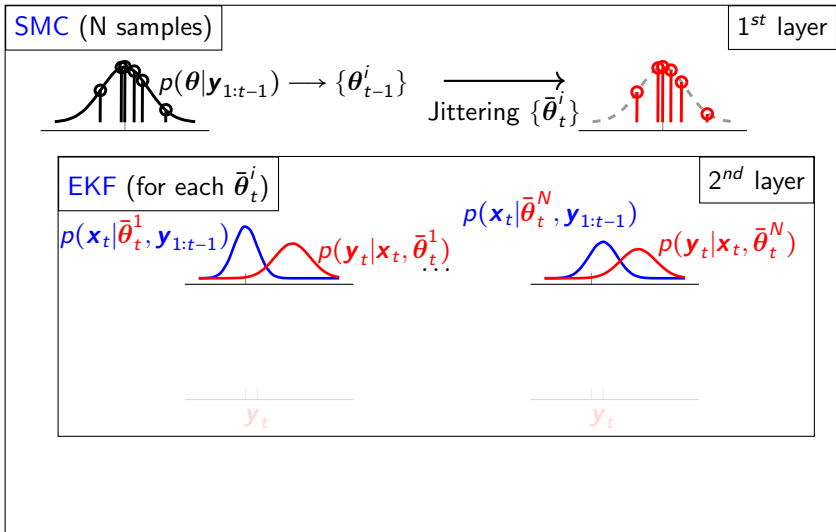
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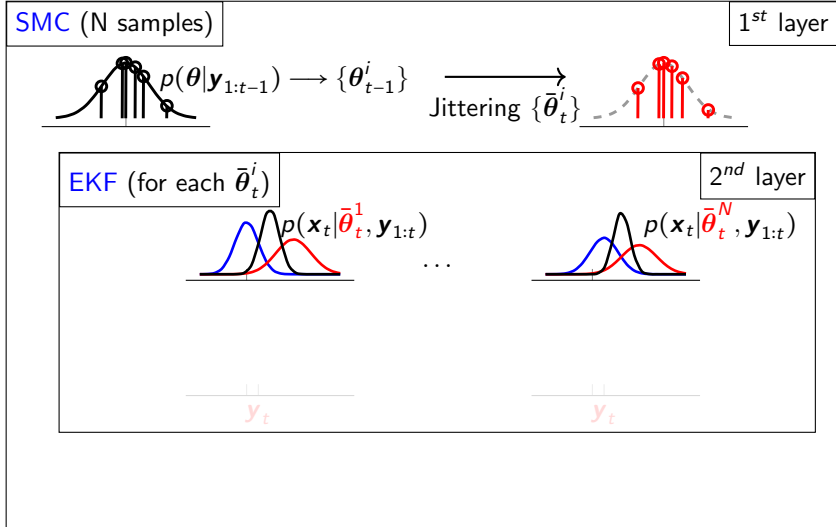
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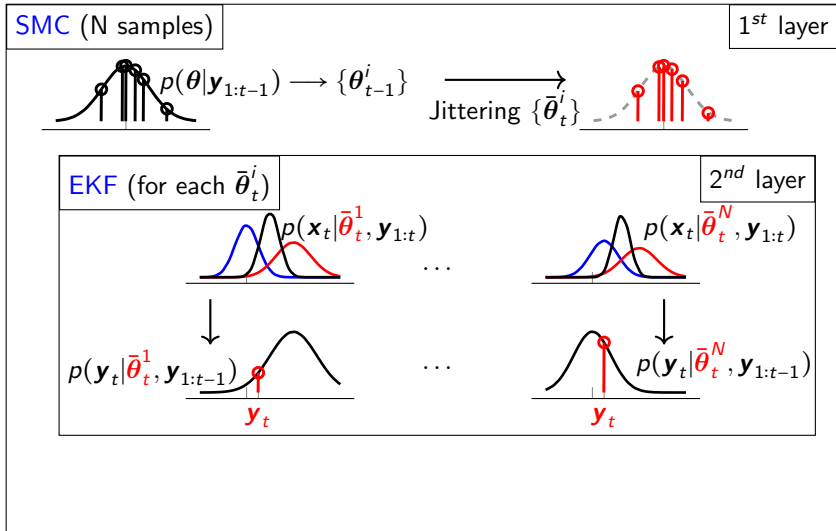
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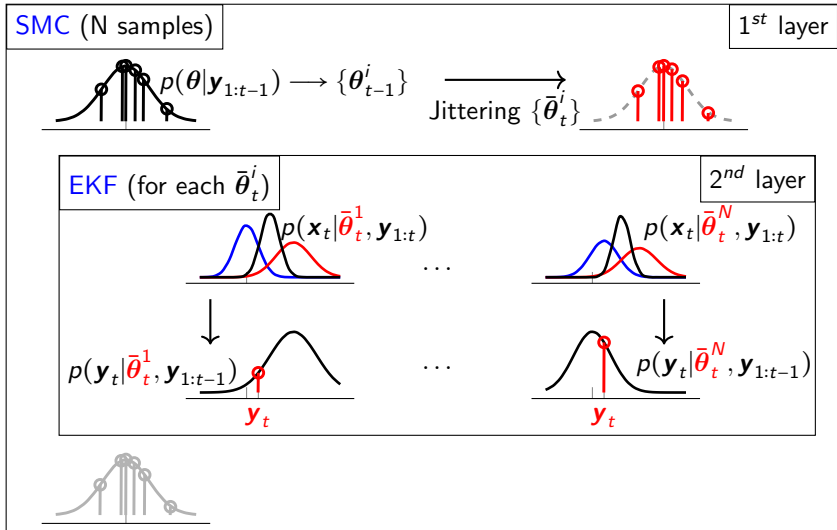
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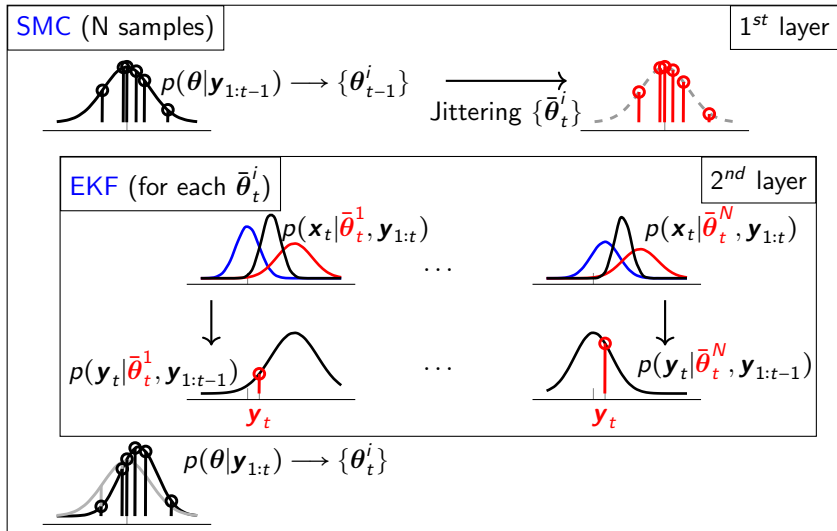
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Convergence Theorem

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

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

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

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

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Convergence Theorem

Theorem 1

Let the sequence of observations $y_{1:t_0}$ be arbitrary but fixed, with $t_0 < \infty$, and choose an arbitrary function $h \in B(D)$. Let $p^N(d\theta|y_{1:t}) = \frac{1}{N} \sum_{i=1}^N \delta_{\theta_i^t}(d\theta)$ be the random probability measure in the parameter space generated by the nested filter. If A.1 holds and under regularity conditions, then

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

for $t = 0, 1, \dots, t_0$, where $\{c_t\}_{0 \leq t \leq t_0}$ is a sequence of constants independent of N . \square

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 $p(\theta|y_{1:t})$, then we obtain the new sequence of measures

$$\bar{p}(\theta|y_{1:t}) \propto \bar{u}_t(\theta) * \bar{p}(\theta|y_{1:t-1}), \quad t = 1, 2, \dots$$

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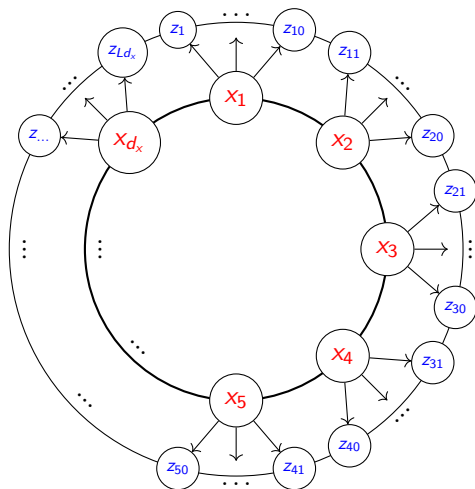
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A stochastic Lorenz 96 model



A stochastic Lorenz 96 model

We consider a **stochastic two-scale Lorenz 96 model** that is described by

- the **slow state** variable, $\mathbf{x} = [x_1, \dots, x_{d_x}]^\top$,
- the **fast state** variable, $\mathbf{z} = [z_1, \dots, z_{d_z}]^\top$, with $d_z = Ld_x$,
- the **static parameters** $\alpha = [F, C, B, H]^\top$ and
- for $j = 1, \dots, d_x$ and $l = 1, \dots, d_z$, the following **SDEs (in continuous time)**

$$\begin{aligned}
 dx_j &= \underbrace{f_{1,j}(\mathbf{x}, \mathbf{z}, \alpha)}_{\left[-x_{j-1}(x_{j-2} - x_{j+1}) - x_j + F - \frac{HC}{B} \sum_{l=(j-1)L}^{Lj-1} z_l \right]} d\tau + \sigma_x dv_j, \\
 dz_l &= \underbrace{f_{2,l}(\mathbf{x}, \mathbf{z}, \alpha)}_{\left[-CBz_{l+1}(z_{l+2} - z_{l-1}) - Cz_l + \frac{CF}{B} + \frac{HC}{B} x_{\lfloor (l-1)L \rfloor} \right]} d\tau + \sigma_z dw_l,
 \end{aligned}$$

A Stochastic Lorenz 96 Model

- Applying a discretization method with a step Δ , we obtain the **discrete-time version**

$$\mathbf{x}_t = \mathbf{x}_{t-1} + \Delta \mathbf{f}_1(\mathbf{x}_{t-1}, \mathbf{z}_{t-1}, \boldsymbol{\alpha}) + \sigma_{\mathbf{x}} \mathbf{v}_t,$$

$$\mathbf{z}_t = \mathbf{z}_{t-1} + \Delta \mathbf{f}_2(\mathbf{x}_{t-1}, \mathbf{z}_{t-1}, \boldsymbol{\alpha}) + \sigma_{\mathbf{z}} \mathbf{w}_t$$

- The **observations** are written as

$$\mathbf{y}_t = \begin{bmatrix} x_{K,tm} \\ x_{2K,tm} \\ \vdots \\ x_{d_y K,tm} \end{bmatrix} + \mathbf{r}_t, \quad (1)$$

→ This model is used to **generate the ground truth values** for the **slow variables** $\{\mathbf{x}_t\}_{t \geq 0}$, and the **synthetic observations**, $\{\mathbf{y}_t\}_{t \geq 0}$.

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A Stochastic Lorenz 96 Model

For the **forecast model**, we use instead the differential equation

$$\dot{x}_j = f_j(\mathbf{x}, \boldsymbol{\theta}) = -x_{j-1}(x_{j-2} - x_{j+1}) - x_j + F - \frac{HC}{B} \sum_{l=(j-1)L}^{Lj-1} z_l \quad (2)$$

where

- function $\ell(x_j, \mathbf{a})$ is a polynomial in x_j of degree 2, for the coupling term $\frac{HC}{B} \sum_{l=(j-1)L}^{Lj-1} \bar{z}_l$.
- $\mathbf{a} = [a_1, a_2]^T$ is a (constant) parameter vector,
- $\boldsymbol{\theta} = [F, \mathbf{a}^T]^T$ contains all the parameters.

A Stochastic Lorenz 96 Model

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Numerical results

We have **implemented four different algorithms** following the **nested hybrid methodology**:

		2nd layer	
		Extended Kalman filter (EKF)	Ensemble Kalman filter (EnKF)
1st layer	Sequential Monte Carlo (SMC)	SMC-EKF	SMC-EnKF
	Sequential quasi-Monte Carlo (SQMC)	SQMC-EKF	SQMC-EnKF

Numerical results

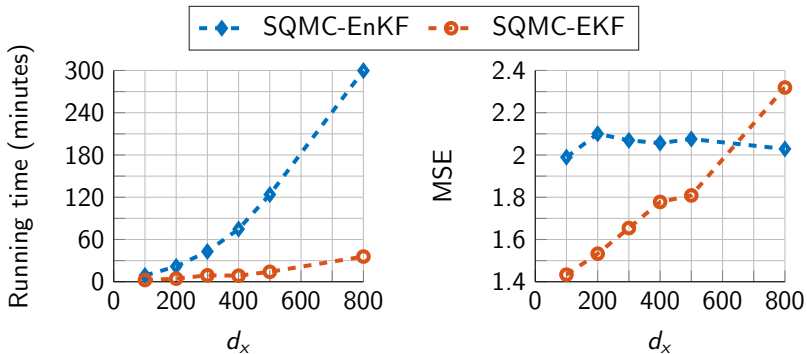
Algorithm	Running time (minutes)	MSE
NHF: SQMC-EKF	2.16	0.46
NHF: SMC-EKF	2.27	0.49
NHF: SQMC-EnKF	6.83	0.62
NHF: SMC-EnKF	7.12	0.95
NPF ($N = M = 800$)	17.96	11.91

→ In the four cases of NHF, the accuracy and the running time are improved in comparison to the NPF.

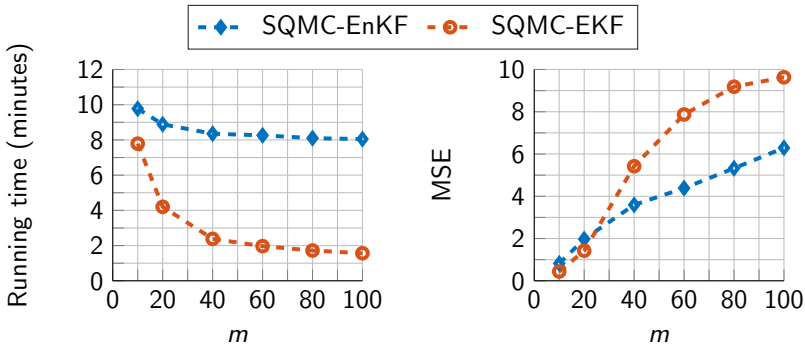
→ The least error and running times are obtained with the NHFs that use the EKF in the second layer.

→ Using the same samples N , the SQMC reduces slightly the running time and the error compared to the SMC.

Numerical results



Numerical results



→ As the **gap between observations** m increases, less data points are effectively available for the estimation task.

Summary of NHFs

- We introduce the **nested hybrid filters (NHFs)**, that use **Monte Carlo**-based methods in the first layer and **Gaussian** methods in the second layer.
- The algorithm **converges to a well defined limit distribution**.
- We have **implemented four algorithms** (SQMC-EKF, SQMC-EnKF, SMC-EKF and SMC-EnKF) that **outperform the NPF**.
- The **selection of the filtering techniques** in each layer depends on the specific problem.

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Nested Gaussian filters

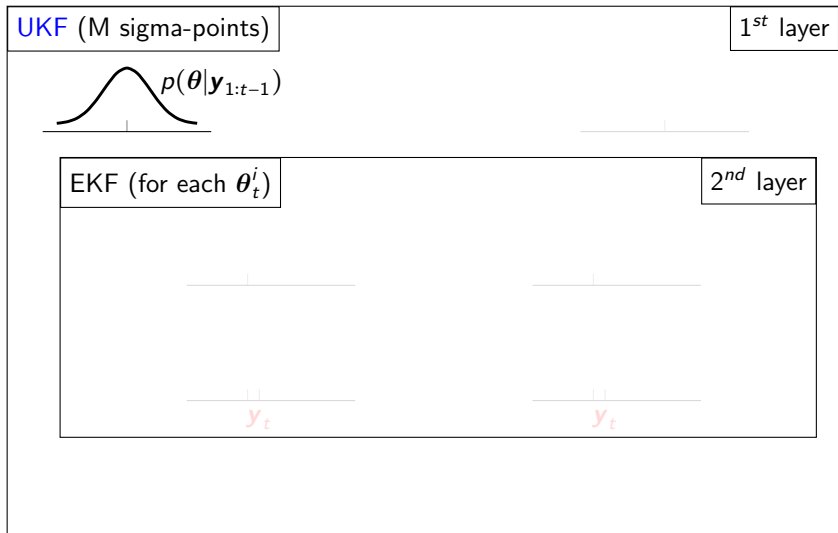
- The algorithm
- Numerical results

Conclusions

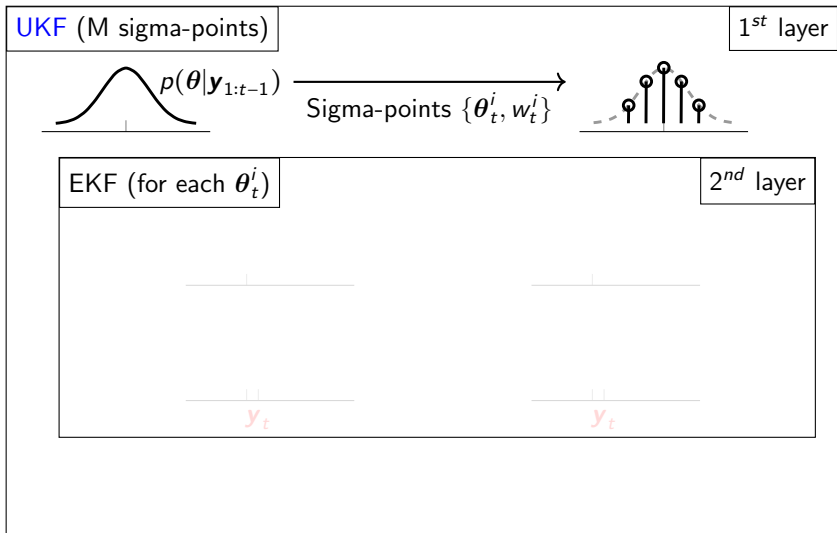
Nested Gaussian filter

- We introduce the use of **deterministic sampling techniques** in the **first layer** of the algorithm, such as the [cubature Kalman filter \(CKF\)](#) and the [unscented Kalman filter \(UKF\)](#).
- We keep applying **Gaussian methods** in the **second layer** of the algorithm.
- We describe how the algorithms can work **sequentially and recursively**.

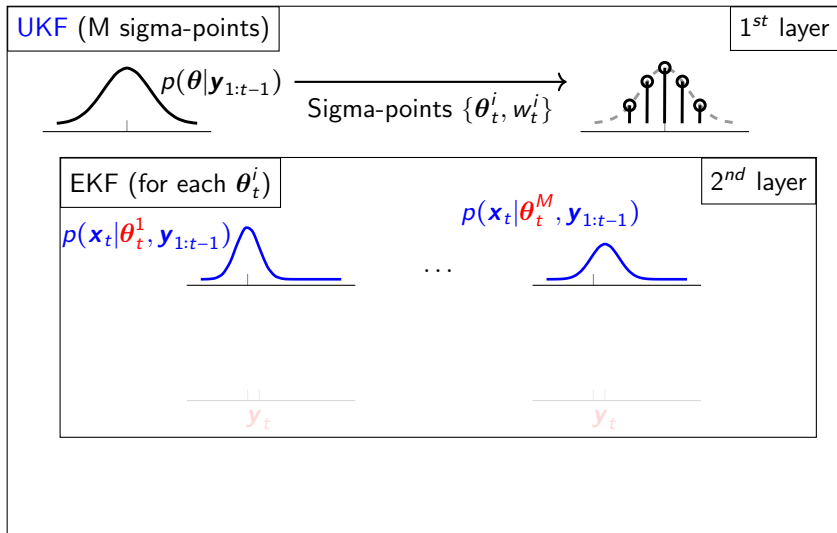
Nested Gaussian filter



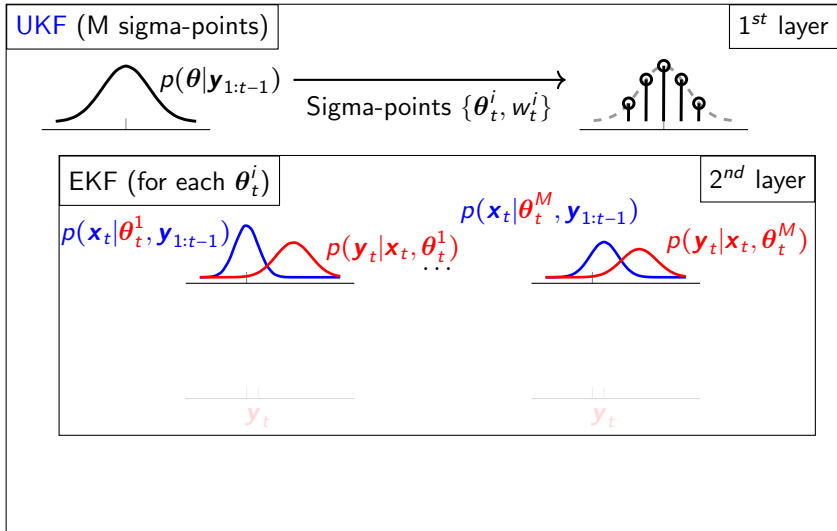
Nested Gaussian filter



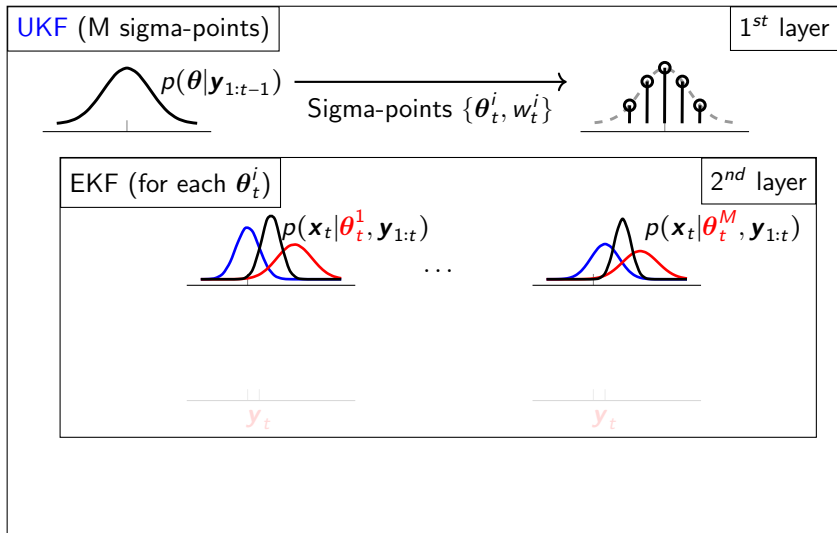
Nested Gaussian filter



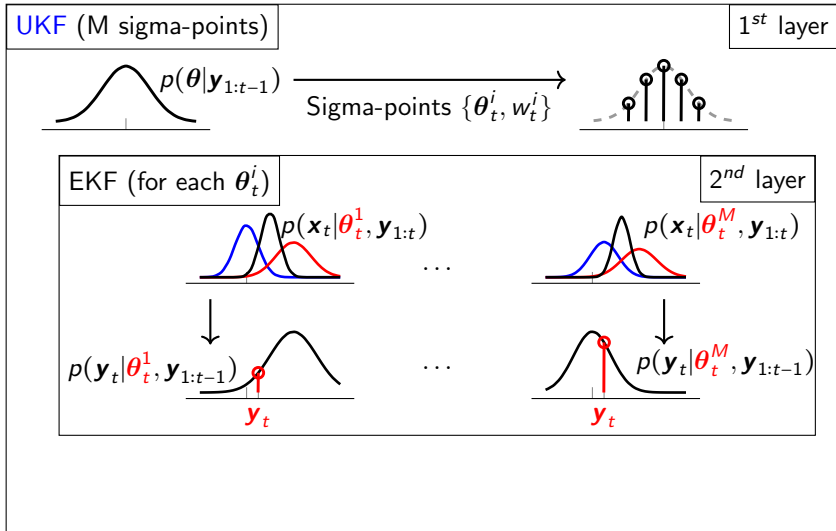
Nested Gaussian filter



Nested Gaussian filter

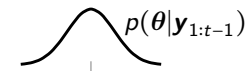
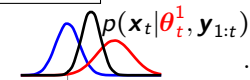


Nested Gaussian filter

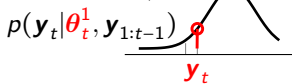


Nested Gaussian filter

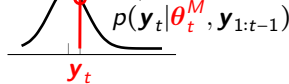
UKF (M sigma-points)

Sigma-points $\{\theta_t^i, w_t^i\}$ 1st layerEKF (for each θ_t^i)

...

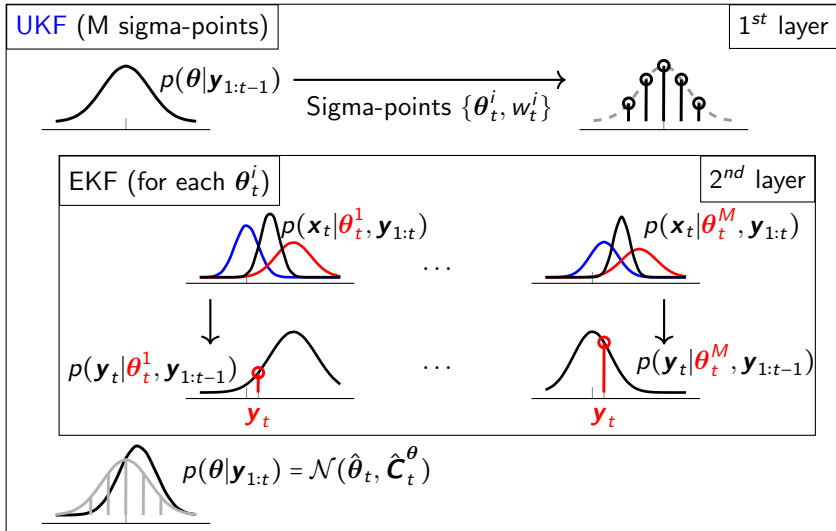


...



$$p(\theta | y_{1:t}) = \mathcal{N}(\hat{\theta}_t, \hat{\mathbf{C}}_t^\theta)$$

Nested Gaussian filter



Recursivity of NGF

→ 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

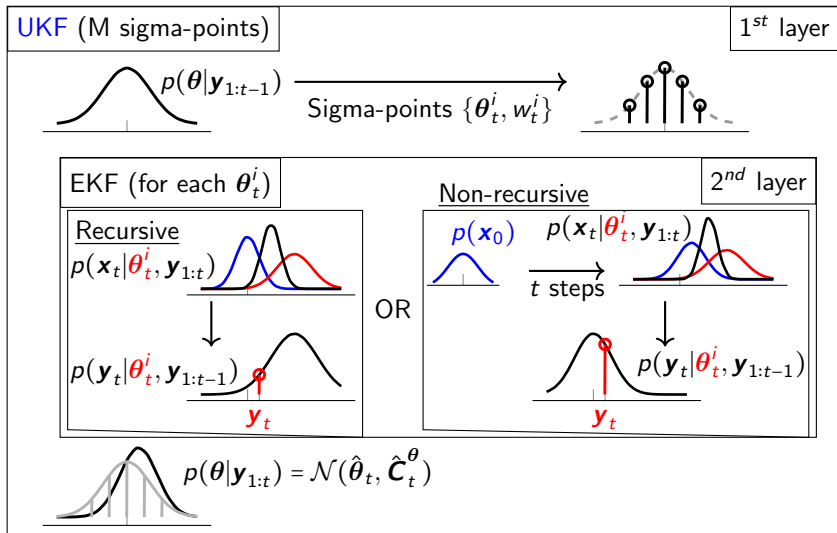
$$p(\mathbf{x}_{t-1} | \mathbf{y}_{1:t-1}, \theta_t^i) \approx p(\mathbf{x}_{t-1} | \mathbf{y}_{1:t-1}, \theta_{t-1}^i).$$

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 $p(\mathbf{x}_{t-1} | \mathbf{y}_{1:t-1}, \boldsymbol{\theta}_t^i) \approx p(\mathbf{x}_{t-1} | \mathbf{y}_{1:t-1}, \boldsymbol{\theta}_{t-1}^i)$.
- If $\|\boldsymbol{\theta}_t^i - \boldsymbol{\theta}_{t-1}^i\|_p > \lambda \|\boldsymbol{\theta}_{t-1}^i\|_p$,
we need to compute the pdf $p(\mathbf{x}_{t-1} | \mathbf{y}_{1:t-1}, \boldsymbol{\theta}_t^i)$ from the **prior** $p(\mathbf{x}_0)$.

Nested Gaussian filter



The Lorenz 63 model

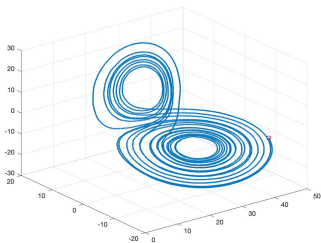
We consider a **stochastic Lorenz 63 model**, whose dynamics are described by

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

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

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

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



The Lorenz 63 model

- Applying a discretization method with step Δ , we obtain

$$x_{1,t+1} = x_{1,t} - \Delta S(x_{1,t} - x_{2,t}) + \sqrt{\Delta} \sigma v_{1,t},$$

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

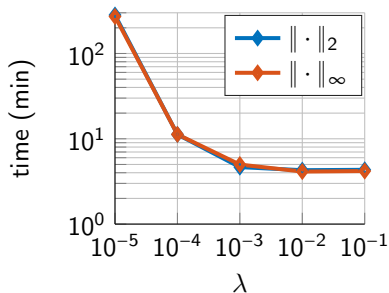
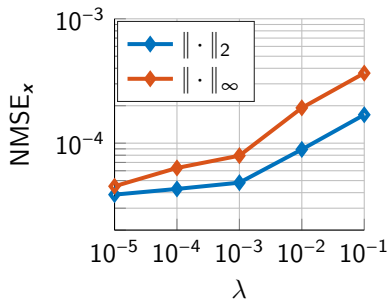
$$x_{3,t+1} = x_{3,t} + \Delta (x_{1,t}x_{2,t} - Bx_{3,t}) + \sqrt{\Delta} \sigma v_{3,t},$$

- We assume linear observations of the form

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

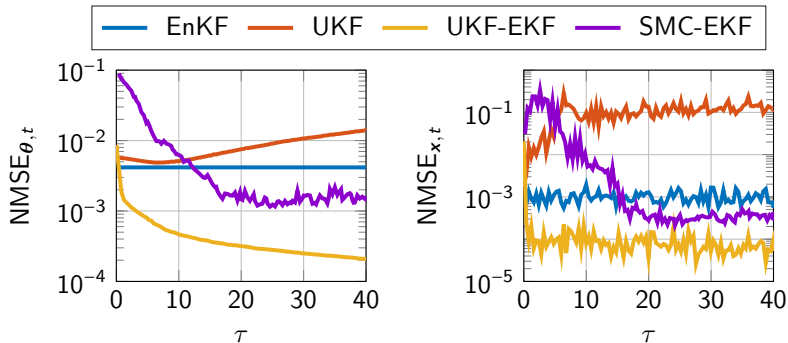
where k_o is a fixed known parameter and $\mathbf{r}_t \sim \mathcal{N}(\mathbf{r}_t | \mathbf{0}, \sigma_y^2 \mathbf{I}_2)$.

Numerical results



→ We observe that below $\lambda = 10^{-3}$ there is almost no improvement in the error of the state.

Numerical results



Summary of NGFs

- We introduce the **nested Gaussian filters (NGFs)**, that use **deterministic sampling** methods in the first layer and **Gaussian** methods in the second layer.
- We have introduced and assessed the values of a **relative threshold** $\lambda > 0$ that enables the algorithm to work **recursively**.
- We have **implemented a UKF-EKF** and compare it to other algorithms.

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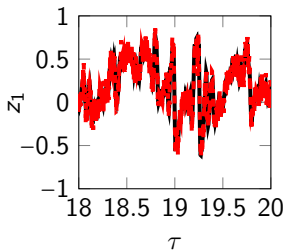
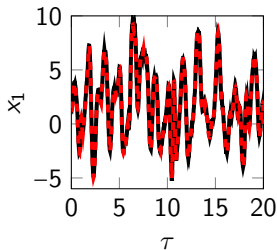
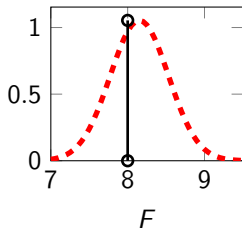
Conclusions

Conclusions

- We have introduced a **generalized nested methodology** that estimates the full posterior distribution of the **static parameters** and **state dynamical variables**.
- This **probabilistic methodology** admits **different types of filtering techniques in each layer**, leading to the nested hybrids filters, the nested Gaussian filters and the NPF.
- We keep the algorithm working **recursively** by applying the **jittering** or by using a **distance dependant on the parameter space**.
- We have proved, under general assumptions, that **the family of nested hybrid filters converges** to a possibly **biased** version of the **posterior distribution of the parameters**.
- The **use of Gaussian filters** in the nested methodology admits **fast implementations** and are well suited to **high-dimensional systems**.

Conclusions

- **Further generalization** of the nested filters to estimate heterogeneous **multi-scale systems**.
- **Three layers of computation** for the static parameters and the two sets of state variables.



List of publications

- Sara Pérez-Vieites and Joaquín Míguez. “Kalman-based nested hybrid filters for recursive inference in state-space models”. *2020 28th European Signal Processing Conference (EUSIPCO)*, 2468-2472.
- Sara Pérez-Vieites and Joaquín Míguez. “A nested hybrid filter for parameter estimation and state tracking in homogeneous multi-scale models”. *2020 IEEE 23rd International Conference on Information Fusion (FUSION)*, 1-8.
- Sara Pérez-Vieites, Inés Pérez Mariño and Joaquín Míguez. “Probabilistic scheme for joint parameter estimation and state prediction in complex dynamical systems”. *Physical Review E*, 98 (6), 063305.
- Sara Pérez-Vieites and Joaquín Míguez. “Nested Gaussian filters for recursive Bayesian inference and nonlinear tracking in state space models”. *Signal Processing*, 189, 108295.

Thank you!