Introduction	State-space Model	Model Inference	Multi-scale nested filters	Results	Conclusions
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A nested hybrid filter for parameter estimation and state tracking in homogeneous multi-scale models

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July 9, 2020



We aim at tracking **homogeneous multi-scale systems**. They are of broad interest since they are found in many fields of science (biology, fluid dynamics, chemistry...).

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The goal is to estimate the time-evolution of a system governed by

- processes with different time-scales,
- that may be described by diverse laws,
- and with cross dependencies among them

State-space Model

Introduction

Model Inference

Multi-scale nested filters

Results

Conclusions

State of the Art Methods

We can find **theoretically-guaranteed solutions** for systems with unknown static parameters and dynamic state variables: a multi-scale problem with only two time scales:

- Sequential Monte Carlo square (SMC²) [Chopin et al., 2011] or particle Markov chain Monte Carlo (PMCMC) [Andrieu et al., 2010] aim at computing the joint posterior probability distribution of all the unknown variables and parameters of the system. Unfortunately, they are batch techniques.
- Nested particle filters (NPFs) [Crisan et al., 2018] is a scheme with two intertwined layers of Monte Carlo methods that approximates the same distribution but in a recursive way. Then, it is better suited for long sequences of observations but the computational cost is prohibitive.
- Nested hybrid filters (NHFs) [S. Pérez-Vieites, 2017] introduce Gaussian filtering techniques in the second layer of the algorithm, reducing considerably the computational cost.

duction	State-space Model	Model Inference	Multi-scale nested filters	Results	Concl
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State-space Model

We are interested in systems described by multidimensional stochastic differential equations (SDEs):

$$d\mathbf{x} = f_{\mathbf{x}}(\mathbf{x}, \boldsymbol{\theta}) dt + g_{\mathbf{x}}(\mathbf{z}, \boldsymbol{\theta}) dt + \sigma_{\mathbf{x}} d\mathbf{v}, \qquad (1)$$

$$dz = f_z(x,\theta)dt + g_z(z,\theta)dt + \sigma_z dw, \qquad (2)$$

where:

- t denotes time.
- $\mathbf{x}(t) \in \mathbb{R}^{d_x}$ are the slow states of the system.
- $\mathbf{z}(t) \in \mathbb{R}^{d_z}$ are the fast states of the system.
- $\boldsymbol{\theta} \in \mathbb{R}^{d_{\theta}}$ are fixed vector of unknown parameters.
- f_x , f_z , g_x and g_z are possibly non-linear functions.
- σ_x, σ_z > 0 are known scale parameters that control the intensity of stochastic perturbations.
- v(t), w(t) are vectors of independent standard Wiener processes with dimension d_x and d_z.

ction	State-space Model	Model Inference	Multi-scale nested filters	Results	Conclusion
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Macro-micro Solver

In order to handle both time scales we apply a macro-micro solver [Weinan et al., 2005]. We use different integration steps: Δ_z for z and $\Delta_x \gg \Delta_z$ for x:

$$\mathbf{x}_{n} = \mathbf{x}_{n-1} + \Delta_{\mathbf{x}} (f_{\mathbf{x}}(\mathbf{x}_{n-1}, \boldsymbol{\theta}) + g_{\mathbf{x}}(\bar{\mathbf{z}}_{n}, \boldsymbol{\theta})) + \sqrt{\Delta_{\mathbf{x}}} \sigma_{\mathbf{x}} \mathbf{v}_{n},$$
(3)

$$\boldsymbol{z}_{k} = \boldsymbol{z}_{k-1} + \Delta_{\boldsymbol{z}}(f_{\boldsymbol{z}}(\boldsymbol{x}_{\lfloor \frac{k-1}{h} \rfloor}, \boldsymbol{\theta}) + \boldsymbol{g}_{\boldsymbol{z}}(\boldsymbol{z}_{k-1}, \boldsymbol{\theta})) + \sqrt{\Delta_{\boldsymbol{x}}}\sigma_{\boldsymbol{x}}\boldsymbol{w}_{k},$$
(4)

where

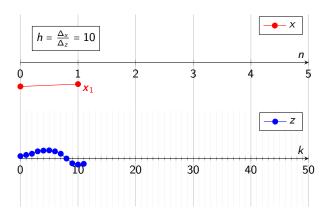
- n ∈ N denotes discrete time in the time scale of x (x_n ≃ x(n∆_x)),
- k ∈ N denotes discrete time in the time scale of z (z_k ≃ z(k∆_z)),
- $h = \frac{\Delta_x}{\Delta_z}$ is the ratio between the two time scales and

$$\bar{z}_n = \frac{1}{h} \sum_{i=h(n-1)+1}^{hn} z_i.$$
 (5)

Introduction	State-space Model	Model Inference	Multi-scale nested filters	Resu
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Results 000 Conclusions

Macro-micro Solver



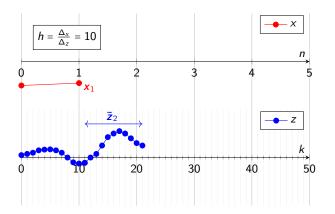
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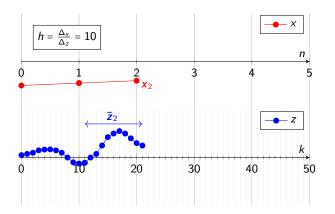
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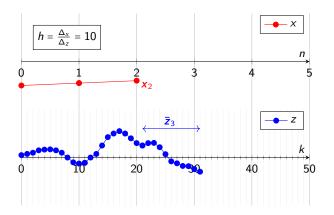
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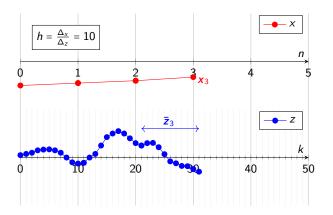
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Introduction	State-space Model	Model Inference	Multi-scale nested filters	Results
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Introduction 00	State-space Model	Model Inference ●○	Multi-scale nested filters 0	Results 000	Conclusions 00

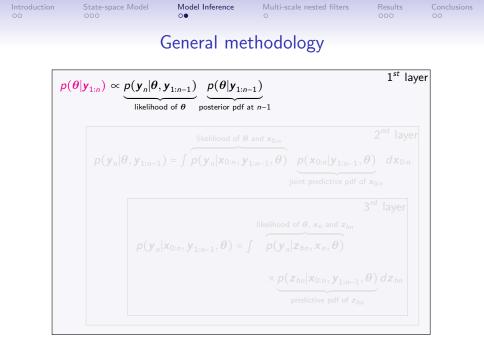
Model Inference

We aim at approximating the joint posterior probability density function (pdf) $p(\theta, \mathbf{x}_{0:n}, \mathbf{z}_{hn} | \mathbf{y}_{1:n})$. Using the chain rule, we can factorize this pdf as

$$p(\boldsymbol{z}_{hn}, \boldsymbol{x}_n, \boldsymbol{\theta} | \boldsymbol{y}_{1:n}) = \underbrace{p(\boldsymbol{z}_{hn} | \boldsymbol{x}_{0:n}, \boldsymbol{y}_{1:n}, \boldsymbol{\theta})}_{3^{rd} | ayer} \underbrace{p(\boldsymbol{x}_{0:n} | \boldsymbol{y}_{1:n}, \boldsymbol{\theta})}_{2^{nd} | ayer} \underbrace{p(\boldsymbol{\theta} | \boldsymbol{y}_{1:n})}_{1^{st} | ayer}$$

 \rightarrow Each of these pdf's can be handled in a different layer of computation.

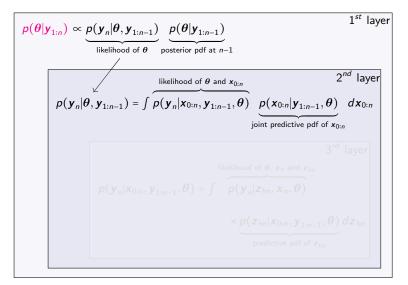
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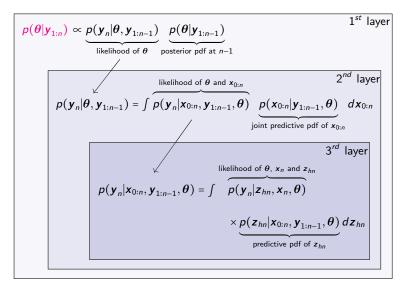
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General methodology

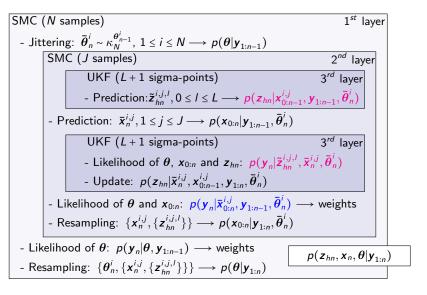


Introduction	State-space Model	Model Inference	Multi-scale nested filters	Results	Conclusio
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General methodology

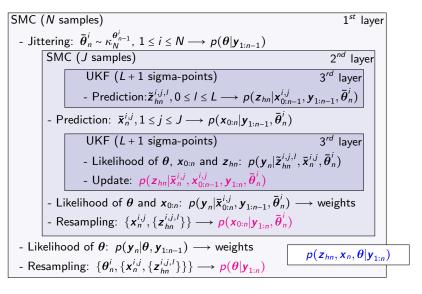


$$\begin{aligned} & \text{SMC } (N \text{ samples}) & 1^{st} \text{ layer} \\ & \text{- Jittering: } \bar{\theta}_n^i \sim \kappa_N^{\theta_{n-1}^i}, 1 \leq i \leq N \longrightarrow p(\theta|\mathbf{y}_{1:n-1}) \\ & \text{SMC } (J \text{ samples}) & 2^{nd} \text{ layer} \\ & \mathbb{U}\text{KF } (L+1 \text{ sigma-points}) & 3^{rd} \text{ layer} \\ & - \text{Prediction: } \tilde{\boldsymbol{z}}_{hn}^{i,j,l}, 0 \leq l \leq L \longrightarrow p(\boldsymbol{z}_{hn}|\boldsymbol{x}_{0:n-1}^{i,j}, \boldsymbol{y}_{1:n-1}, \bar{\theta}_n^i) \\ & - \text{Prediction: } \tilde{\boldsymbol{x}}_n^{i,j}, 1 \leq j \leq J \longrightarrow p(\boldsymbol{x}_{0:n}|\boldsymbol{y}_{1:n-1}, \bar{\theta}_n^i) \\ & \mathbb{U}\text{KF } (L+1 \text{ sigma-points}) & 3^{rd} \text{ layer} \\ & - \text{Likelihood of } \boldsymbol{\theta}, \boldsymbol{x}_{0:n} \text{ and } \boldsymbol{z}_{hn}: p(\boldsymbol{y}_n|\tilde{\boldsymbol{z}}_{hn}^{i,j,l}, \bar{\boldsymbol{x}}_n^{i,j}, \bar{\theta}_n^i) \\ & - \text{Update: } p(\boldsymbol{z}_{hn}|\bar{\boldsymbol{x}}_n^{i,j}, \boldsymbol{x}_{0:n-1}^{i,j,l}, \boldsymbol{y}_{1:n-1}, \bar{\theta}_n^i) \\ & - \text{Likelihood of } \boldsymbol{\theta} \text{ and } \boldsymbol{x}_{0:n}: p(\boldsymbol{y}_n|\bar{\boldsymbol{x}}_{0:n}^{i,j}, \boldsymbol{y}_{1:n-1}, \bar{\theta}_n^i) \\ & - \text{Likelihood of } \boldsymbol{\theta} \text{ and } \boldsymbol{x}_{0:n}: p(\boldsymbol{y}_n|\bar{\boldsymbol{x}}_{0:n}^{i,j}, \boldsymbol{y}_{1:n-1}, \bar{\theta}_n^i) \\ & - \text{Likelihood of } \boldsymbol{\theta} \text{ and } \boldsymbol{x}_{0:n}: p(\boldsymbol{y}_n|\bar{\boldsymbol{x}}_{0:n}^{i,j}, \boldsymbol{y}_{1:n-1}, \bar{\theta}_n^i) \\ & - \text{Likelihood of } \boldsymbol{\theta} \text{ and } \boldsymbol{x}_{0:n}: p(\boldsymbol{y}_n|\bar{\boldsymbol{x}}_{0:n}^{i,j}, \boldsymbol{y}_{1:n-1}, \bar{\theta}_n^i) \\ & - \text{Likelihood of } \boldsymbol{\theta} \text{ and } \boldsymbol{x}_{0:n}: p(\boldsymbol{y}_n|\bar{\boldsymbol{x}}_{0:n}^{i,j}, \boldsymbol{y}_{1:n-1}, \bar{\theta}_n^i) \\ & - \text{Likelihood of } \boldsymbol{\theta} \text{ p}(\boldsymbol{y}_n|\boldsymbol{\theta}, \boldsymbol{y}_{1:n-1}) \longrightarrow \text{weights} \\ & - \text{Resampling: } \{\boldsymbol{\theta}_n^i, \{\boldsymbol{x}_n^{i,j}, \{\boldsymbol{z}_{hn}^{i,j}\}\} \longrightarrow p(\boldsymbol{\theta}|\boldsymbol{y}_{1:n}) \\ & p(\boldsymbol{z}_{hn}, \boldsymbol{x}_n, \boldsymbol{\theta}|\boldsymbol{y}_{1:n}) \\ \end{array} \right$$



$$\begin{aligned} & \text{SMC } (N \text{ samples}) & 1^{st} \text{ layer} \\ & \text{- Jittering: } \bar{\theta}_n^i \sim \kappa_N^{\theta_{n-1}^i}, 1 \leq i \leq N \longrightarrow p(\theta|\mathbf{y}_{1:n-1}) \\ & \text{SMC } (J \text{ samples}) & 2^{nd} \text{ layer} \\ & \mathbb{U}\text{KF } (L+1 \text{ sigma-points}) & 3^{rd} \text{ layer} \\ & - \text{Prediction: } \tilde{\boldsymbol{z}}_{hn}^{i,j,l}, 0 \leq l \leq L \longrightarrow p(\boldsymbol{z}_{hn}|\mathbf{x}_{0:n-1}^{i,j}, \mathbf{y}_{1:n-1}, \bar{\theta}_n^i) \\ & - \text{Prediction: } \tilde{\boldsymbol{x}}_n^{i,j,1} 1 \leq j \leq J \longrightarrow p(\mathbf{x}_{0:n}|\mathbf{y}_{1:n-1}, \bar{\theta}_n^i) \\ & \mathbb{U}\text{KF } (L+1 \text{ sigma-points}) & 3^{rd} \text{ layer} \\ & - \text{Likelihood } of \boldsymbol{\theta}, \mathbf{x}_{0:n} \text{ and } \boldsymbol{z}_{hn}: p(\mathbf{y}_n|\tilde{\boldsymbol{z}}_{hn}^{i,j,l}, \tilde{\boldsymbol{x}}_n^{i,j}, \bar{\theta}_n^i) \\ & - \text{Update: } p(\boldsymbol{z}_{hn}|\tilde{\mathbf{x}}_n^{i,j}, \mathbf{x}_{0:n-1}^{i,j,l}, \mathbf{y}_{1:n}, \bar{\theta}_n^i) \\ & - \text{Likelihood } of \boldsymbol{\theta} \text{ and } \mathbf{x}_{0:n}: p(\mathbf{y}_n|\tilde{\mathbf{x}}_{0:n}^{i,j}, \mathbf{y}_{1:n-1}, \bar{\theta}_n^i) \\ & - \text{Likelihood } of \boldsymbol{\theta} \text{ and } \mathbf{x}_{0:n}: p(\mathbf{y}_n|\tilde{\mathbf{x}}_{0:n}^{i,j}, \mathbf{y}_{1:n-1}, \bar{\theta}_n^i) \\ & - \text{Likelihood } of \boldsymbol{\theta} \text{ and } \mathbf{x}_{0:n}: p(\mathbf{y}_n|\tilde{\mathbf{x}}_{0:n}^{i,j}, \mathbf{y}_{1:n-1}, \bar{\theta}_n^i) \\ & - \text{Likelihood } of \boldsymbol{\theta} \text{ and } \mathbf{x}_{0:n}: p(\mathbf{y}_n|\tilde{\mathbf{x}}_{0:n}^{i,j}, \mathbf{y}_{1:n}, \bar{\theta}_n^i) \\ & - \text{Likelihood } of \boldsymbol{\theta} \text{ and } \mathbf{x}_{0:n}: p(\mathbf{y}_n|\mathbf{x}_{0:n}, \mathbf{y}_{1:n}, \bar{\theta}_n^i) \\ & - \text{Likelihood } f \boldsymbol{\theta} \text{ is } p(\mathbf{y}_n|\boldsymbol{\theta}, \mathbf{y}_{1:n-1}) \longrightarrow \text{ weights} \\ & - \text{Resampling: } \{\boldsymbol{\theta}_n^i, \{\mathbf{x}_n^{i,j}, \{\mathbf{z}_{hn}^{i,j}\}\} \longrightarrow p(\boldsymbol{\theta}|\mathbf{y}_{1:n}) \\ & p(\boldsymbol{z}_{hn}, \mathbf{x}_n, \boldsymbol{\theta}|\mathbf{y}_{1:n}) \\ \end{array} \right$$

$$\begin{aligned} & \text{SMC } (N \text{ samples}) & 1^{\text{st }} \text{ layer} \\ & \text{- Jittering: } \bar{\theta}_n^i \sim \kappa_N^{\theta_{n-1}^i}, 1 \leq i \leq N \longrightarrow p(\theta|\mathbf{y}_{1:n-1}) \\ & \text{SMC } (J \text{ samples}) & 2^{nd} \text{ layer} \\ & \mathbb{U}\text{KF } (L+1 \text{ sigma-points}) & 3^{rd} \text{ layer} \\ & - \text{Prediction: } \bar{\mathbf{z}}_{hn}^{i,j,l}, 0 \leq l \leq L \longrightarrow p(\mathbf{z}_{hn}|\mathbf{x}_{0:n-1}^{i,j}, \mathbf{y}_{1:n-1}, \bar{\theta}_n^i) \\ & - \text{Prediction: } \bar{\mathbf{x}}_n^{i,j,1} \leq j \leq J \longrightarrow p(\mathbf{x}_{0:n}|\mathbf{y}_{1:n-1}, \bar{\theta}_n^i) \\ & \mathbb{U}\text{KF } (L+1 \text{ sigma-points}) & 3^{rd} \text{ layer} \\ & - \text{Likelihood } of \ \theta, \ \mathbf{x}_{0:n} \text{ and } \mathbf{z}_{hn}: \ p(\mathbf{y}_n|\tilde{\mathbf{z}}_{hn}^{i,j,l}, \bar{\mathbf{x}}_n^{i,j}, \bar{\theta}_n^i) \\ & - \text{Update: } p(\mathbf{z}_{hn}|\bar{\mathbf{x}}_n^{i,j}, \mathbf{x}_{0:n-1}^{i,j,l}, \mathbf{y}_{1:n-1}, \bar{\theta}_n^i) \\ & - \text{Likelihood } of \ \theta \text{ and } \mathbf{x}_{0:n}: \ p(\mathbf{y}_n|\bar{\mathbf{x}}_{0:n}^{i,j,l}, \mathbf{y}_{1:n-1}, \bar{\theta}_n^i) \\ & - \text{Likelihood } of \ \theta \text{ and } \mathbf{x}_{0:n}: p(\mathbf{y}_n|\bar{\mathbf{x}}_{0:n}^{i,j,l}, \mathbf{y}_{1:n-1}, \bar{\theta}_n^i) \\ & - \text{Likelihood } of \ \theta \text{ and } \mathbf{x}_{0:n}: p(\mathbf{y}_n|\bar{\mathbf{x}}_{0:n}^{i,j,l}, \mathbf{y}_{1:n-1}, \bar{\theta}_n^i) \\ & - \text{Likelihood } of \ \theta \text{ and } \mathbf{x}_{0:n}: p(\mathbf{y}_n|\bar{\mathbf{x}}_{0:n}^{i,j,l}, \mathbf{y}_{1:n-1}, \bar{\theta}_n^i) \\ & - \text{Likelihood } of \ \theta \text{ and } \mathbf{x}_{0:n}: p(\mathbf{y}_n|\mathbf{x}_{0:n}, \mathbf{y}_{1:n-1}, \bar{\theta}_n^i) \\ & - \text{Likelihood } f \ \theta \text{ and } \mathbf{x}_{0:n}: p(\mathbf{y}_n|\mathbf{x}_{0:n}, \mathbf{y}_{1:n-1}, \bar{\theta}_n^i) \\ & - \text{Likelihood } f \ \theta \text{ and } \mathbf{x}_{0:n}: p(\mathbf{y}_n|\mathbf{x}_{0:n}, \mathbf{y}_{1:n-1}, \bar{\theta}_n^i) \\ & - \text{Likelihood } f \ \theta \text{ and } \mathbf{x}_{0:n}: p(\mathbf{y}_n|\mathbf{x}_{0:n}, \mathbf{y}_{1:n-1}, \bar{\theta}_n^i) \\ & - \text{Likelihood } f \ \theta \text{ and } \mathbf{x}_{0:n}: p(\mathbf{y}_n|\mathbf{x}_{0:n}, \mathbf{y}_{1:n}, \bar{\theta}_n^i) \\ & - \text{Likelihood } f \ \theta \text{ and } \mathbf{x}_{0:n}: p(\mathbf{y}_{1:n}, \mathbf{y}_{1:n}) \\ & - p(\theta|\mathbf{y}_{1:n}) \\ \end{array} \right$$





Numerical results

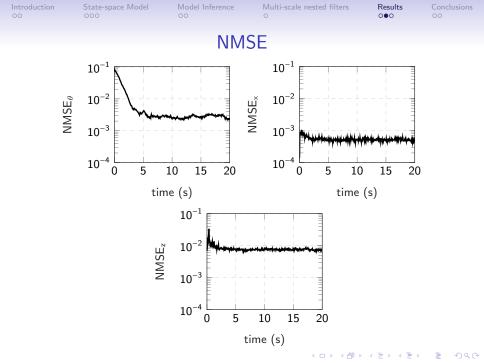
We consider a stochastic two-scale Lorenz 96 model that is described, in continuous time, by the SDEs

$$dx_{j} = \left[-x_{j-1}(x_{j-2} - x_{j+1}) - x_{j} + F - \frac{HC}{B} \sum_{l=(j-1)L}^{Lj-1} z_{l} \right] dt + \sigma_{x} dv_{j},$$
(6)
$$dz_{l} = \left[-CBz_{l+1}(z_{l+2} - z_{l-1}) - Cz_{l} + \frac{CF}{B} + \frac{HC}{B} x_{\lfloor (l-1)L \rfloor} \right] dt + \sigma_{z} dw_{l},$$
(7)

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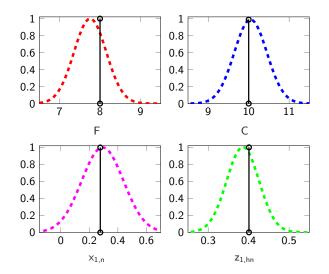
where

- the slow variables, x, are a d_x -dimensional vector,
- the fast variables, z, are d_z -dimensional $(d_z > d_x)$ and
- we assume static parameters H and B are known, while we need to estimate θ = [F, C]T.



Introduction	State-space Model	Model Inference	Multi-scale nested filters	Results	Conclu
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Approximate posterior density functions



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Introduction 00	State-space Model	Model Inference	Multi-scale nested filters 0	Results 000	Conclusions ●○		
Conclusions							

- We have introduced a new recursive methodology for tracking the time evolution and evaluate any static parameters of homogeneous multi-scale systems.
- It is a nested multilayered structure that allows different computation schemes at each layer. Specifically, we have explored the use of sequential Monte Carlo in both first and second layers of the filter, and in the third layer, Gaussian filters (UKF).
- We have analyzed a dynamical system of 3 time-scales (static parameters, slow dynamic state variables and fast dynamic state variables), showing the average performance of the method in terms of estimation errors.

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