

# Adaptive parameter-space exploration for online Bayesian inference

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## State-space model

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

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

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

- $\mathbf{f}$ ,  $\mathbf{g}$ : state transition function and observation function
- $\mathbf{v}_t$ ,  $\mathbf{r}_t$ : 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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## State estimation

Classical filtering methods:

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

Every time step  $t$ :

1. Predictive distribution:

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

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

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

In practice,  $\theta^*$  is not known. It is needed to estimate both  $\theta$  and  $\mathbf{x}_t$ , i.e.,  $p(\mathbf{x}_t, \theta|\mathbf{y}_{1:t})$ .

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# State-of-the-art methods

Methods for Bayesian inference of both  $\theta$  and  $\mathbf{x}_t$ :

- **particle Markov chain Monte Carlo (PMCMC)**<sup>1</sup>
- **sequential Monte Carlo square (SMC<sup>2</sup>)**<sup>2</sup>
- **nested particle filters (NPFs)**<sup>3</sup>

- They can **quantify the uncertainty** or estimation error.
- They can be applied to a **broad class of models**.
- They provide **theoretical guarantees**.
- Both PMCMC and SMC<sup>2</sup> are **batch techniques**, while the NPF is a **recursive method**.

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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

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

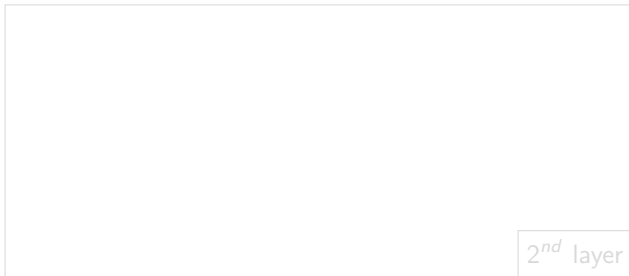
→ The **key difficulty** in this class of models is **the Bayesian estimation of the parameter vector  $\boldsymbol{\theta}$** .

# Model inference

At every time step  $t$ :

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

1<sup>st</sup> layer



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

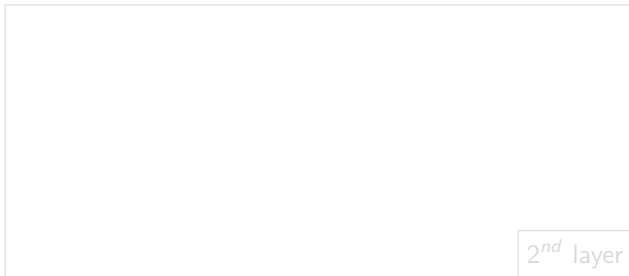
$$\underbrace{p(\theta|\mathbf{y}_{1:t})}_{\text{Post. pdf of } \theta} \propto p(\mathbf{y}_t|\theta, \mathbf{y}_{1:t-1})p(\theta|\mathbf{y}_{1:t-1})$$

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Likelihood:  $p(\mathbf{y}_t|\mathbf{x}_t, \theta)$

Posterior pdf of  $\mathbf{x}$ :  $p(\mathbf{x}_t|\mathbf{y}_{1:t}, \theta)$

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

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# Naive importance sampling approximation

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

At  $t \geq 1$  and for every  $\theta^i$ ,  $i = 1, \dots, N$ :

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

For  $j = 1, \dots, M$ :

SMC ( $M$  samples)  
to approximate  $p(\mathbf{y}_t | \mathbf{y}_{1:t-1}, \theta^i)$

- Draw  $\bar{\mathbf{x}}_t^{i,j} \sim p(\mathbf{x}_t | \theta^i, \mathbf{y}_{1:t-1})$
- Weights:  $\tilde{u}_t^{i,j} \propto p(\mathbf{y}_t | \bar{\mathbf{x}}_t^{i,j}, \theta^i)$
- Resampling: for  $m = 1, \dots, M$ ,  $\tilde{\mathbf{x}}_t^{i,j} = \bar{\mathbf{x}}_t^{i,m}$   
with prob.  $u_t^{i,m} = \frac{\tilde{u}_t^{i,m}}{\sum_{j=1}^M \tilde{u}_t^{i,j}}$

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

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



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## Naive importance sampling approximation

- Careful with  $p(\theta)$ : after several time steps the filter **degenerates**
- Possible solution: drawing  $\{\theta_t^i\} \sim p(\theta | \mathbf{y}_{1:t-1})$  at each time step  $\rightarrow$  **re-running from scratch the filter for  $\mathbf{x}$**  (i.e., not recursive anymore)

- NPF  $\rightarrow$  **jittering**:  $\bar{\theta}_t^i \sim \kappa_N(d\theta | \theta')$ , where

$$\kappa_N(d\theta | \theta') = (1 - \epsilon_N) \delta_{\theta'}(\theta) + \epsilon_N \kappa(d\theta | \theta')$$

- $0 < \epsilon_N \leq \frac{1}{\sqrt{N}}$
- $\kappa(d\theta | \theta')$  is an arbitrary Markov kernel with mean  $\theta'$  and finite variance, e.g.,  $\kappa(d\theta | \theta') = \mathcal{N}(\theta | \theta', \tilde{\sigma}^2 I)$ , with  $\tilde{\sigma}^2 < \infty$ .
- Guarantees convergence to the true posterior when  $N \rightarrow \infty$

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Nested particle filter (NPF)<sup>4</sup>For  $i = 1, \dots, N$ :

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<sup>4</sup>Crisan and Miguez 2017.

# Family of nested filters

## 1. Nested particle filters (NPFs)<sup>5</sup>.

- Both layers → Sequential Monte Carlo (SMC) methods  
High computational complexity:  $N \times M$

## 2. Nested hybrid filters (NHF)<sup>6</sup>.

- $\theta$ -layer → Monte Carlo-based methods (e.g., SMC or SQMC)
- $x$ -layer → Gaussian techniques (e.g., EKF or EnKF)

## 3. Nested Gaussian filters (NGF)<sup>7</sup>.

- $\theta$ -layer → Deterministic sampling methods (e.g., UKF).
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## Reducing number of particles online

**Problem:** Great amount of samples ( $N \times M$ ) and **waste of computational effort** when they are not well chosen.

Possible approach: reducing automatically the number of samples,  $N$ , when the performance is no longer compromised.

We studied the case for a nested Gaussian filter that implements:

- **Quadrature or cubature rules in the  $\theta$ -layer**, i.e., we generate  $N$  quadrature points such that

$$N = \alpha^{d_\theta}, \quad \text{for } \alpha \in \mathbb{N}, \alpha > 1. \quad (3)$$

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



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## Adaptive reduction rule

New statistic to decide when to reduce  $N_t$ :

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

The statistic takes

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

The adaptive reduction rule. Given  $\epsilon$  and  $\alpha_{\min}$ :

- If  $\frac{\rho_t}{N_t} > 1 - \epsilon$  ( $\rho_t$  is close to its maximum value),

$$\text{Set } \alpha_{t+1} = \max(\alpha_{\min}, \alpha_t - 1).$$

- Otherwise,  $\alpha_{t+1} = \alpha_t$ .

$$\text{Set } N_{t+1} = \alpha_{t+1}^{d_\theta}.$$

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

The statistic takes

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

The **adaptive reduction rule**. Given  $\epsilon$  and  $\alpha_{\min}$ :

- If  $\frac{\rho_t}{N_t} > 1 - \epsilon$  ( $\rho_t$  is close to its maximum value),

Set  $\alpha_{t+1} = \max(\alpha_{\min}, \alpha_t - 1)$ .

- Otherwise,  $\alpha_{t+1} = \alpha_t$ .

Set  $N_{t+1} = \alpha_{t+1}^{d_\theta}$ .

## Numerical results - Lorenz 63

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

- **state variables**  $\mathbf{x}_t$  of dimension  $d_x = 3$ ,

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

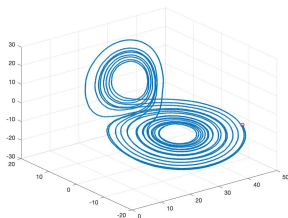
$$dx_2 = [Rx_1 - x_2 - x_1x_3]d\tau + \sigma dv_2,$$

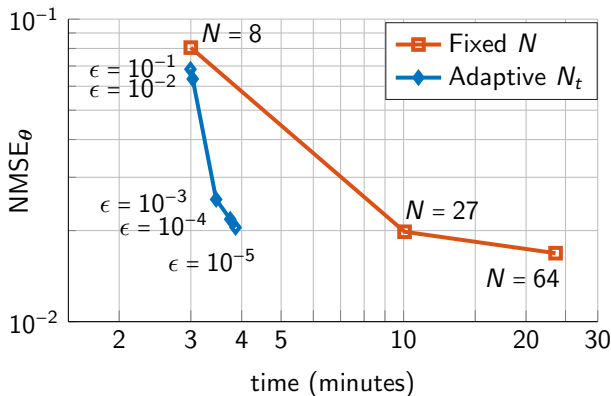
$$dx_3 = [x_1x_2 - Bx_3]d\tau + \sigma dv_3,$$

- **static parameters**  
 $\theta = [S, R, B]^T$ , and
- **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<sup>8</sup>

1. **Nested Gaussian filter with fixed  $N$ .** Different fixed  $\alpha = \{2, 3, 4\}$ , i.e.,  $N = \{8, 27, 64\}$ .
2. **Nested Gaussian filter with adaptive  $N_t$ .** We set  $\alpha_0 = 4$  and  $\alpha_{\min} = 2$ , i.e.,  $N_0 = 64$  and  $N_{\min} = 8$ .

<sup>8</sup>Pérez-Vieites and Elvira 2023.

# Conclusions

1. The nested methodology is **online and flexible**. It admits different types of filtering techniques in each layer, leading to a **set of algorithms**.
2. For a **further reduction of the computational complexity**. Automatic reduction of  $N$  when points become less informative → reduction of cost for a given performance.



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