Monte Carlo and Empirical Methods for Stochastic Inference (MASM11/FMSN50)

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Lecture 7
Sequential Monte Carlo methods III
February 12, 2019
Plan of today’s lecture

1. Last time: Sequential importance sampling (SIS)
   - SIS in a nutshell
   - Example: filtering in HMMs

2. Sequential importance sampling with resampling (SISR)
   - SIS + multinomial selection = SISR
   - Alternative selection strategies
   - A slide on convergence

3. Home assignment 2 (HA2)
1. Last time: Sequential importance sampling (SIS)
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3. **Home assignment 2 (HA2)**
In the sequential MC framework, we aim at sequentially estimating sequences \((\tau_n)_{n \geq 0}\) of expectations

\[ \tau_n = \mathbb{E}_{\phi_n}(\phi(X_{0:n})) = \int_{X_n} \phi(x_{0:n})f_n(x_{0:n}) \, dx_{0:n} \]

over spaces \(X_n\) of increasing dimension, where the densities \((f_n)\) are known up to normalizing constants only, i.e., for every \(n \geq 0\),

\[ f_n(x_{0:n}) = \frac{z_n(x_{0:n})}{c_n}, \]

where \(c_n\) is an unknown constant.
To derive the SIS algorithm we proceeded recursively. Assume that we have generated particles \((X^0_i)\) from \(g_n(x_{0:n})\) so that

\[
\sum_{i=1}^{N} \frac{\omega^i_n}{\sum_{\ell=1}^{N} \omega^\ell_n} \phi(X^0_i) \approx \mathbb{E}_{f_n}(\phi(X_{0:n})),
\]

where, as usual, \(\omega^i_n = \omega_n(X^0_i) = z_n(X^0_i)/g_n(X^0_i)\).

**Key trick:** Choose an instrumental distribution satisfying

\[
g_{n+1}(x_{0:n+1}) = g_{n+1}(x_{n+1}|x_{0:n})g_n(x_{0:n}).
\]
Consequently, $X_{i}^{0:n+1}$ and $\omega_{n+1}^{i}$ can be generated by

- keeping the previous $X_{i}^{0:n}$,
- simulating $X_{i}^{n+1} \sim g_{n+1}(x_{n+1}|X_{i}^{0:n})$,
- setting $X_{i}^{0:n+1} = (X_{i}^{0:n}, X_{i}^{n+1})$, and
- computing

$$\omega_{n+1}^{i} = \frac{z_{n+1}(X_{i}^{0:n+1})}{g_{n+1}(X_{i}^{0:n+1})}$$

$$= \frac{z_{n+1}(X_{i}^{0:n+1})}{z_{n}(X_{i}^{0:n}) g_{n+1}(X_{i}^{n+1}|X_{i}^{0:n})} \times \frac{z_{n}(X_{i}^{0:n})}{g_{n}(X_{i}^{0:n})} \times \omega_{n}^{i}.$$
So, SIS updates the estimator

$$\sum_{i=1}^{N} \frac{\omega_n^i}{\sum_{\ell=1}^{N} \omega_n^\ell} \phi(X_{i}^{0:n}) \approx \mathbb{E}_{f_n}(\phi(X_{0:n}))$$

to the estimator

$$\sum_{i=1}^{N} \frac{\omega_{n+1}^i}{\sum_{\ell=1}^{N} \omega_{n+1}^\ell} \phi(X_{i}^{0:n+1}) \approx \mathbb{E}_{f_{n+1}}(\phi(X_{0:n+1}))$$

by only adding a component $X_{i}^{n+1}$ to $X_{i}^{0:n}$ and sequentially updating the weights. The algorithm is initialized by standard importance sampling of $\tau_0$. We note that for each $n$, an unbiased estimate of $c_n$ can, as usual, be obtained as

$$\frac{1}{N} \sum_{i=1}^{N} \omega_n^i \approx c_n.$$
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3. Home assignment 2 (HA2)
HMMs

Graphically:

\[ Y_{k-1} \rightarrow X_{k-1} \rightarrow X_k \rightarrow X_{k+1} \rightarrow Y_k \rightarrow Y_{k+1} \]

\[ Y_k | X_k = x_k \sim p(y_k | x_k) \]  
\[ X_{k+1} | X_k = x_k \sim q(x_{k+1} | x_k) \]  
\[ X_0 \sim \chi(x_0) \]

(Observations)

(Markov chain)

(Observation density)

(Transition density)

(Initial distribution)
Consider the linear HMM

\[
Y_k = X_k + S \varepsilon_k, \quad \sim p(y_k|x_k)
\]

\[
X_{k+1} = AX_k + R \eta_{k+1}, \quad \sim q(x_{k+1}|x_k)
\]

\[
X_0 = R/\sqrt{1 - A^2 \eta_0}, \quad \sim \chi(x_0)
\]

where \(|A| < 1\) and \((\eta_k)\) and \((\varepsilon_k)\) are independent standard Gaussian variables.

Given \textit{fixed} observations \((y_k)\), we want to estimate sequentially the \textit{filter} means

\[
\tau_n = \mathbb{E}(X_n|Y_{0:n} = y_{0:n})
\]

\[
= \int_{\phi(x_{0:n})} \underbrace{\chi(x_0)p(y_0|x_0) \prod_{k=0}^{n-1} q(x_{k+1}|x_k)p(y_{k+1}|x_{k+1})}_{L_n(y_{0:n})} \frac{z_n(x_{0:n})}{c_n} \, dx_{0:n}.
\]
To obtain a SIS implementation, we set

\[ g_{n+1}(x_{n+1}|x_{0:n}) = q(x_{n+1}|x_n) = \mathcal{N}(x_{k+1}; Ax_n, R^2), \]

implying

\[
\omega_{n+1}^i = \frac{z_{n+1}(X^0_{i:n+1})}{z_n(X^0_{i:n})g_{n+1}(X_{i}^{n+1}|X^0_{i:n})} \times \omega^i_n \]

\[
= \frac{\chi(X_i^0) p(y_0|X_i^0) \prod_{k=0}^{n} q(X_{i}^{k+1}|X_{i}^k) p(y_{k+1}|X_{i}^{k+1})}{\chi(X_i^0) p(y_0|X_i^0) \prod_{k=0}^{n-1} q(X_{i}^{k+1}|X_{i}^k) p(y_{k+1}|X_{i}^{k+1})} \times \omega^i_n \]

\[
= p(y_{n+1}|X_{i}^{n+1}) \times \omega^i_n \]

\[
= \mathcal{N}(y_{n+1}; X_{i}^{n+1}, S^2) \times \omega^i_n. \]
This gives the following scheme.

Assume that

$$\sum_{i=1}^{N} \frac{\omega_{n}^{i}}{\sum_{\ell=1}^{N} \omega_{n}^{\ell}} X_{i}^{n} \approx \mathbb{E}(X_{n}|Y_{0:n} = y_{0:n});$$

then, for $i = 1, 2, \ldots, N$,

- draw $X_{i}^{n+1} \sim \mathcal{N}(AX_{i}^{n}, R^{2})$,
- set $\omega_{n+1}^{i} = \mathcal{N}(y_{n+1}; X_{i}^{n+1}, S^{2}) \times \omega_{n}^{i}$,

yielding the approximation

$$\sum_{i=1}^{N} \frac{\omega_{n+1}^{i}}{\sum_{\ell=1}^{N} \omega_{n+1}^{\ell}} X_{i}^{n+1} \approx \mathbb{E}(X_{n+1}|Y_{0:n+1} = y_{0:n+1}).$$
In Matlab:

```matlab
N = 1000;
n = 60;
tau = zeros(1,n); % vector of estimates
p = @(x,y) normpdf(y,x,S); % observation density, for weights
part = R*sqrt(1/(1 - A^2))*randn(N,1); % initialization
w = p(part,Y(1));
tau(1) = sum(part.*w)/sum(w);
for k = 1:n, % main loop
    part = A*part + R*randn(N,1); % mutation
    w = w.*p(part,Y(k + 1)); % weighting
    tau(k + 1) = sum(part.*w)/sum(w); % estimation
end
```
Linear/Gaussian HMM, SIS implementation

Comparison of SIS (○) with exact values (∗) provided by the Kalman filter (possible only for linear/Gaussian models):

![Graph showing filtered means for Kalman filter and SIS]
Distribution of importance weights: 😞

- $n = 1$
- $n = 5$
- $n = 15$
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   - SIS + multinomial selection = SISR
   - Alternative selection strategies
   - A slide on convergence

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2. Sequential importance sampling with resampling (SISR)
   - $SIS + \text{multinomial selection} = SISR$
   - Alternative selection strategies
   - A slide on convergence

3. Home assignment 2 (HA2)
Multinomial resampling

A simple—but revolutionary!—idea: duplicate/kill particles with large/small weights! (Gordon et al., 1993)

The most natural approach to such selection is to simply draw, with replacement, new particles \( \tilde{X}^0:n_1, \tilde{X}^0:n_2, \ldots, \tilde{X}^0:n_N \) among the SIS-produced particles \( X^0:n_1, X^0:n_2, \ldots, X^0:n_N \) with probabilities given by the normalized importance weights.

Formally, this amounts to setting, for \( i = 1, 2, \ldots, N \),

\[
\tilde{X}^0:n_i = X^0:n_j \quad \text{with probability} \quad \frac{\omega^i_n}{\sum_{\ell=1}^N \omega^\ell_n}.
\]
Criteria for good resampling strategies

Let $N^i_n$ be the number of resampled copies of particle $i$.

- The total number of particles should remain constant.
- The weights should be set equal after resampling.
- It should hold that

$$\mathbb{E}[N^i_n | X^{0:n}] = N \frac{\omega^i_n}{\sum_{\ell=1}^{N} \omega^\ell_n}, \quad i = 1, 2, \cdots, N.$$  

Assures that the resampling gives no additional bias.
After this, the resampled particles \((\tilde{X}_i^{0:n})\) are assigned equal weights \(\tilde{\omega}_n^i = 1\), say, and we replace

\[
\sum_{i=1}^{N} \frac{\omega_n^i}{\sum_{\ell=1}^{N} \omega_n^\ell} \phi(X_i^{0:n}) \quad \text{by} \quad \frac{1}{N} \sum_{i=1}^{N} \phi(\tilde{X}_i^{0:n}).
\]

Multinomial resampling does not add bias to the estimator:

**Theorem**

*For all* \(N \geq 1\) *and* \(n \geq 0\),

\[
\mathbb{E} \left( \frac{1}{N} \sum_{i=1}^{N} \phi(\tilde{X}_i^{0:n}) \right) = \mathbb{E} \left( \sum_{i=1}^{N} \frac{\omega_n^i}{\sum_{\ell=1}^{N} \omega_n^\ell} \phi(X_i^{0:n}) \right).
\]

The operation adds however some variance due to additional randomness.
Sequential importance sampling with resampling (SISR)

After selection, we proceed with standard SIS and move the selected particles \( \tilde{X}_i^{0:n} \) according to \( g_{n+1}(x_{n+1}|x_{0:n}) \).

The full scheme goes as follows. Given \( (X_i^{0:n}, \omega_i^n) \),

- **(selection)** draw, with replacement, \( \tilde{X}_i^{0:n} \) among \( X_i^{0:n} \) according to probabilities \( \omega_i^n / \sum_{\ell=1}^N \omega_\ell^n \)
- **(mutation)** draw, for all \( i \), \( X_i^{n+1} \sim g_{n+1}(x_{n+1}|\tilde{X}_i^{0:n}) \),
- set, for all \( i \), \( X_i^{0:n+1} = (\tilde{X}_i^{0:n}, X_i^{n+1}) \), and
- set, for all \( i \),

\[
\omega_i^{n+1} = \frac{z_{n+1}(X_i^{0:n+1})}{z_n(\tilde{X}_i^{0:n})g_{n+1}(X_i^{n+1}|\tilde{X}_i^{0:n})}.
\]
SISR, estimation of $\tau_n$ and $c_n$

At every time step $n$, both

$$\sum_{i=1}^{N} \frac{\omega^i_n}{\sum_{\ell=1}^{N} \omega^\ell_n} \phi(X^0:n)$$

and

$$\frac{1}{N} \sum_{i=1}^{N} \phi(\tilde{X}^0:n)$$

are valid estimators of $\tau_n$. The former has however somewhat lower variance. For estimation of normalizing constants using SISR, set

$$c_{N,n}^{SISR} = \prod_{k=0}^{n} \left( \frac{1}{N} \sum_{i=1}^{N} \omega^i_k \right) .$$

**Theorem**

For all $n \geq 0$ and $N \geq 1$,

$$\mathbb{E} \left( c_{N,n}^{SISR} \right) = c_n.$$
Example: Linear/Gaussian HMM, SISR implementation

In Matlab:

N = 1000;
n = 60;
tau = zeros(1,n); % vector of filter means
w = zeros(N,1);
p = @(x,y) normpdf(y,x,S); % observation density, for weights
part = R*sqrt(1/(1 - A^2))*randn(N,1); % initialization
w = p(part,Y(1));
tau(1) = sum(part.*w)/sum(w);
for k = 1:n, % main loop
    part = A*part + R*randn(N,1); % mutation
    w = p(part,Y(k + 1)); % weighting
    tau(k + 1) = sum(part.*w)/sum(w); % estimation
    ind = randsample(N,N,true,w); % selection
    part = part(ind);
end
The Essential part of the randsample function

The Matlab (R2016a) function `randsample` has 178 lines of code but we actually could just use the essential part of the code

\[
\text{CW}=\text{cumsum}([0 \ W]);
\]
\[
[~,\text{ind}] = \text{histc}(\text{rand}(1,N),\text{CW}/\text{CW}(<\text{end}));
\]

where `histc` is the builtin and very efficiently coded function for counting the number of points in each in bin and the indices of which bin we fall in for doing histograms.

We here use the normalised cumulative weightsum as bin boundaries and only look at the bin indices for points \( \in U(0,1) \). This gives us exactly the correct resampling distribution of the indicies `ind`.

It is also easy to modify the code to do a version of stratified resampling (see below).
Example: Linear/Gaussian HMM, SIS implementation

Comparison of SIS (○) and SISR (∗, blue) with exact values (∗, red) provided by the Kalman filter:

![Graph showing filtered means for Kalman filter, SIS, and SISR]
A comparison between Kalman filter $\mathbb{E}[X_k|Y_{0:k} = y_{0:k}]$ and Smoother $\mathbb{E}[X_k|Y_{0:n} = y_{0:n}]$ for $k = 0, 1, \cdots, n$: 

![Graph comparing Kalman filter and Smoother]
Film time! 😊
Last time: Sequential importance sampling (SIS)
Sequential importance sampling with resampling (SISR)
Home assignment 2 (HA2)

SIS + multinomial selection = SISR
Alternative selection strategies
A slide on convergence
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SIS + multinomial selection = SISR

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Sequential importance sampling with resampling (SISR)
Home assignment 2 (HA2)

SIS + multinomial selection = SISR
Alternative selection strategies
A slide on convergence
Last time: Sequential importance sampling (SIS) and Sequential importance sampling with resampling (SISR)

Home assignment 2 (HA2)

SIS + multinomial selection = SISR

Alternative selection strategies

A slide on convergence
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Home assignment 2 (HA2)

\[ \text{SIS + multinomial selection} = \text{SISR} \]

Alternative selection strategies
A slide on convergence

\[ \rightarrow \text{prédiction correction sélection} \]
Last time: Sequential importance sampling (SIS)
Sequential importance sampling with resampling (SISR)
Home assignment 2 (HA2)

SIS + multinomial selection = SISR
Alternative selection strategies
A slide on convergence
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3. Home assignment 2 (HA2)
There are several alternatives to multinomial selection. In the residual resampling scheme the number $N^i_n$ of offspring of particle $i$ is—"semi-deterministically"—set to

$$N^i_n = \left\lfloor N \frac{\omega^i_n}{\sum_{\ell=1}^N \omega^\ell_n} \right\rfloor + \tilde{N}^i_n,$$

where the $\tilde{N}^i_n$’s are random integers obtained by randomly distributing the remaining $N - R$ offspring, with

$$R \overset{\text{def}}{=} \sum_{j=1}^N \left\lfloor N \frac{\omega^j_n}{\sum_{\ell=1}^N \omega^\ell_n} \right\rfloor,$$

among the ancestors as follows.
Residual resampling, pseudo-code

for $i = 1 \rightarrow N$ do
    set $\tilde{N}_n^i \leftarrow 0$
    set $\bar{\omega}_n^i \leftarrow \frac{1}{N - R} \left( N \frac{\omega_n^i}{\sum_{\ell=1}^{N} \omega_n^\ell} - \left[ N \frac{\omega_n^i}{\sum_{\ell=1}^{N} \omega_n^\ell} \right] \right)$
end for

for $r = 1 \rightarrow N - R$ do
    set $I_r \leftarrow j$ with probability $\bar{\omega}_n^j$
    set $\tilde{N}_n^{I_r} \leftarrow \tilde{N}_n^{I_r} + 1$
end for

return $(\tilde{N}_n^i)$
Consequently, the residual resampling operation replaces the estimator

\[
\sum_{i=1}^{N} \frac{\omega_n^i}{\sum_{\ell=1}^{N} \omega_n^\ell} \phi(X_0^{i:n}) \quad \text{by} \quad \frac{1}{N} \sum_{i=1}^{N} N_n^i \phi(X_0^{i:n}).
\]

Also residual resampling is unbiased (exercise!):

**Theorem**

For all \( N \geq 1 \) and \( n \geq 0 \),

\[
\mathbb{E} \left( \frac{1}{N} \sum_{i=1}^{N} N_n^i \phi(X_0^{i:n}) \right) = \mathbb{E} \left( \sum_{i=1}^{N} \frac{\omega_n^i}{\sum_{\ell=1}^{N} \omega_n^\ell} \phi(X_0^{i:n}) \right).
\]

One can also show that the variance of the estimator is smaller than the variance of the estimator obtained with multinomial selection.
Other selection strategies are

- Stratified resampling
- Bernoulli branching
- Poisson branching
- ...
Stratified resampling

A simple modification of the code gives stratified resampling instead!

\[
\text{CW} = \text{cumsum}([0 \ W]);
\]
\[
[\sim, \text{ind}] = \text{histc}((\text{rand}(1, N) + (0 : (N - 1))) / N, \text{CW} / \text{CW}(\text{end}));
\]

**Compare with original multinomial resampling (as before)**

\[
\text{CW} = \text{cumsum}([0 \ W]);
\]
\[
[\sim, \text{ind}] = \text{histc}(\text{rand}(1, N), \text{CW} / \text{CW}(\text{end}));
\]
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3. Home assignment 2 (HA2)
SISR: Some theoretical results

Even though the theory of SISR is hard, there is a number of results establishing the convergence of the algorithm as \( N \) tends to infinity. For instance,

\[
\sqrt{N} \left( \sum_{i=1}^{N} \frac{\omega_n^i}{\sum_{\ell=1}^{N} \omega_n^{\ell}} \phi(X_0^n) - \tau_n \right) \xrightarrow{d} \mathcal{N}(0, \sigma_n^2),
\]

where \( \sigma_n^2 \) in general lack a closed form expression. Thus, the convergence rate is still \( \sqrt{N} \).

**Open problem:** find an online estimator of \( \sigma_n^2 \)!

The dependence of \( \sigma_n^2 \) on \( n \) is crucial. However, for filtering in HMMs (particle filtering) one may prove, under weak assumptions,

\[
\sigma_n^2 \leq c
\]

for a constant \( c < \infty \). Thus, the SISR estimates are stable in \( n \).
A few references on SMC


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3. Home assignment 2 (HA2)
HA2 deals exclusively with the self-avoiding walk (SAW) in $\mathbb{Z}^d$. Let $c_n(d)$ be the number of SAW:s of length $n$ in dimension $d$. The home assignment has the following tasks:

- two minor theoretical questions on the asymptotics of the number $c_n(d)$ of SAW:s as the length $n$ tends to infinity,
- two questions dealing with SIS-based approaches to estimation of $c_n(2)$,
- two questions dealing with an SISR-based approach to estimation of $c_n(2)$ and $A_2, \mu_2$ and $\gamma_2$, and
- three additional questions dealing with SAW:s in $\mathbb{Z}^d$ for $d \geq 3$. 
Submission of HA2

As for HA1, the following is to be submitted:

- A written report in PDF format (No MS Word-files). The pair Sverker Persson and Lilith Nilsson name their report file proj2-nlps.pdf. A printed and stitched copy of the report is given to the lecturer at the very beginning of the lecture on Tuesday 26 Feb.

- An email containing the report file as well as all your m-files with a file proj2.m that runs your analysis. This email has to be sent to fms091@matstat.lu.se before Tuesday 26 Feb, 13:00:00 (that is, 15 minutes before the beginning of the lecture). Use your STIL-IDs in the subject line of the email. Set the subject line to: “Project 2 by “STILID1” and “STILID2” “

- Late submissions do not qualify for marks higher than 3.