

# State-space models: bootstrap filter and particle MCMC

MVE187-MSA101 “Computational methods for Bayesian statistics”, 2022

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- We look at how to perform parameter inference by embedding particle filters into Metropolis-Hastings.

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and mentioned that we wanted to approximate the likelihood via importance sampling as

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Then, it was discussed that, in practice, instead of trying to approximate the  $t + 1$ -dimensional integral above in one-go, it was easier to design a sequential strategy that recursively approximate the integral.

We had that we can approximate  $p(y_t|y_{1:t-1})$  with

$$\hat{p}(y_t|y_{1:t-1}) = \sum_{i=1}^N \frac{p(y_t|x_t^i)p(x_t^i|x_{t-1}^i)}{h(x_t^i|x_{0:t-1}^i, y_{1:t})} \tilde{w}_{t-1}^i, \quad i = 1, \dots, N$$

Then I mentioned that, except for the simplest models, it is often difficult to “construct” an importance function  $h(\cdot|x_{0:t-1}, y_{0:t})$  that is able to “look ahead” and see the next observation  $y_t$ , we simply take

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Thanks to this simplification (which has downsides, as we will see) we get

$$\hat{p}(y_t|y_{1:t-1}) = \sum_{i=1}^N p(y_t|x_t^i) \tilde{w}_{t-1}^i, \quad i = 1, \dots, N$$

or, by setting  $w_t^i = p(y_t|x_t^i)$  and  $\tilde{w}_t^i = w_t^i / \sum_{i=1}^N w_t^i$ ,

$$\hat{p}(y_t|y_{1:t-1}) = \sum_{i=1}^N w_t^i \tilde{w}_{t-1}^i, \quad i = 1, \dots, N$$

## (simplified) Sequential importance sampling

Then we obtained the following sequential algorithm where we “propagate forward” from the transition density:

1.  $t = 0$  (initialize)  $x_0^i \sim p(x_0)$ , assign  $\tilde{w}_0^i = 1/N$ ,  $i = 1, \dots, N$
2. at the current  $t$  assume we have the particles  $x_t^i$
3. From your model *propagate forward*  $x_{t+1}^i \sim p(x_{t+1}|x_t^i)$ ,  $i = 1, \dots, N$ .
4. Compute (unnormalised weights)

$$w_{t+1}^i \propto p(y_{t+1}|x_{t+1}^i) \times \tilde{w}_t^i.$$

5. we can finally approximate ([Creal, p. 253](#) ← hyperlink)

$$\hat{p}(y_{t+1}|y_{1:t}) = \sum_{i=1}^N w_{t+1}^i \tilde{w}_t^i$$

and normalise weights  $\tilde{w}_{t+1}^i = w_{t+1}^i / \sum_{i=1}^N w_{t+1}^i$

6. set  $t := t + 1$  and if  $t < T$  go to step 2.

We found out that even for a simple example the approximation was poor, even when using  $N$  very large.

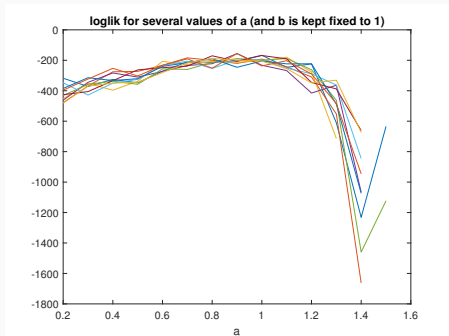
Let's see what happened for the usual model

In `demo_sis.m` we use the following model:

$$\begin{cases} y_t = b \cdot x_t + \epsilon_t^{(1)}, & \epsilon_t^{(1)} \sim_{iid} N(0, 0.3^2) \\ x_t = a \cdot x_{t-1} + \epsilon_t^{(2)}, & \epsilon_t^{(2)} \sim_{iid} N(0, 1) \\ x_0 = 0 \end{cases}$$

and in the previous lecture, just for illustration, we set  $b = 1$  constant to the true value that generated data and let  $a$  vary on a grid of values.

## Ten runs with $N=10000$



The data-generating value was  $a = 1$ , but the likelihood approximation does not seem very informative about the optimal value of  $a$ .

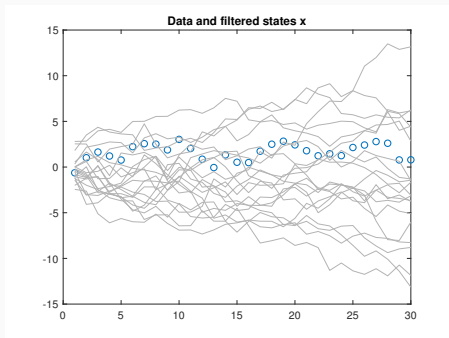
Notice: sometimes observed data are not informative enough (eg too small dataset). But it is NOT the case here, it is something else.



## How do the simulated $x$ values look?

[notice I uploaded a new, slightly modified SIS file  
`demo_sis_with_states.m`]

I collect the simulated  $x$  values and they look like (here  $N=20$  just to make things not too messy to read)



Clearly the  $x$  values go all over the place and won't get much weight in  $p(y_t|x_t) = N(x_t, 0.3^2)$ . So the likelihood is badly approximated.

The trick will be to **not allow particles that have low weight  $w_t$  at time  $t$  to keep existing at time  $t + 1$ .**

We want to kill those state values (particles) that seem improbable.

An in fact, if particle  $x_{t-1}^i$  has low weight  $w_{t-1}^i$ , then

$$\tilde{w}_{t-1}^i = w_{t-1}^i / \sum_i w_{t-1}^i$$

will become small and this particle will be forever doomed, see next slide.

It is not unusual that a particle gets an exactly zero weight, since your computer sets to zero a very small yet in principle strictly positive  $w_t$ . This is called *numerical underflow*, and that particle is doomed! Since

$$w_t^i \propto \frac{p(y_t|x_t^i)p(x_t^i|x_{t-1}^i)}{h(x_t^i|x_{0:t-1}^i, y_{1:t})} \tilde{w}_{t-1}^i.$$

if for a given  $i$  we have  $\tilde{w}_{t-1}^i = 0$ , then particle  $i$  will get zero weight for *all subsequent times*.

## Example of underflow

example, say that you want to evaluate particle value  $x_t^i = 40$  in  
 $p(y_t|x_t^i) = N(x_t^i; 0, 1)$

```
dnorm(40, 0, 1)
```

```
[1] 0
```

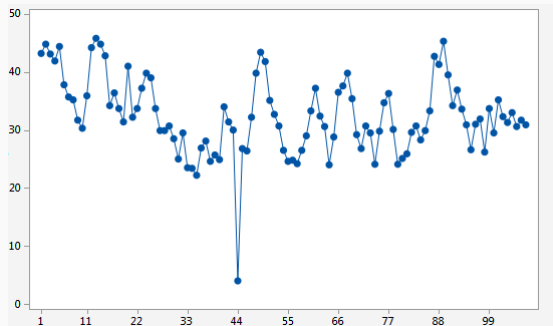
and even if you work on the log-density domain

```
> logw=dnorm(40, 0, 1, log=TRUE)
```

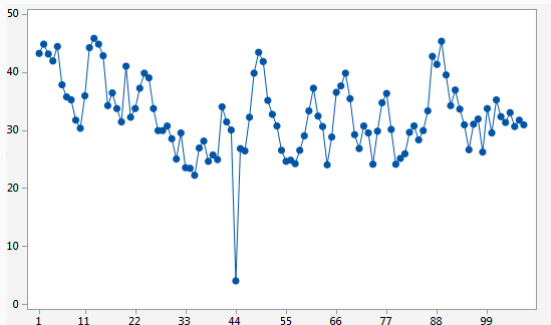
```
> exp(logw)
```

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So, as I said we really need to get rid of unpromising particles and let them die ( $\rightarrow$  no propagation forward from those ones).

The key idea is to do resampling with replacement according to normalised weights.

# The Resampling idea

A life saving solution is to use *resampling with replacement*.

Say that we are at time  $t$  and obtained the particles  $x_t^1, \dots, x_t^N$  and their unnormalised weights  $w_t^1, \dots, w_t^N$ .

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2. draw  $N$  particles with replacement from the weighted set. Call the drawn particles  $\{\tilde{x}_t^1, \dots, \tilde{x}_t^N\}$  and replace the original ones with  $\{\tilde{x}_t^1, \dots, \tilde{x}_t^N\}$ .

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3. After resampling, consider the new particles as all having the same importance, that is give them all  $w_t^i = 1/N$ .
4. Now propagate forward each of the particles  $\tilde{x}_t^i \rightarrow x_{t+1}$  as usual by running your model.

The key part was that in the last step we wrote

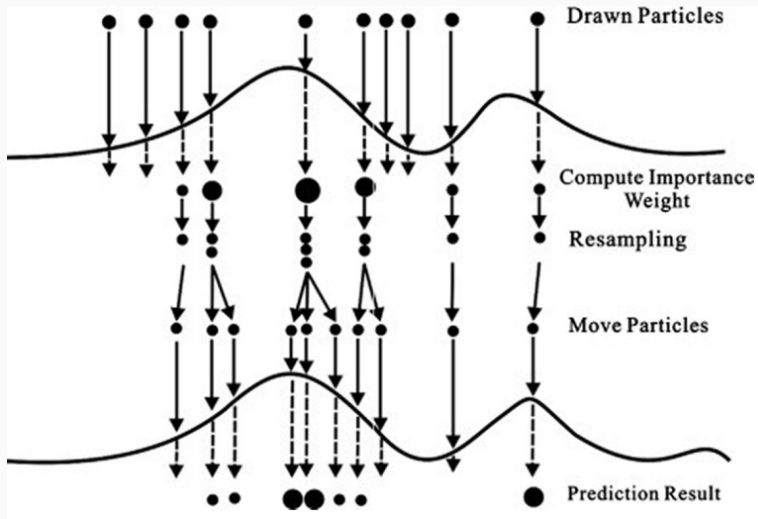
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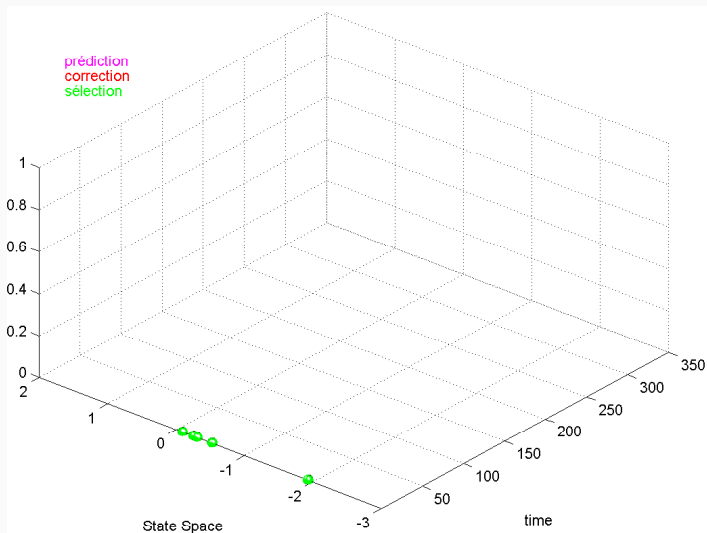
This means that **we propagate forward only the resampled particles**. The others peacefully **die out!**

Propagation→weighting→resampling→propagation of resampled particles→weighting→etc

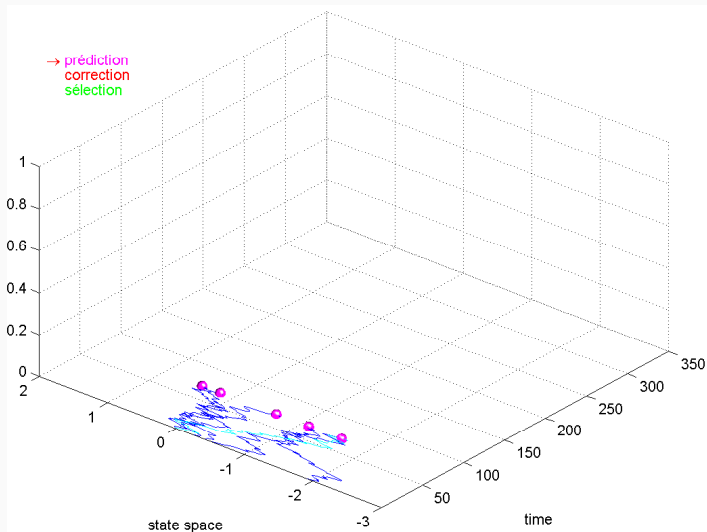


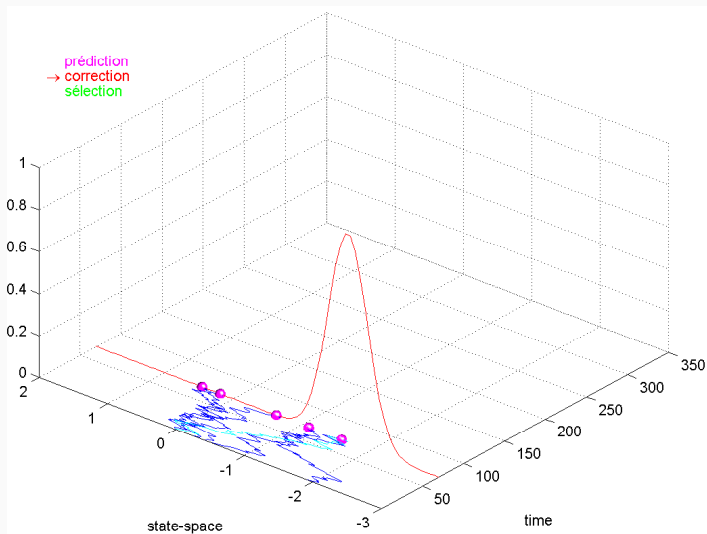
The next animation illustrates the concept of sequential importance sampling resampling with  $N = 5$  particles.

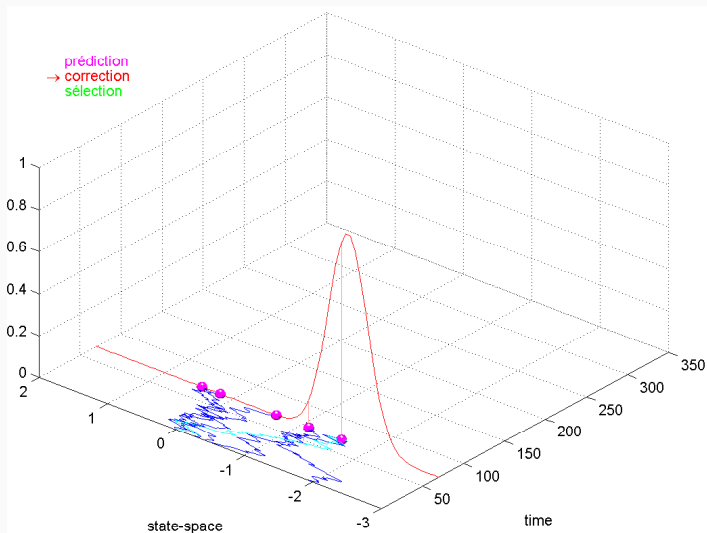
- Cyan: observed trajectory (data)
- dark blue: simulation of the latent process  $\{X_t\}$
- pink balls: particles  $x_t^i$
- green balls: selected particles  $\tilde{x}_t^i$  from resampling
- red curves: density  $p(y_t|x_t)$

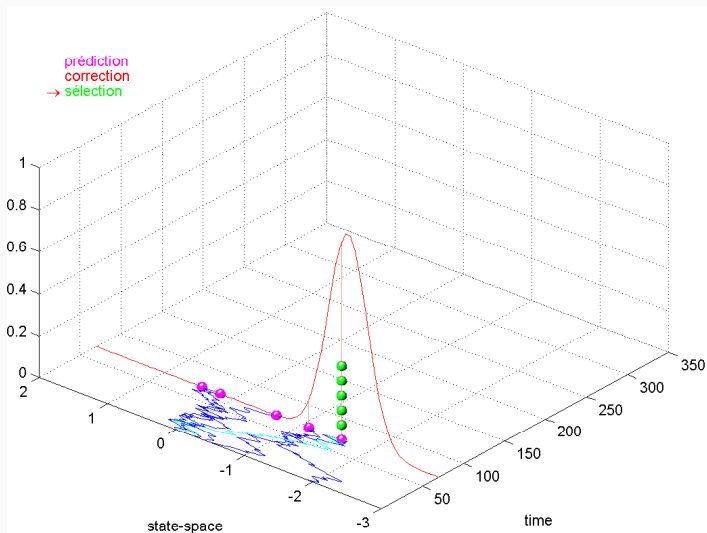


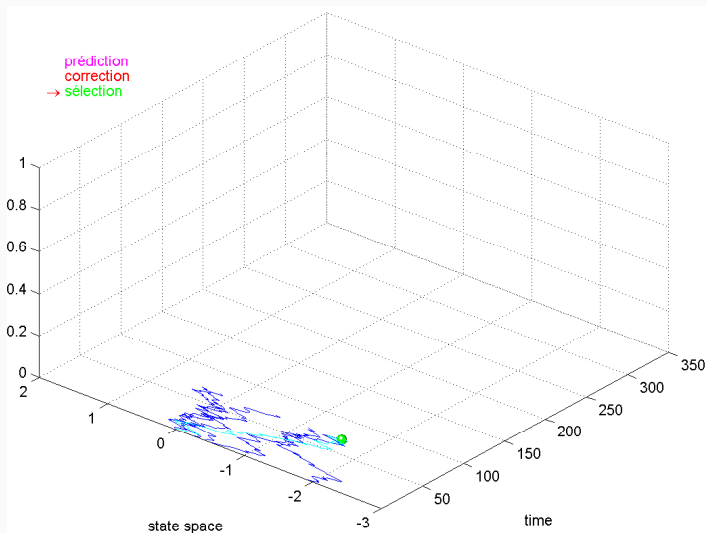


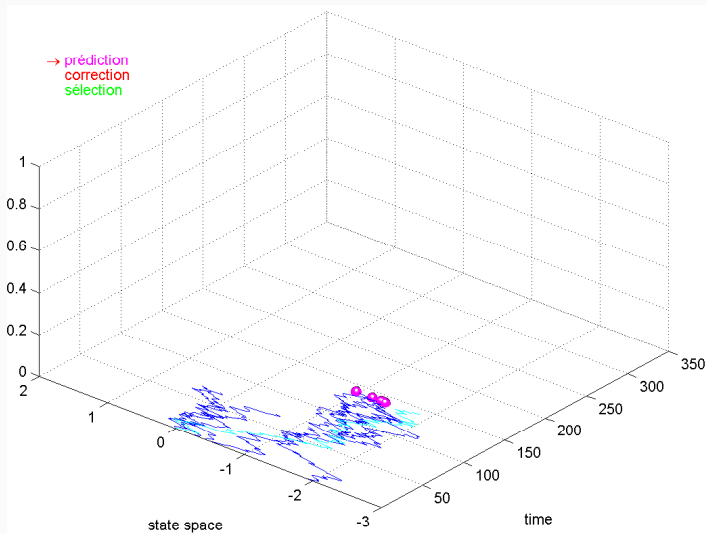


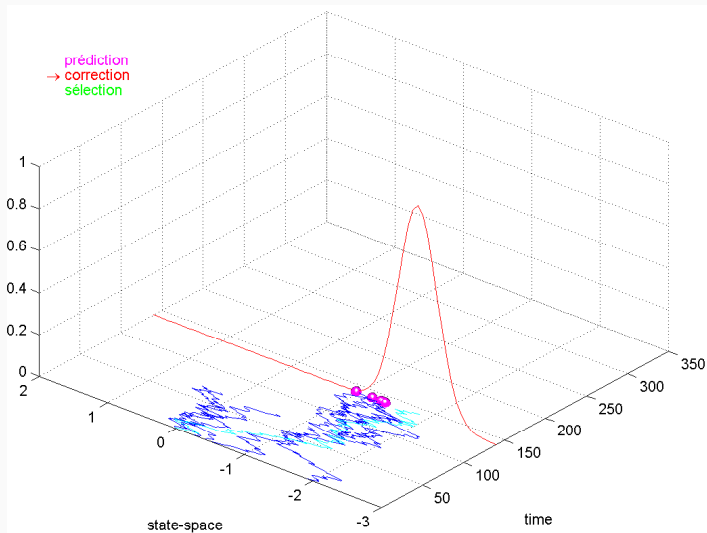


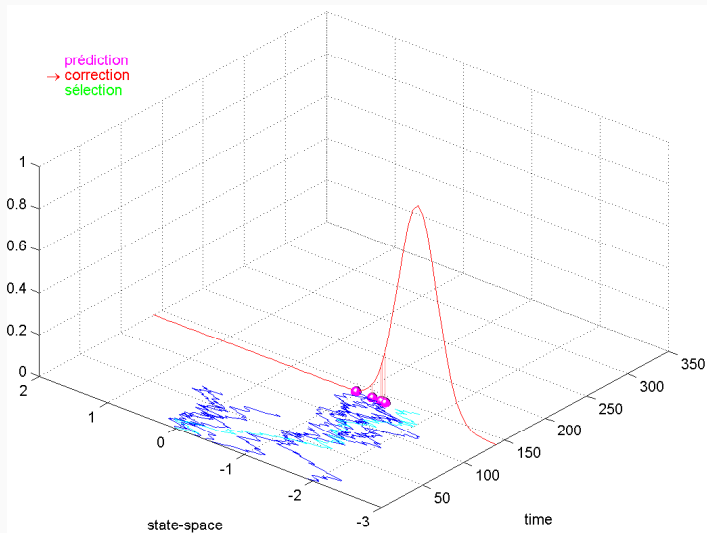




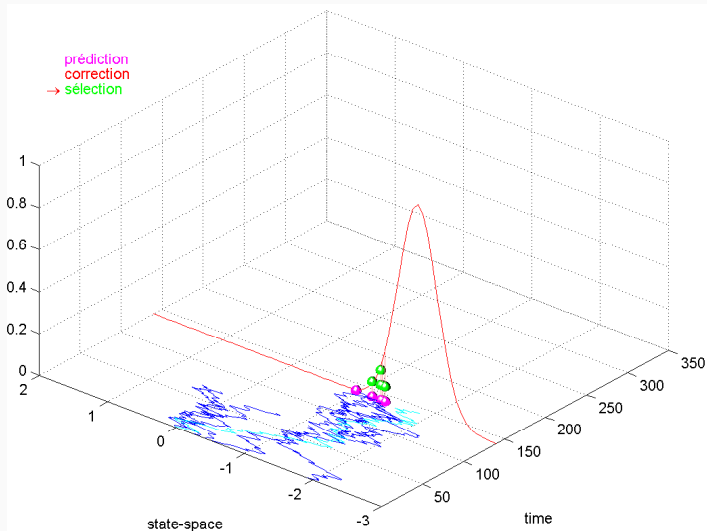


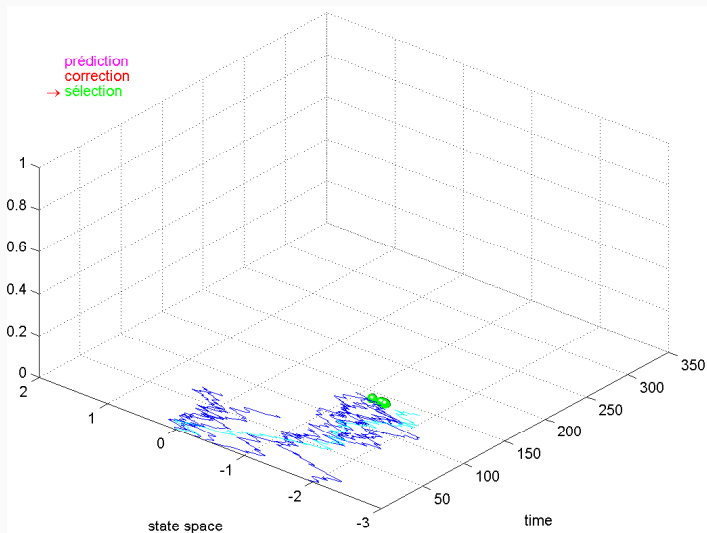


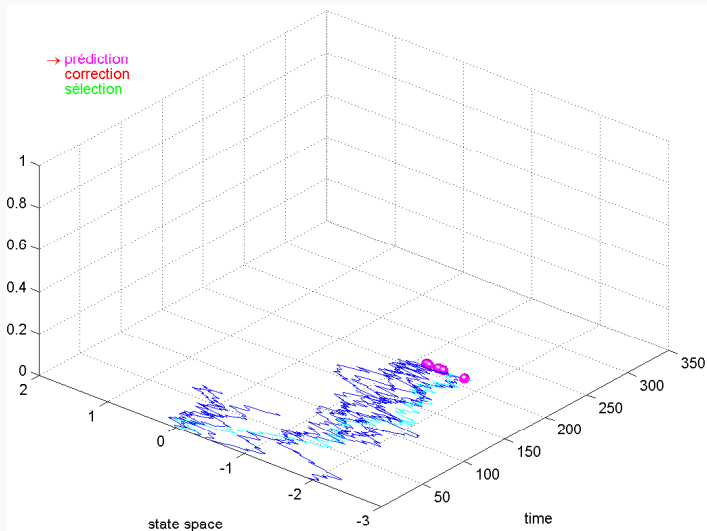


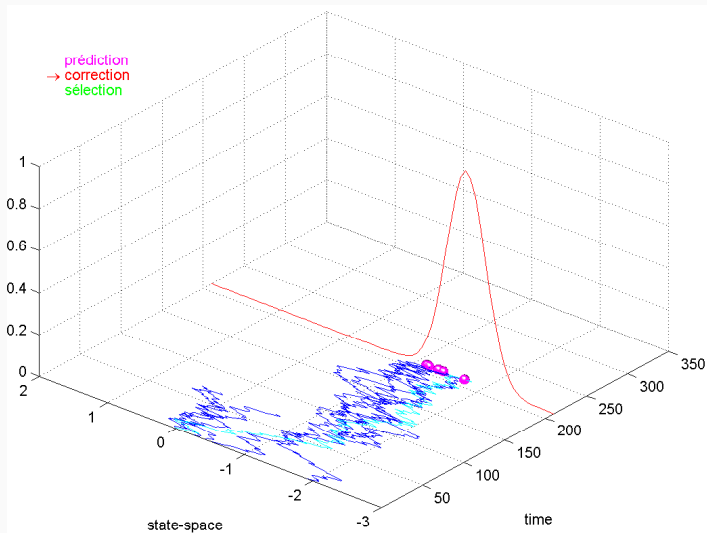


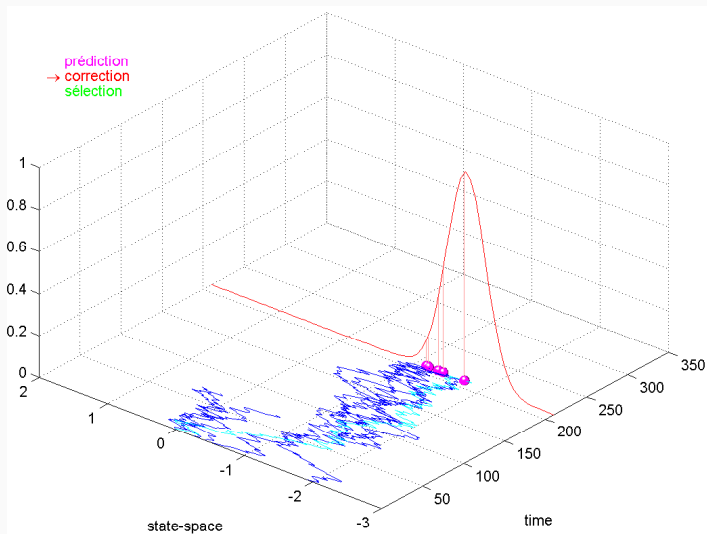


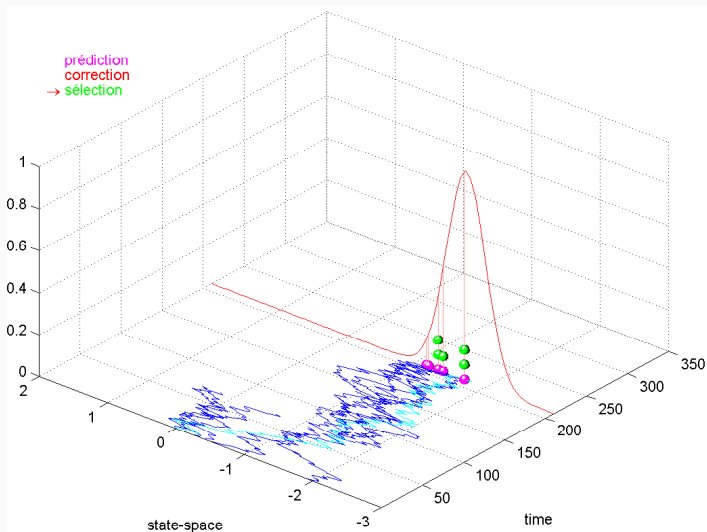


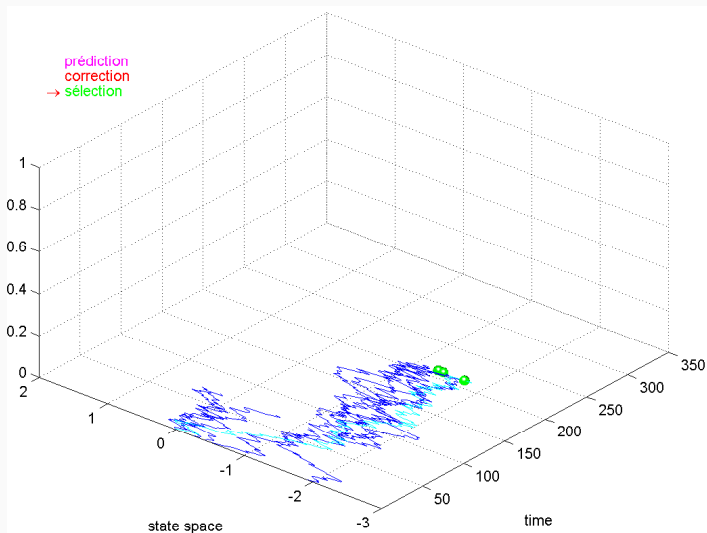


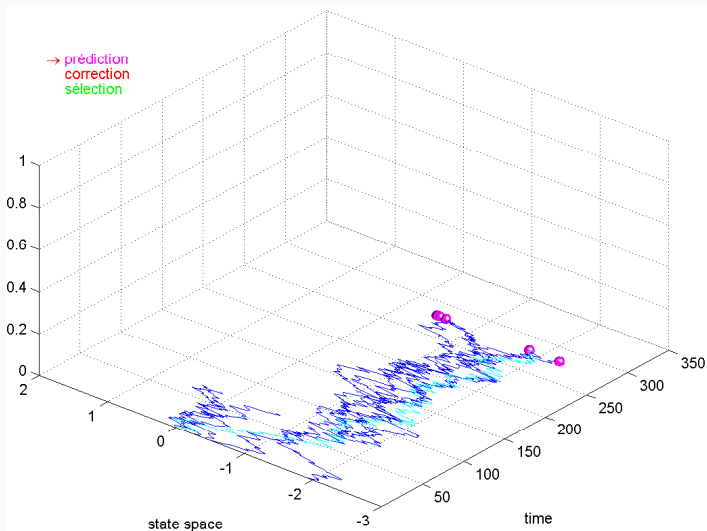




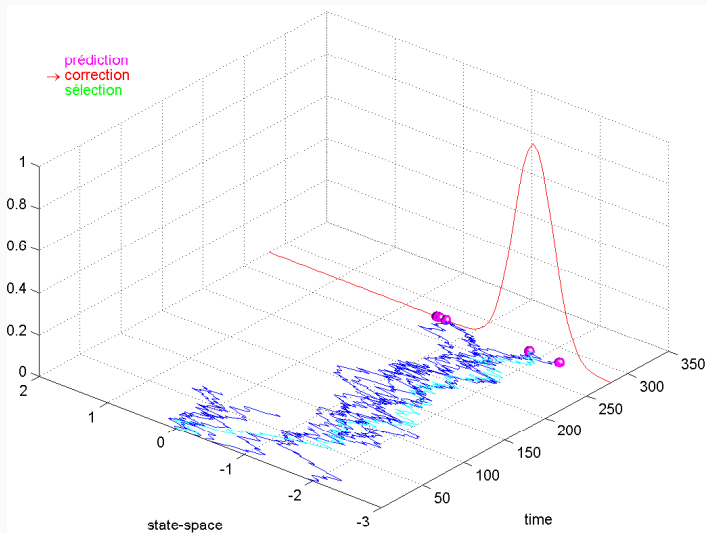


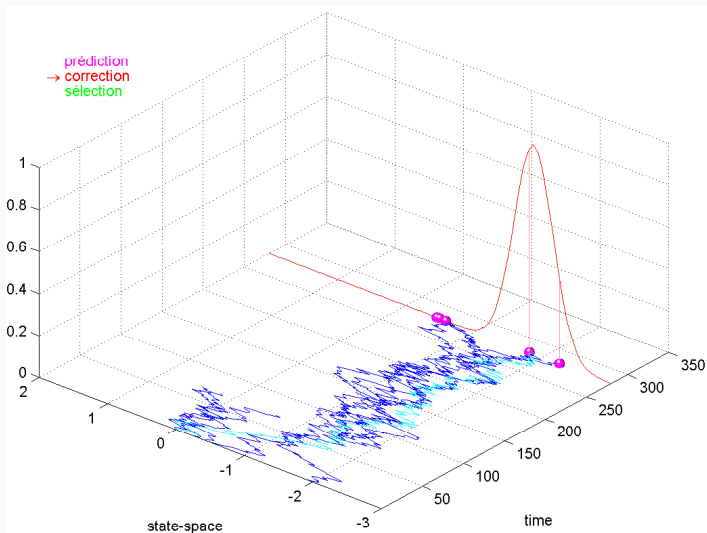


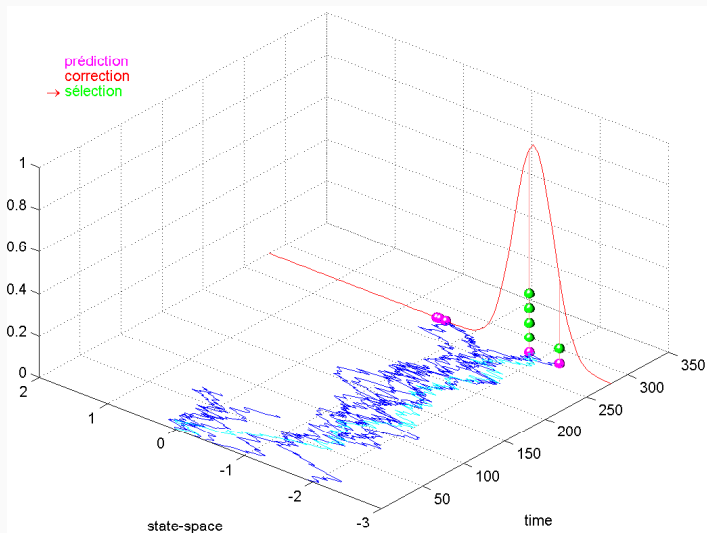


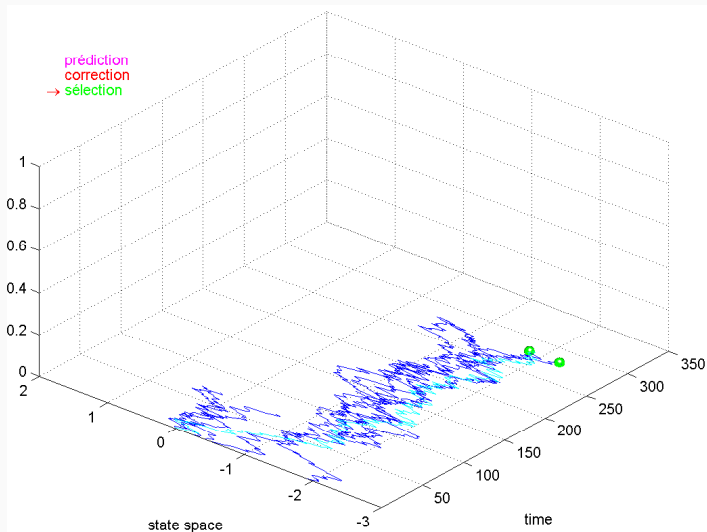


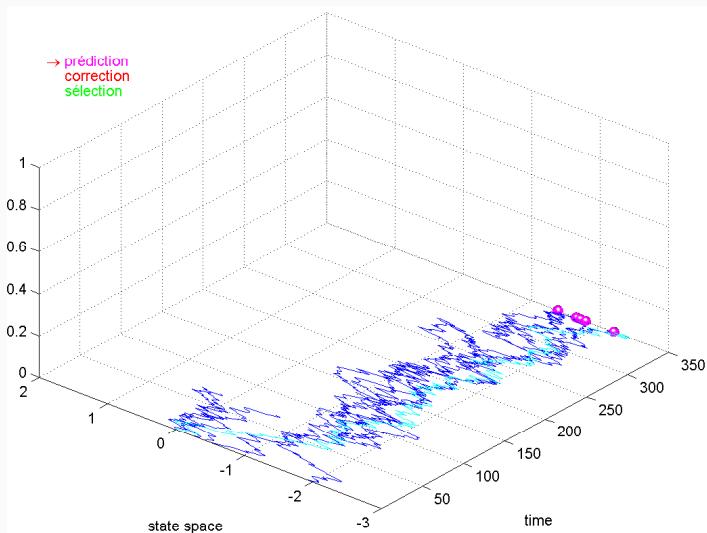


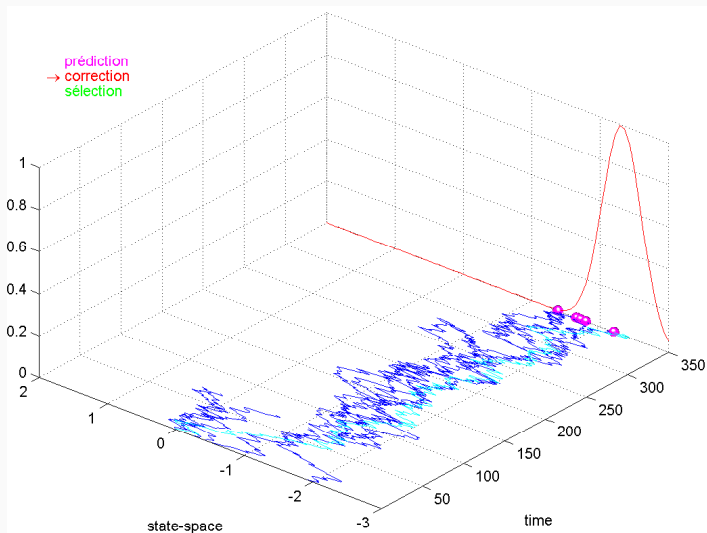


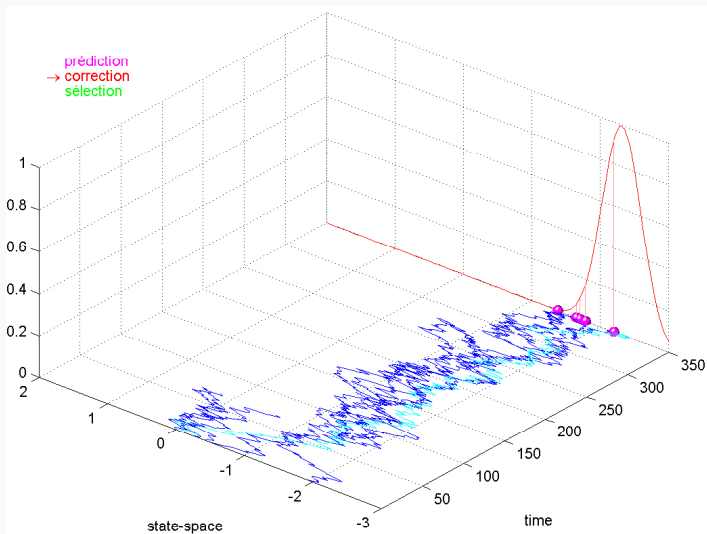












## Bootstrap filter for likelihood approximation

This is also aptly named *SIS with resampling*:

1.  $t = 0$  (initialize)  $x_0^i \sim p(x_0)$ , assign  $\tilde{w}_0^i = 1/N$ , for  $i = 1, \dots, N$
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6. approximate the likelihood term as usual

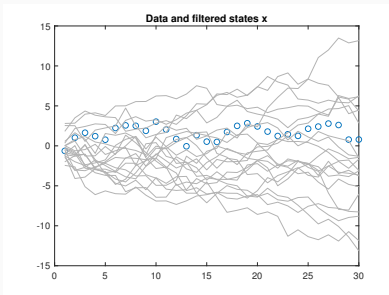
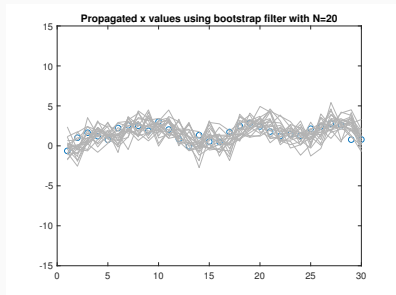
$$\hat{p}(y_{t+1}|y_{1:t}) = \sum_{i=1}^N w_{t+1}^i \tilde{w}_t^i = \sum_{i=1}^N w_{t+1}^i / N$$

## The usual example

Let's look at how the propagated trajectories look, with as little as  $N = 20$  with bootstrap filter (left) and SIS (right).

## The usual example

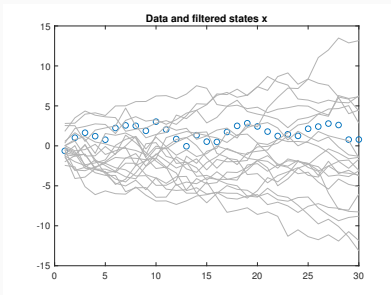
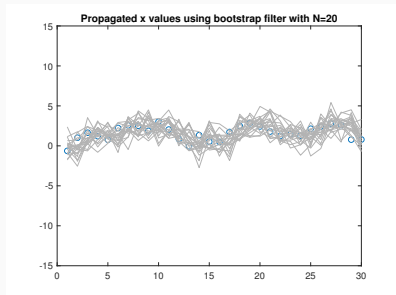
Let's look at how the propagated trajectories look, with as little as  $N = 20$  with bootstrap filter (left) and SIS (right).



Of course we could use a larger  $N$  but visually the plots would look too dense.

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Let's now look at the loglikelihood approximation.

## LogLikelihood approximations for varying $a$ and fixed $b$

Same as we did with SIS: let  $a$  vary and  $b$  is kept fixed to truth  $b = 1$ . Here  $N = 1,000$ , and we approximate the loglikelihood functions across 10 independent runs.

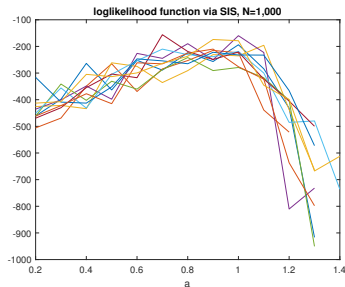
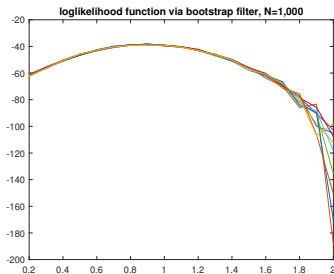
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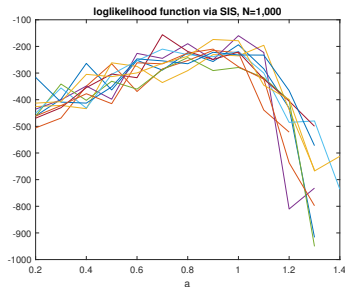
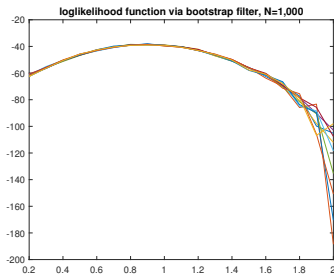


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Also notice SIS is unable to return values for  $a > 1.4$ .

## LogLikelihood approximations for varying $a$ and fixed $b$

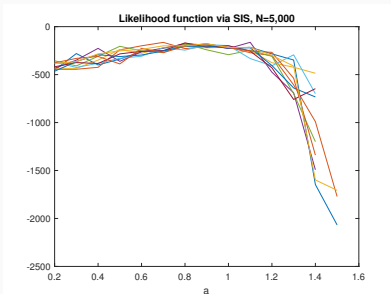
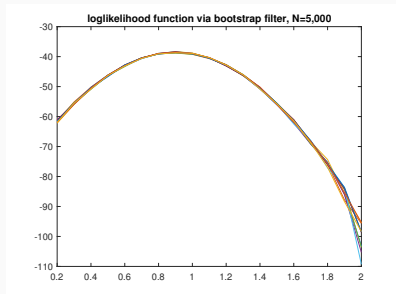
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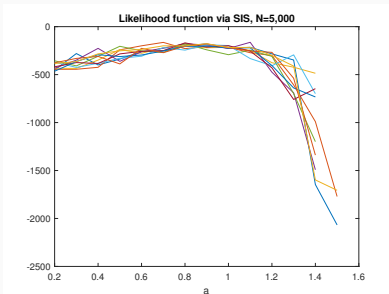
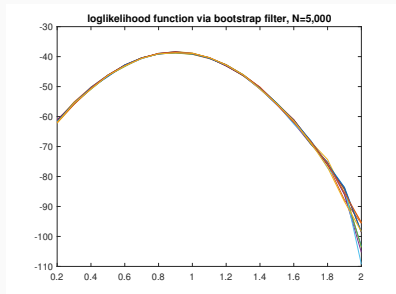


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# LogLikelihood approximations for varying $a$ and fixed $b$

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We use bootstrap filter (left) and SIS (right).



Notice the y-axis are on **very different scales**.

We have finally found a criterion that clearly displays a maximizer around  $a = 1$  as wanted.

So the bootstrap filter by Gordon et al. (1993)<sup>1</sup> easily provides what we need!

- $\hat{p}(y_t|y_{1:t-1}; \theta) = \frac{1}{N} \sum_{i=1}^N w_t^i$
- Finally a **likelihood approximation**:

$$\hat{p}(y_{1:T}|\theta) = \hat{p}(y_1) \prod_{t=2}^T \hat{p}(y_t|y_{1:t-1}; \theta)$$

We could use it for:

- **approximate** maximum likelihood

$$\theta_{mle} = \operatorname{argmax}_{\theta} \hat{p}(y_{1:T}; \theta)$$

or

- **Bayesian inference** by plugging  $\hat{p}(y_{1:T}|\theta)$  inside Metropolis-Hastings.

---

<sup>1</sup>Gordon, Salmond and Smith. IEEE Proceedings F. 140(2) 1993.

## Resampling particles using some software

To resample particles you can make use of built-in routines. Always remember that in this context we wish to sample **with replacement**. Below `normw` denotes the normalised weights  $\tilde{w}$  at a given time and `xres` is the vector of resampled particles obtained from the current `x`.

- In R you can use `xres <- sample(x, size = N, replace = TRUE, prob = normw)`
- Or, again in R, I believe the most efficient way is to first sample *indices* of the particles via `index <- sample.int(N, size = N, replace = TRUE, prob = normw)`  
and then create `xres <- x[, index]` (assuming you created `x` to be a matrix with  $N$  columns).

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Luckily, you have already seen the tool that we need to use. It is MCMC via Metropolis-Hastings.

Let's refresh our memory.

We wish to sample from the posterior  $\pi(\theta|y_{1:T}) \propto p(y_{1:T}|\theta) \times \pi(\theta)$ .

However in practice we can only sample from

$$\hat{\pi}(\theta|y_{1:T}) \propto \hat{p}(y_{1:T}|\theta) \times \pi(\theta),$$

with  $\hat{p}(y_{1:T}|\theta)$  approximated via particle filters, eg via bootstrap filter.

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with  $\hat{p}(y_{1:T}|\theta)$  approximated via particle filters, eg via bootstrap filter.

Since we embed a particle filter inside an MCMC algorithm, this strategy is often called **particle MCMC**<sup>2</sup>.

For our usual example,  $\theta = (a, b)$  and we need to specify priors for  $a$  and  $b$ .

---

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## Metropolis-Hastings (“particle MCMC” in this context)

**Initialization:** Set a starting value  $\theta_1 = \theta^*$ , eg the mean of the priors of  $a$  and  $b$ . Set  $N$  and  $R$  the number of iterations for Metropolis-Hastings. Compute the initial  $\hat{p}(y_{1:T}|\theta^*)$ . Define a proposal  $g(\theta'|\theta)$ . Set  $r = 1$ .

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1. Propose a move  $\theta^\# \sim g(\theta|\theta^*)$  and run the bootstrap filter using  $\theta^\#$  to obtain  $\hat{p}(y_{1:T}|\theta^\#)$ .
2. Generate a uniform random draw  $u \sim U(0, 1)$ , and calculate the acceptance probability

$$\alpha = \min \left[ 1, \frac{\hat{p}(y_{1:T}|\theta^\#)}{\hat{p}(y_{1:T}|\theta^*)} \times \frac{g(\theta^*|\theta^\#)}{g(\theta^\#|\theta^*)} \times \frac{\pi(\theta^\#)}{\pi(\theta^*)} \right].$$

If  $u > \alpha$ , set  $\theta_{r+1} := \theta_r$  otherwise set  $\theta_{r+1} := \theta^\#$ ,  $\theta^* := \theta^\#$  and  $\hat{p}(y_{1:T}|\theta^*) := \hat{p}(y_{1:T}|\theta^\#)$ . Set  $r := r + 1$  and go to step 3.

3. Repeat steps 1–2 as long as  $r \leq R$ .

The resulting sequence  $\theta_1, \dots, \theta_R$  (possibly after having discarded some initial burnin iterations) is a Markov chain having  $\hat{\pi}(\theta|y_{1:T})$  as stationary distribution.



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## Bayesian inference for $a$ and $b$

The following is coded in `demo_pmcmc.m`.

I made the following assumptions but this is just for illustration, you are free to change this.

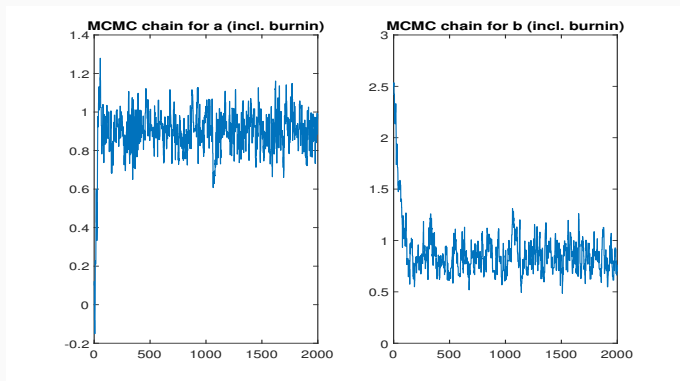
- Joint prior for  $\theta = (a, b)$  given by  $\pi(\theta) = \pi(a)\pi(b)$  ( $a$  and  $b$  a-priori independent) with  $\pi(a) = N(0.5, 1)$ ,  $\pi(b) = N(1.5, 0.5^2)$ .
- $g(\theta|\theta^*) = MVN(\theta^*, \Sigma)$ , a multivariate Gaussian with mean  $\theta^*$  and diagonal covariance matrix

$$\Sigma = \begin{bmatrix} 0.1^2 & 0 \\ 0 & 0.1^2 \end{bmatrix}$$

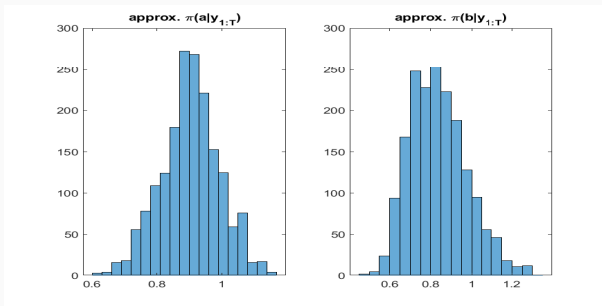
Notice the chosen  $g(\cdot|\cdot)$  is **symmetric**, eg  $g(\theta^\#|\theta^*) = g(\theta^*|\theta^\#)$ , so it simplifies out in  $\alpha$  (no need to code it in the ratio).

Recall the used data have been generated with  $a = b = 1$  so we hope to recover these values to some extent.

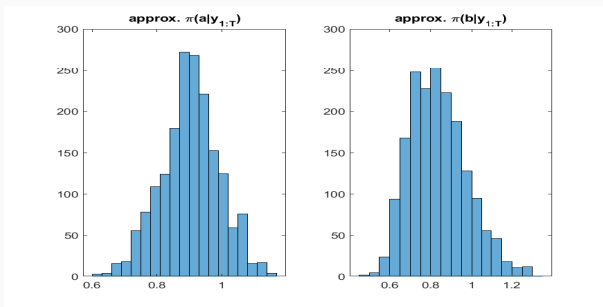
These results used  $N = 1,000$  particles,  $R = 2000$  MCMC iterations. I used a starting  $\theta_1 = (a_1 = 0.1, b_1 = 2.5)$ .



The marginal posteriors below are produced by disregarding the first 200 iterations (burnin).



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True values  $a = b = 1$  are likely in the posterior (which is good) but we also have some uncertainty.

If you didn't know that in reality true values are  $a=b=1$ , what you would concluded is that, conditional to observed data, the true value of  $a$  should be with high probability somewhere between 0.6 and 1.1, while for  $b$  is somewhere between 0.6 and 1.2.

Would you have expected less variability? You can do the following:

- When constructing the experiment, try to get more data (posterior converges to truth as data size grows to infinity).

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- When constructing the experiment, try to get more data (posterior converges to truth as data size grows to infinity).
- For real studies: learn from previous literature and previous experiment (or construct experts), so you can encode a more informative prior that could have some effect on the posterior.
- The results are depending on the quality of the model you design: if the model is inappropriate, inferences will be flawed. But we never know the true model generating the data (except in simulation studies like the one we did).



## Tips for Metropolis-Hastings

As usual, best to code things on log-scale for numerical stability.

In `demo_pmcmmcmc.m` I did the following: **instead of coding** (notice I simplified-out the ratio of symmetric proposal densities)

$$\alpha = \min \left[ 1, \frac{\hat{p}(y_{1:T}|\theta^\#)}{\hat{p}(y_{1:T}|\theta^*)} \times \frac{\pi(\theta^\#)}{\pi(\theta^*)} \right].$$

If  $u > \alpha$ , set  $\theta_{r+1} := \theta_r \dots$

**I coded**

$$\log \alpha = \min \left[ 0, \log \hat{p}(y_{1:T}|\theta^\#) - \log \hat{p}(y_{1:T}|\theta^*) + \log \pi(\theta^\#) - \log \pi(\theta^*) \right].$$

If  $\log u > \log \alpha$ , set  $\theta_{r+1} := \theta_r \dots$  etc.

The latter is a completely equivalent but safer approach.

(optional for those interested: more Metropolis-Hastings tips [here](#).)

You find on Canvas:

- `demo_sis_with_states.m`: this is a better version of `demo_sis.m`. You can delete the latter. The new version is also able to plot the  $x$  states, so it is more useful.
- `demo_bootstrap.m` which illustrates the bootstrap filter.
- `demo_pmcmc.m` which illustrates particle MCMC, i.e. produces Bayesian inference via Metropolis-Hastings + bootstrap particle filter.
- `demo_nimbleSMC.R` which illustrates the bootstrap particle filter in R using nimbleSMC, without specifying parameters  $a$  and  $b$ .
- `demo_nimbleSMC_with_parameters.R` same as above, but here you can easily provide values for parameters  $a$  and  $b$ .

## A possible exercise

- If you did last week's exercise (constructing the SIS filter in R), building the bootstrap filter will be a trivial modification of the SIS filter. Of course you can look at the uploaded Matlab version for inspiration.
- Once the above is done, you may build your own particle MCMC sampler for  $a$  and  $b$ , for example using the same setup I used, or a different one, and obtain draws from  $\hat{\pi}(a|y_{1:T})$  and  $\hat{\pi}(b|y_{1:T})$ .
- What happens if you start at very unlikely (extreme) values of  $a$  and  $b$ ? Do you observe a lot of rejections? If yes, can you repair this by increasing  $N$ ? Any intuition why  $N$  could have anything to do with MCMC rejections?
- To verify that your custom R code for particle MCMC worked as expected, you may also compare against a version using loglikelihoods obtained via the bootstrap filter as in `nimbleSMC` (as illustrated in `demo_nimbleSMC_with_parameters.R`), at any given proposed parameter value.