STAT 576 Bayesian Analysis

Lecture 11: State-space Models and Sequential Monte Carlo II

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Sequential Monte Carlo

- Last time, we introduced the state-space models.
- For linear Gaussian state-space models, we can use Kalman filter and smoother to estimate the latent states and parameters.
- The key idea behind the Kalman filter and smoother is to recursively update the filtering and smoothing distributions.

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- The key idea behind the Kalman filter and smoother is to recursively update the filtering and smoothing distributions.
- For general state-space models, we usualy do not have closed-form solutions as in the linear Gaussian case.
- Sequential Monte Carlo (SMC) methods provide a general framework for estimating the filtering and smoothing distributions in general state-space models through Monte Carlo sampling.

The Sequential Structure (MC version)

- In our previous discussion for the Kalman filter and smoother, we have the following recursive structure:

$$X_t \mid \boldsymbol{Y}_t \sim \mathcal{N}(\boldsymbol{\mu}_t, \boldsymbol{V}_t) \implies X_{t+1} \mid \boldsymbol{Y}_t \sim \mathcal{N}(\boldsymbol{\mu}_{t+1}, \boldsymbol{V}_{t+1}).$$

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- (**MC version**) Similarly, if we have samples $(\boldsymbol{X}_t^{(i)}, w_t^{(i)})_{i=1}^N$ from the filtering distribution $p(\boldsymbol{X}_t \mid \boldsymbol{Y}_t)$, we can generate samples from the filtering distribution $p(\boldsymbol{X}_{t+1} \mid \boldsymbol{Y}_{t+1})$ by the following steps:

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  1. Sample $X_{t+1}^{(i)} \sim q_{t+1}(X_{t+1})$ for some proposal distribution q_{t+1}
  2. Let $\boldsymbol{X}_{t+1}^{(i)} = (\boldsymbol{X}_t^{(i)}, X_{t+1}^{(i)})$ and assign weights

$$w_{t+1}^{(i)} = w_t^{(i)} \frac{f_{t+1}(X_{t+1}^{(i)} \mid \boldsymbol{X}_t^{(i)}) g_{t+1}(Y_{t+1} \mid X_{t+1}^{(i)})}{q_{t+1}(X_{t+1}^{(i)})}$$

Sequential Importance Sampling (SIS)

1. **Initialization:**
   1.1 Generate N independent samples $X_0^{(i)}$ from the proposal distribution $q_0(X_0)$.
   1.2 Assign weights $w_0^{(i)} \propto f_0(X_0^{(i)})/q_0(X_0^{(i)})$.
2. **Iteration:** For $t = 1, 2, \ldots, T$,
   2.1 Sample $X_t^{(i)} \sim q_t(X_t)$ for $i = 1, \ldots, N$.
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Then:

- The weighted samples $(\boldsymbol{X}_t^{(i)}, w_t^{(i)})_{i=1}^N$ are samples from the filtering distribution $p(\boldsymbol{X}_t \mid \boldsymbol{Y}_t)$.
- The weighted samples $(\boldsymbol{X}_T^{(i)}, w_T^{(i)})_{i=1}^N$ are samples from the smoothing distribution $p(\boldsymbol{X}_T \mid \boldsymbol{Y}_{1:T})$.

Justification on the Importance Sampling

- From the principle of impoartance sampling, if $X^{(i)}$ are samples from $q(X)$ and $(X^{(i)}, w^{(i)})$ are (weighted) samples from the target $p(X)$, then

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$$q(\boldsymbol{X}_t) = q_0(X_0) \prod_{s=1}^{t} q_s(X_s)$$

- The target filtering distribution is

$$p(\boldsymbol{X}_t \mid \boldsymbol{Y}_t) \propto f_0(X_0) \prod_{s=1}^{t} f_s(X_s \mid \boldsymbol{X}_{s-1}) g_s(Y_s \mid X_s)$$

Justification on the Importance Sampling

- The proper weight for the i-th sample at time t is

$$w_t^{(i)} \propto \frac{p(\boldsymbol{X}_t^{(i)} \mid \boldsymbol{Y}_t)}{q(\boldsymbol{X}_t^{(i)})} \propto \frac{q_0(X_0^{(i)})}{f_0(X_0^{(i)})} \prod_{s=1}^{t} \frac{f_s(X_s^{(i)} \mid \boldsymbol{X}_{s-1}^{(i)}) g_s(Y_s \mid X_s^{(i)})}{q_s(X_s^{(i)})}$$

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- On the one hand, this is the cumulated product of the importance weights for the samples up to time t:

$$w_t^{(i)} \propto w_0^{(i)} \prod_{s=1}^{t} \frac{w_s^{(i)}}{w_{s-1}^{(i)}}$$

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- On the other hand, the sequential update for the weights is

$$w_t^{(i)} \propto w_{t-1}^{(i)} \frac{f_t(X_t^{(i)} \mid \boldsymbol{X}_{t-1}^{(i)}) g_t(Y_t \mid X_t^{(i)})}{q_t(X_t^{(i)})}$$

Different Choices for the Proposal Distribution

- Particle Filter / Bootstrap Filter:

$$q_t(X_t) = f_t(X_t \mid \boldsymbol{X}_{t-1})$$

- Independent Filter:

$$q_t(X_t) \propto g_t(Y_t \mid X_t)$$

- Conditional Optimal Filter:

$$q_t(X_t) \propto f_t(X_t \mid \boldsymbol{X}_{t-1}) g_t(Y_t \mid X_t)$$

- Auxiliary Particle Filter:

$$q_t(X_t) \propto p(Y_{t+1} \mid X_t)$$

Likelihood Estimation with SIS

Suppose the state-space model dynamics is parametrized by $\boldsymbol{\theta}$ and we want to estimate the likelihood $p(\boldsymbol{Y}_{1:T} \mid \boldsymbol{\theta})$.

Likelihood Estimation with SIS

Suppose the state-space model dynamics is parametrized by $\boldsymbol{\theta}$ and we want to estimate the likelihood $p(\boldsymbol{Y}_{1:T} \mid \boldsymbol{\theta})$.

- The likelihood can be written as a high-dimensional integral:

$$p(\boldsymbol{Y}_T \mid \boldsymbol{\theta}) = \int p(\boldsymbol{Y}_T, \boldsymbol{X}_T \mid \boldsymbol{\theta}) d\boldsymbol{X}_T$$
$$= \int f_0(X_0 \mid \boldsymbol{\theta}) \prod_{s=1}^{T} f_s(X_s \mid \boldsymbol{X}_{s-1}; \boldsymbol{\theta}) g_s(Y_s \mid X_s; \boldsymbol{\theta}) d\boldsymbol{X}_T$$

- Directly estimate the likelihood is infeasible due to the high-dimensional integral.

Likelihood Estimation with SIS

With SIS, we observe that

$$
\begin{aligned}
\mathbb{E}_{\text{SIS}}\left[\frac{w_t}{w_{t-1}}\right] &= \mathbb{E}_{\text{SIS}}\left[\frac{f_t(X_t \mid \boldsymbol{X}_{t-1};\boldsymbol{\theta})g_t(Y_t \mid X_t;\boldsymbol{\theta})}{q_t(X_t)}\right] \\
&= \int \frac{f_t(X_t \mid \boldsymbol{X}_{t-1};\boldsymbol{\theta})g_t(Y_t \mid X_t;\boldsymbol{\theta})}{q_t(X_t)} q_t(X_t) p(\boldsymbol{X}_{t-1} \mid \boldsymbol{Y}_{t-1};\boldsymbol{\theta}) dX_t d\boldsymbol{X}_{t-1} \\
&= \int f_t(X_t \mid \boldsymbol{X}_{t-1};\boldsymbol{\theta})g_t(Y_t \mid X_t;\boldsymbol{\theta}) p(\boldsymbol{X}_{t-1} \mid \boldsymbol{Y}_{t-1};\boldsymbol{\theta}) dX_t d\boldsymbol{X}_{t-1} \\
&= \int \left(\int f_t(X_t \mid \boldsymbol{X}_{t-1};\boldsymbol{\theta}) p(\boldsymbol{X}_{t-1} \mid \boldsymbol{Y}_{t-1};\boldsymbol{\theta}) d\boldsymbol{X}_{t-1}\right) g_t(Y_t \mid X_t;\boldsymbol{\theta}) dX_t \\
&= \int p(X_t \mid \boldsymbol{Y}_{t-1};\boldsymbol{\theta}) g_t(Y_t \mid X_t;\boldsymbol{\theta}) dX_t \\
&= p(Y_t \mid \boldsymbol{Y}_{t-1};\boldsymbol{\theta})
\end{aligned}
$$

Likelihood Estimation with SIS

Notice that

$$p(\boldsymbol{Y}_t; \boldsymbol{\theta}) = \prod_{s=1}^{T} p(Y_t \mid \boldsymbol{Y}_{t-1}; \boldsymbol{\theta})$$

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$$p(\mathbf{Y}_t; \boldsymbol{\theta}) = \prod_{s=1}^{T} p(Y_t \mid \mathbf{Y}_{t-1}; \boldsymbol{\theta})$$

1. **Initialization:**
   1.1 Set $L = 1$.
   1.2 Generate N independent samples $X_0^{(i)}$ from the proposal distribution $q_0(X_0)$.
   1.3 Assign weights $w_0^{(i)} \propto f_0(X_0^{(i)})/q_0(X_0^{(i)})$.
2. **Iteration:** For $t = 1, 2, \ldots, T$,
   2.1 Sample $X_t^{(i)} \sim q_t(X_t)$ for $i = 1, \ldots, N$.
   2.2 Assign weights

$$w_t^{(i)} = w_{t-1}^{(i)} \frac{f_t(X_t^{(i)} \mid \boldsymbol{X}_{t-1}^{(i)}) g_t(Y_t \mid X_t^{(i)})}{q_t(X_t^{(i)})}$$

   2.3 Update the likelihood estimate

$$L = L \cdot \frac{\sum_{i=1}^{N} w_t^{(i)}}{\sum_{i=1}^{N} w_{t-1}^{(i)}}$$

Example

Consider a simple state-space model with the following dynamics:

$$X_t \mid X_{t-1} \sim \mathcal{N}(\phi X_{t-1}, 1)$$
$$Y_t \mid X_t \sim \mathcal{N}(X_t, 1)$$

where ϕ is the parameter to be estimated.

Example

Simulate data from the model with $\phi = 0.6$.

```
T = 20
Y = rep(0, T)
X = 0
for(t in 1:T){
    X = 0.6 * X + rnorm(1)
    Y[t] = X + rnorm(1)
}
```

Example

Compute the likelihood with SIS:

```
llh <- function(phi){
    n = 1000
    x = rep(0, n)
    logw = rep(0, n)
    loglik = 0
    for(t in 1:T){
        z = rnorm(n)/sqrt(2)
        xx = (phi*x + Y[t])/2 + z
        dlogw = -0.5*(xx - phi*x)**2
        dlogw = dlogw - 0.5*(Y[t]-xx)**2
        dlogw = dlogw + z**2
        x = xx
        loglik = loglik + log(sum(exp(logw+dlogw)))
        loglik = loglik - log(sum(exp(logw)))
        logw = logw + dlogw
        logw  = logw - mean(logw)
    }
    return(loglik)
}
```

Example

Compute the MLE:

```
phi.hat = optimize(llh, c(-1, 1), maximum = T)$maximum
```

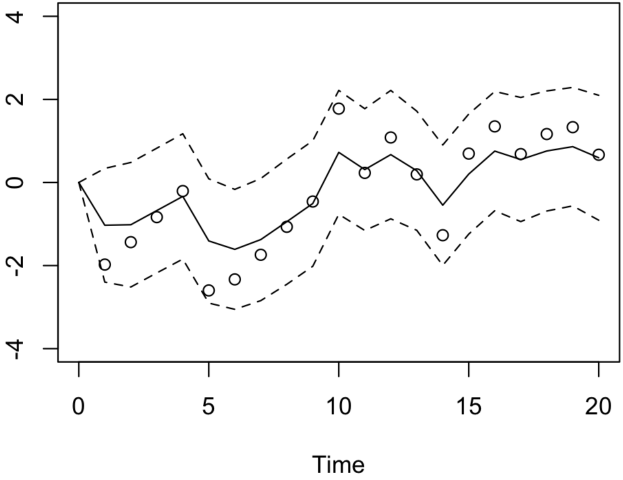
The outcome is $\hat{\phi} = 0.61$. (The result can be noisy due to the randomness in the SIS algorithm and lack of resampling.)

Example

Draw samples from the posterios:

```
smc <- function(phi){
    n = 1000
    x = array(0, c(n, T+1))
    logw = rep(0, n)
    for(t in 1:T){
        z = rnorm(n)/sqrt(2)
        x[,t+1] = (phi*x[,t] + Y[t])/2 + z
        dlogw = -0.5*(x[,t+1] - phi*x[,t])**2
        dlogw = dlogw - 0.5*(Y[t]-x[,t+1])**2
        dlogw = dlogw + z**2
        logw = logw + dlogw
        logw  = logw - mean(logw)
    }
    return(x)
}
```

Example



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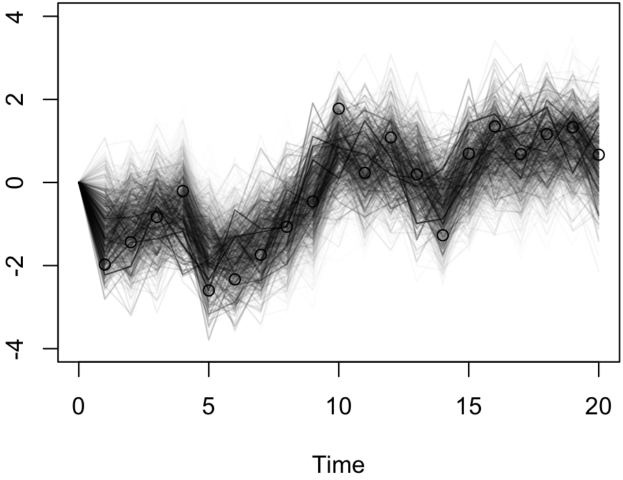

Degeneracy

One of the problem is the degeneracy of the SIS algorithm. The weights of the particles can be very skewed, leading to poor performance of the algorithm.

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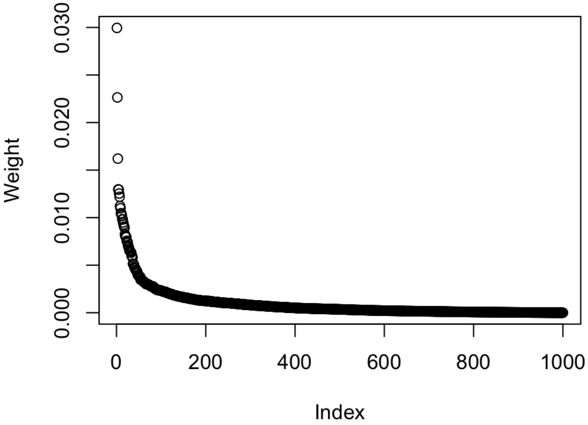

Degeneracy

One way to evaluate the performance of the SIS algorithm is to look at the effective sample size (ESS):

$$\mathrm{ESS}_t = \frac{\left(\sum_{i=1}^{N} w_t^{(i)}\right)^2}{\sum_{i=1}^{N} (w_t^{(i)})^2}$$

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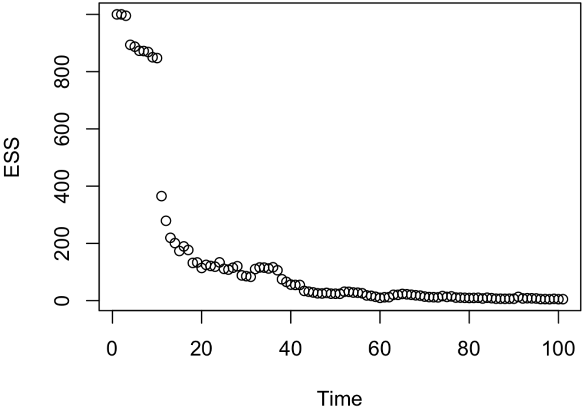
- The ESS of the previous example at time T is $\sim 183 \ll 1000$.
- If the observation equation is restrictive, the weight adjustedment step can lead to a large variance in the weights, resulting in a low ESS.
- We refer to the problem of **reduced effective sample size** as **degeneracy**.

Example

For the previous Autoregressive example, if we set $T = 100$, the ESS is tracked over time as follows.



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- Suppose now we have $N = 5$ samples at time t:

$$(X_t^{(1)}, 0.8),\ (X_t^{(2)}, 0.17),\ (X_t^{(3)}, 0.01),\ (X_t^{(4)}, 0.01),\ (X_t^{(5)}, 0.01),$$

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  where the second element is the weight.

- **Without resampling**, the samples at time $t + 1$ will be dominated by the first sample:

$$(X_{t+1}^{(1)}, 0.83),\ (X_{t+1}^{(2)}, 0.14),\ (X_{t+1}^{(3)}, 0.01),\ (X_{t+1}^{(4)}, 0.01),\ (X_{t+1}^{(5)}, 0.01)$$

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- **With resampling**, we draw $N = 5$ samples from the current samples with replacement:

$$(X_t^{(1)}, 0.2),\ (X_t^{(1)}, 0.2),\ (X_t^{(1)}, 0.2),\ (X_t^{(1)}, 0.2),\ (X_t^{(2)}, 0.2),$$

SIS with Resampling (SISR)

1. **Initialization:**
   1.1 Generate N independent samples $X_0^{(i)}$ from the proposal distribution $q_0(X_0)$.
   1.2 Assign weights $w_0^{(i)} \propto f_0(X_0^{(i)})/q_0(X_0^{(i)})$.
2. **Iteration:** For $t = 1, 2, \ldots, T$,
   2.1 Sample $X_t^{(i)} \sim q_t(X_t)$ for $i = 1, \ldots, N$.
   2.2 Assign weights
   $$w_t^{(i)} = w_{t-1}^{(i)} \frac{f_t(X_t^{(i)} \mid \boldsymbol{X}_{t-1}^{(i)}) g_t(Y_t \mid X_t^{(i)})}{q_t(X_t^{(i)})}$$
   2.3 (Optional) Resample N samples from $\{X_t^{(i)}\}_{i=1}^N$ with replacement according to the weights $\{w_t^{(i)}\}_{i=1}^N$ and set weights to be $\propto 1$.

When to Resample?

- Resampling is a trade-off between the variance reduction and the information loss.
- If the weights are very skewed, resampling can help to reduce the variance of the weights.
- If the weights are not very skewed, resampling can lead to information loss.

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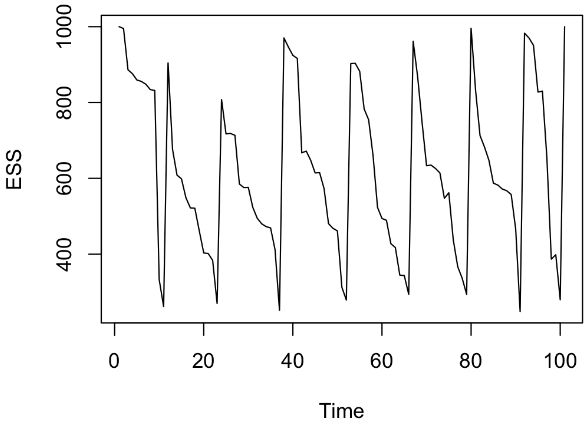
Resampling schedules:

- Deterministic schedule: Resample every K steps.
- Dynamic schedule: Resample when the ESS is below a threshold.

Example

For the previous Autoregressive example, if we set resample when ESS is below $0.3N$, the ESS is tracked over time as follows.



Resampling w.r.t. the Priority Scores

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- The resampling step w.r.t. the priority scores β_i is:
  1. Draw N samples $\{j_1, \ldots, j_N\}$ with replacement from $\{1, \ldots, N\}$ with probabilities (proportional to) $\{\beta_i\}_{i=1}^N$.
  2. Set the new samples to be $\{X_t^{(j_1)}, \ldots, X_t^{(j_N)}\}$.
  3. Set the new weights to be

$$w^{(j_i)} \leftarrow \frac{w^{(j_i)}}{\beta_{j_i}}$$

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- The previous example is a special case with $\beta_i = w_t^{(i)}$.
- **Least Aggresive Resampling:** Set $\beta_i = \sqrt{w_t^{(i)}}$ for all i.

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- **Simple Random Resampling**: Draw N samples with replacement from $\{1, \ldots, N\}$ with probabilities $\{\beta_i\}_{i=1}^{N}$.
- **Residual Resampling**:
  1. Retain $k_i = \lfloor N\tilde{w}^{(i)}$ copies of $X^{(i)}$, where $\tilde{w}^{(i)} = w^{(i)} / \sum_i w^{(i)}$.
  2. Obtain $N - \sum_i k_i$ samples by drawing with replacement from $\{1, \ldots, N\}$ with probabilities $N\tilde{w}^{(i)} - k_i$.

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   2.3 Conduct computation w.r.t. to the filtering sample here.
   2.4 (Optional Resampling):
      2.4.1 Draw N samples with replacement from $\{1, \ldots, N\}$ with probabilities $\{\beta_i\}_{i=1}^N$.
      2.4.2 Set the new samples to be $\{\boldsymbol{X}_t^{(j_1)}, \ldots, \boldsymbol{X}_t^{(j_N)}\}$.
      2.4.3 Set the new weights to be

$$w^{(j_i)} \leftarrow \frac{w^{(j_i)}}{\beta_{j_i}}$$

3. Conduct computation w.r.t. to the smoothing sample here.

Example

We consider the following 1D random walk with noisy observations:

$$X_t = X_{t-1} + \mathcal{N}(0, 1)$$
$$Y_t = X_t + \mathcal{N}(0, 1)$$

The starting point is $X_0 = 0$.

Example

Simulate data from the model:

```
T = 100
x = cumsum(rnorm(T))
y = x + rnorm(T)
```

Example

```
smc <- function(n, y, resample=FALSE){
    T = length(y)
    X = array(0, dim=c(n, T+1))
    logw = rep(0, n)
    out.filter = rep(0, T)
    ess = rep(n, T)
    for(t in 1:T){
        z = rnorm(n) / sqrt(2)
        X[,t+1] = (X[,t] + y[t]) / 2 + z
        logw = logw -0.5*(y[t]-X[,t+1])**2 - 0.5*(X[,t+1]-X[,t])
            **2
        logw = logw + 0.5*z**2
        logw = logw - mean(logw)
        w = exp(logw)
        w = w / sum(w)
        out.filter[t] = X[,t+1]%*%w
        ess[t] = sum(w)**2/sum(w**2)
```

Example

```
        if(resample && ess[t] < 0.3*n){
            index = sample(n, n, replace=T, prob=w)
            logw = rep(0, n)
            X = X[index,]
        }
    }
    w = exp(logw)
    w = w / sum(w)
    out.smoothing = w%*%X
    return(list(filtering=out.filter, smoothing=out.smoothing,
        ess=ess))
}
```