

Sequential Monte Carlo

Geir Storvik

Geilo Winter school 2023



UiO : Universitetet i Oslo



Outline

- 1 Sequential Monte Carlo
- 2 Details on SMC
- 3 Feynman-Kac formulation
- 4 Smoothing algorithms
- 5 A Case study - Covid-19
- 6 SMC and parameter estimation
 - Offline methods
 - Online methods
 - Online methods

Sequential Monte Carlo

Static versus dynamic inference

- MCMC/INLA: Inference when **all** data is collected
- Assume now $\mathbf{y}_1, \mathbf{y}_2, \dots$ are collected dynamically in time
- Want to do inference based on $\mathbf{y}_{1:t}$ **at each time point t**
- Can in principle start MCMC/INLA from scratch
- Possible to utilize computation performed at time $t - 1$?
 - YES: by **sequential Monte Carlo**

Sequential updating

- Aim now: **Sequential sampling** from $\pi_t(\mathbf{x}_t)$ for $t = 1, 2, \dots$
- **State space** settings:

$$\mathbf{x}_t \sim p(\mathbf{x}_t | \mathbf{x}_{t-1}; \theta)$$

State process

$$\mathbf{y}_t \sim p(\mathbf{y}_t | \mathbf{x}_t; \theta)$$

Observation process

Aim: $\pi_t(\mathbf{x}_t) = p(\mathbf{x}_t | \mathbf{y}_{1:t})$ or $\pi_t(\mathbf{x}_{1:t}) = p(\mathbf{x}_{1:t} | \mathbf{y}_{1:t})$

- **Complex Bayesian settings**
 - $p(\mathbf{x} | \mathbf{y})$ complex, $p(\mathbf{x})$ simple
 - Construct $\pi_t(\mathbf{x}) \propto p(\mathbf{x}) p(\mathbf{y} | \mathbf{x})^{\gamma_t}$ with $\gamma_t = \frac{t}{T}$, $t = 0, \dots, T$
- Sequential updating: Breaks down high-dimensional sampling to many low-dimensional ones
- References:
 - Dai et al. (2022): *An invitation to sequential Monte Carlo samplers*
 - Naesseth et al. (2019): *Elements of sequential Monte Carlo*
 - Doucet et al. (2001): *Sequential Monte Carlo methods in practice*
 - Chopin et al. (2020): *An introduction to sequential Monte Carlo*

Sequential Monte Carlo

- Assume $\mathbf{x} = \mathbf{x}_{1:t} = (\mathbf{x}_1, \dots, \mathbf{x}_t)$ have a **Markov** structure

$$\pi_t(\mathbf{x}_{1:t}) = \pi_1(\mathbf{x}_1) \prod_{s=2}^t \pi_s(\mathbf{x}_s | \mathbf{x}_{s-1})$$

Sequential Monte Carlo

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- Also assume a **proposal** distribution with **Markov property**:

$$g_t(\mathbf{x}_{1:t}) = g_1(\mathbf{x}_1) \prod_{s=2}^t g_s(\mathbf{s}_s | \mathbf{x}_{s-1})$$

Sequential Monte Carlo

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$$g_t(\mathbf{x}_{1:t}) = g_1(\mathbf{x}_1) \prod_{s=2}^t g_s(\mathbf{s}_s | \mathbf{x}_{s-1})$$

- Importance weights:

$$w(\mathbf{x}_{1:t}) = \frac{\pi_t(\mathbf{x}_{1:t})}{g_t(\mathbf{x}_{1:t})} = \frac{\pi_1(\mathbf{x}_1)}{g_1(\mathbf{x}_1)} \prod_{s=2}^t \frac{\pi_s(\mathbf{x}_s | \mathbf{x}_{s-1})}{g_s(\mathbf{x}_s | \mathbf{x}_{s-1})} = w(\mathbf{x}_{1:t-1}) \frac{\pi_t(\mathbf{x}_t | \mathbf{x}_{t-1})}{g_t(\mathbf{x}_t | \mathbf{x}_{t-1})}$$

Sequential Monte Carlo

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- Opens up for **sequential** sampling/estimation
- Note: Possible to generalize to non-Markov settings as well
 - More computing at each step

Sequential Monte Carlo

Algorithm 1 SMC

- 1: Sample $\mathbf{x}_1 \sim g_1(\cdot)$. Let $w_1 = u_1 = \pi_1(\mathbf{x}_1)/g_1(\mathbf{x}_1)$. Set $t = 2$
 - 2: Sample $\mathbf{x}_t | \mathbf{x}_{t-1} \sim g_t(\mathbf{x}_t | \mathbf{x}_{t-1})$.
 - 3: Append \mathbf{x}_t to $\mathbf{x}_{1:t-1}$, obtaining \mathbf{x}_t
 - 4: Let $u_t = \pi_t(\mathbf{x}_t | \mathbf{x}_{t-1}) / g_t(\mathbf{x}_t | \mathbf{x}_{t-1})$
 - 5: Let $w_t = w_{t-1} u_t$, the importance weight for $\mathbf{x}_{1:t}$
 - 6: Increment t and return to step 2
-

Sequential Monte Carlo

Algorithm 2 SMC

- 1: Sample $\mathbf{x}_1 \sim g_1(\cdot)$. Let $w_1 = u_1 = \pi_1(\mathbf{x}_1)/g_1(\mathbf{x}_1)$. Set $t = 2$
 - 2: Sample $\mathbf{x}_t | \mathbf{x}_{t-1} \sim g_t(\mathbf{x}_t | \mathbf{x}_{t-1})$.
 - 3: Append \mathbf{x}_t to $\mathbf{x}_{1:t-1}$, obtaining \mathbf{x}_t
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 - 5: Let $w_t = w_{t-1} u_t$, the importance weight for $\mathbf{x}_{1:t}$
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- Can simulate N sequences **in parallel!**
- Approximation: $p(\mathbf{x}_t | \mathbf{y}_{1:t}) \approx \sum_{i=1}^N w_t^i \delta_{\mathbf{x}_t^i}(\mathbf{x}_t)$
 - Typically one would **normalize** weights

$$w_t^i \rightarrow w_t^i / \sum_j w_t^j$$

Weight degeneracy

- General rule:

$$\text{var}[Y] = E[\text{var}[Y|Z]] + \text{var}[E[Y|Z]] \geq \text{var}[E[Y|Z]]$$

Weight degeneracy

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- $Y = w_t, Z = \mathbf{x}_{1:t-1}$ (w_{t-1} given by $\mathbf{x}_{1:t-1}$):

$$\begin{aligned} E[w_t | \mathbf{x}_{1:t-1}] &= w_{t-1} E\left[\frac{\pi_t(\mathbf{x}_t | \mathbf{x}_{t-1})}{g_t(\mathbf{x}_t | \mathbf{x}_{t-1})} \mid \mathbf{x}_{1:t-1}\right] \\ &= w_{t-1} \cdot 1 = w_{t-1} \end{aligned}$$

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implying that

$$\text{var}[w_t] \geq \text{var}[w_{t-1}]$$

which indicates that the variance will **increase at each time-step**.

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which indicates that the variance will **increase at each time-step**.

- **Practical consequence:**
 - Only a few samples will dominate the others
 - Variability of estimate will increase

Bootstrap filter for state space models

- Introduce **resampling**
 - Discard samples (particles) with small weight
 - Duplicate particles with high weight

Algorithm 3 SMC

- 1: Simulate $\mathbf{x}_1^i \sim p(\mathbf{x}_1)$ for $i = 1, \dots, N$. ▷ Initialization
 - 2: Put weights $w_1^i = p(\mathbf{y}_1 | \mathbf{x}_1^i)$.
 - 3: Sample $\{B_1^1, \dots, B_1^N\}$ from $\{1, \dots, N\}$ with probabilities $\{w_1^i\}$.
 - 4: **for** $t = 2, 3, \dots$ **do** ▷ Sequential Monte Carlo
 - 5: Simulate $\mathbf{x}_t^i \sim p(\mathbf{x}_t | \mathbf{x}_{t-1}^{B_t^i})$ for $i = 1, \dots, N$.
 - 6: Put weights $w_t^i = p(\mathbf{y}_t | \mathbf{x}_t^i)$.
 - 7: Sample $\{B_t^1, \dots, B_t^N\}$ from $\{1, \dots, N\}$ with probabilities $\{w_t^i\}$.
 - 8: **end for**
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- Approximation: $p(\mathbf{x}_t | \mathbf{y}_{1:t}) \approx \sum_{i=1}^N w_t^i \delta_{\mathbf{x}_t^i}(\mathbf{x}_t)$
- More general: Optional resampling with weights propagated if no resampling

State space models

- Model

$$\mathbf{x}_t \sim p(\mathbf{x}_t | \mathbf{x}_{t-1}; \theta)$$

State process

$$\mathbf{y}_t \sim p(\mathbf{y}_t | \mathbf{x}_t; \theta)$$

Observation process

- Target distributions (assuming for now θ known):

$$\pi(\mathbf{x}_{1:t}) = p(\mathbf{x}_{1:t} | \mathbf{y}_{1:t}) \propto p(\mathbf{x}_1) p(\mathbf{y}_1 | \mathbf{x}_1) \prod_{s=2}^t p(\mathbf{x}_s | \mathbf{x}_{s-1}) p(\mathbf{y}_s | \mathbf{x}_s)$$

- Unknown normalization constant(s):

$$p(\mathbf{x}_t | \mathbf{y}_{1:t}) \approx \sum_{i=1}^N W_t^i \delta_{\mathbf{x}_t^i}(\mathbf{x}_t)$$

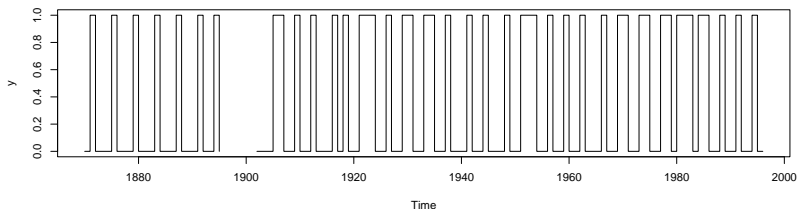
$$\text{with } W_t^i = \frac{w_t^i}{\sum_j w_t^j}$$

Lemmings data

- Observations: $y_t \in \{0, 1\}$, =1 if "lemming year"
- Possible simple model: $\mathbf{x}_t = \log(N_t)$

$$x_t = ax_{t-1} + x_{t-2} + \sigma \varepsilon_t$$

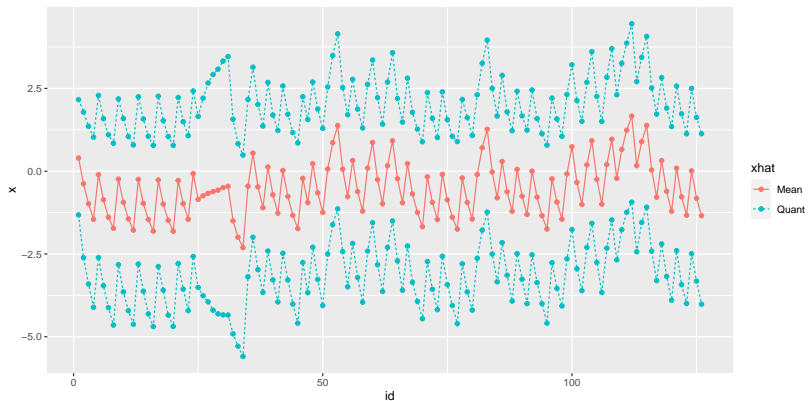
$$\varepsilon_t \sim N(0, 1)$$



- Of interest: $p(N_t | y_{1:t})$

Lemmings - results

Script: SMC_lemmings.R



The many uses of Markov

- **Markov** chain Monte Carlo
- **Markov** assumption in **Ising** model:

$$p(x_i | \mathbf{x}_{-i}) = p(x_i | \mathbf{x}_{N_i})$$

- SMC: **Markov structure** in $\pi_t(\mathbf{x}_{1:t}) = \pi_1(\mathbf{x}_1) \prod_{s=2}^t \pi_s(\mathbf{x}_s | \mathbf{x}_{s-1})$
- SMC: **Markov structure** in $g_t(\mathbf{x}_{1:t}) = g_1(\mathbf{x}_1) \prod_{s=2}^t g_s(\mathbf{s}_s | \mathbf{x}_{s-1})$

Discuss the different uses of Markov assumptions

Effective sample size

- Assume $w_i = w(\mathbf{x}_i)$, $i = 1, \dots, N$ are **normalized** weights
- Define **effective sample size** by

$$\hat{N}_{eff} = \frac{1}{\sum_{i=1}^N w_i^2}$$

$$= N$$

$$\text{if } w_i = \frac{1}{n} \text{ for all } i$$

$$= N - z$$

$$\text{if } w_i = 0, i \leq z, w_i = \frac{1}{N-z}, i > z$$

$$= 1$$

$$\text{if } w_j = 1, w_i = 0, i \neq j$$

- General: Resampling introduce extra Monte Carlo variability
- Rule of tump: Resample only if $\hat{N}_{eff} < 0.5N$

Resampling

- Simplest option:
 - Resample with probabilities equal to w_t^i .
 - Put weights on resample to $\tilde{w}_t^i = N^{-1}$
 - Number of repeats of \mathbf{x}_t^i , N_t^i is Binomial(N , w_t^i)
 - $E[N_t^i \tilde{w}_t^i] = N w_t^i$

Resampling

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 - $E[N_t^i \tilde{w}_t^i] = Nw_t^i$
- More general resampling strategies are possible
- **Sufficient requirement:** $E[N_t^i \tilde{w}_t^i] = Nw_t^i$

Resampling

- Simplest option:

- Resample with probabilities equal to w_t^i .
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- More general resampling strategies are possible

- Sufficient requirement:** $E[N_t^i \tilde{w}_t^i] = N w_t^i$

- Optimal strategy (for equally weighted samples)

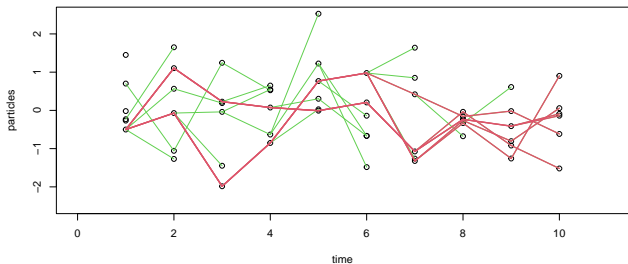
- For $i = 1, \dots, N$, put $\lfloor a \rfloor$ is the largest integer smaller than a)

$$\tilde{N}_t^i = \lfloor N w_t^i \rfloor \quad (\text{Some will be zero})$$

- Let $\delta_t^i = w_t^i - \tilde{N}_t^i / N$
- Define $K = N - \sum_{i=1}^N \tilde{N}_t^i$ (remaining particles that have not been allocated)
- Sample (D_t^1, \dots, D_t^K) from the multinomial distribution with probabilities proportional to $(\delta_t^1, \dots, \delta_t^K)$.
- Put $N_t^i = \tilde{N}_t^i + D_t^i$
- Make N_t^i replicates of \mathbf{x}_t^i , but all weights to $1/N$

Resampling - degeneracy

- At time t : Samples $\{\mathbf{x}_{1:t}^i, i = 1, \dots, N\}$ from $p(\mathbf{x}_{1:t}|\mathbf{y}_{1:t})$
- When resampling, resample whole vector $\mathbf{x}_{1:t}$
- When repeated resampling at many time-steps, \mathbf{x}_1 is resampled each time, less and less unique values



Why did it work in the Lemmings example?

- The results based on $p(x_t | \mathbf{y}_{1:t})$
- Degeneracy problem related to $p(\mathbf{x}_{1:t} | \mathbf{y}_{1:t})$
 - but would be a problem also for $p(x_t | \mathbf{y}_{1:t})$ if no resampling!
- Theoretical properties:
 - If interest in $p(x_t | \mathbf{y}_{1:t})$: Error will be uniform over time
 - If interest in $p(\mathbf{x}_{1:t} | \mathbf{y}_{1:t})$: Error will increase (exponential) over time

Marginal likelihood

- We have

$$L(\theta) = p(\mathbf{y}_{1:T}|\theta) = p(\mathbf{y}_1|\theta) \prod_{t=2}^T p(\mathbf{y}_t|\mathbf{y}_{1:t-1}; \theta)$$

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

$$\hat{p}(\mathbf{y}_t|\mathbf{y}_{1:t-1}) = \frac{1}{N} \sum_{i=1}^N w_t^i$$

- Estimate of marginal likelihood:

$$\hat{L}(\theta) = \prod_{t=1}^T \left(\frac{1}{N} \sum_{i=1}^N w_t^i \right)$$

- Can show that $\hat{L}(\theta)$ is an **unbiased** estimator of $L(\theta)$

Feynman-Kac formulation

Reformulation of target density

- State space models:

$$p(\mathbf{x}_{1:t}|\mathbf{y}_{1:t}) \propto p(x_1)p(y_1|x_1) \prod_{s=2}^t p(x_s|x_{s-1})p(y_s|x_s)$$

- Using that $p(x_s|x_{s-1})p(y_s|x_s) = p(x_s, y_s|x_{s-1}) = p(x_s|x_{s-1}, y_s)p(y_s|x_{s-1})$, we have

$$p(\mathbf{x}_{1:t}|\mathbf{y}_{1:t}) \propto p(x_1|y_1)p(y_1) \prod_{s=2}^t p(x_s|x_{s-1}, y_s)p(y_s|x_{s-1})$$

- Indicate different sampling strategy:
 - Simulate $x_s \sim p(x_s|x_{s-1}, y_s)$
 - Update weights with $u_t = p(y_s|x_{s-1})$
- Will typically give better proposals
 - But more difficulty in calculating weights

Algorithm general

Algorithm 4 Guided Particle filter

- 1: Simulate $\mathbf{x}_1^i \sim q(\mathbf{x}_1)$ for $i = 1, \dots, N$. ▷ Initialization
 - 2: Put weights $w_1^i = p(\mathbf{y}_1 | \mathbf{x}_1^i) \frac{p(\mathbf{x}_1)}{q(\mathbf{x}_1^i)}$.
 - 3: Sample $\{B_1^1, \dots, B_1^N\}$ from $\{1, \dots, N\}$ with probabilities $\{w_1^i\}$.
 - 4: Put $w_1^i = 1/N$.
 - 5: **for** $t = 2, 3, \dots$ **do** ▷ Sequential Monte Carlo
 - 6: Simulate $\mathbf{x}_t^i \sim q(\mathbf{x}_t | \mathbf{x}_{t-1}^{B_t^i}, \mathbf{y}_t)$ for $i = 1, \dots, N$.
 - 7: Put weights $w_t^i = p(\mathbf{y}_t | \mathbf{x}_t^i) \frac{p(\mathbf{x}_t^i | \mathbf{x}_{t-1}^{B_t^i})}{q(\mathbf{x}_t^i | \mathbf{x}_{t-1}^{B_t^i}, \mathbf{y}_t)}$.
 - 8: Sample $\{B_t^1, \dots, B_t^N\}$ from $\{1, \dots, N\}$ with probabilities $\{w_t^i\}$.
 - 9: Put $w_t^i = 1/N$.
 - 10: **end for**
-

- Approximation: $p(\mathbf{x}_t | \mathbf{y}_{1:t}) \approx \sum_{i=1}^N w_t^i \delta_{\mathbf{x}_t^i}(\mathbf{x}_t)$
- More general: Optimal resampling with weights propagated if no resampling

Feynman-Kac formulation - Chopin et al. (2020)

- Assume a general set of target distributions

$$Q_t(x_{1:t}) = \frac{1}{L_t} G_1(x_1) \left\{ \prod_{s=2}^t G_s(x_{s-1}, x_s) \right\} M_t(x_{1:t})$$

$$M_t(x_{1:t}) = M_1(x_1) \prod_{s=2}^t M_s(x_{s-1}, x_s)$$

Markov process

- Ordinary state space model:

$$M_s(x_{s-1}, x_s) = p(x_s | x_{s-1})$$

$$G_s(x_{s-1}, x_s) = p(y_s | x_s)$$

Feynman-Kac formulation - Chopin et al. (2020)

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$$M_t(x_{1:t}) = M_1(x_1) \prod_{s=2}^t M_s(x_{s-1}, x_s)$$

Markov process

- Ordinary state space model:

$$M_s(x_{s-1}, x_s) = p(x_s | x_{s-1})$$

$$G_s(x_{s-1}, x_s) = p(y_s | x_s)$$

- Reformulated model

$$M_s(x_{s-1}, x_s) = p(x_s | x_{s-1}, y_s)$$

$$G_s(x_{s-1}, x_s) = p(y_s | x_{s-1})$$

- Possible with other reformulations as long as

$$G_s(x_{s-1}, x_s) M_s(x_{s-1}, x_s) = p(y_s | x_s) p(x_s | x_{s-1})$$

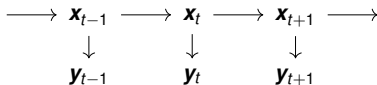
Why Feynman-Kac formalism?

- Different formulations share the same fundamental structure
 - Can be exploited for obtaining theoretical results
 - Can construct/exploit a variety of SMC algorithms in a common framework
- Ideal for development of generic software
 - [Chopin et al. \(2020\)](#): `particles` library (python)
 - Different algorithms correspond to "Bootstrap filter" for reformulated models
 - Bootstrap filter: Use $M_s(x_{s-1}, x_s)$ as proposal, use $G_s(x_{s-1}, x_s)$ as weight update.

Smoothing algorithms

Smoothing algorithms

- Algorithms so far target $p(\mathbf{x}_t|\mathbf{y}_{1:t})$ or $p(\mathbf{x}_{1:t}|\mathbf{y}_{1:t})$ - **filtering**
- In many cases interest in $p(\mathbf{x}_t|\mathbf{y}_{1:T})$ or $p(\mathbf{x}_{1:t}|\mathbf{y}_{1:T})$
 - State space models (parameters known)



Process

Observations

Smoothing algorithms - cont

$$p(\mathbf{x}_t | \mathbf{x}_{t+1:T}, \mathbf{y}_{1:T}) = p(\mathbf{x}_t | \mathbf{x}_{t+1}, \mathbf{y}_{1:t}) = \frac{p(\mathbf{x}_{t+1} | \mathbf{x}_t) p(\mathbf{x}_t | \mathbf{y}_{1:t})}{p(\mathbf{x}_{t+1} | \mathbf{y}_{1:t})}$$

- From filter algorithm:

$$p(\mathbf{x}_t | \mathbf{y}_{1:t}) \approx \sum_{i=1}^N w_t^i \delta_{\mathbf{x}_t^i}(\mathbf{x}_t)$$

$$p(\mathbf{x}_{t+1} | \mathbf{y}_{1:t}) = \int_{\mathbf{x}_t} p(\mathbf{x}_{t+1} | \mathbf{x}_t) p(\mathbf{x}_t | \mathbf{y}_{1:t}) d\mathbf{x} \approx \sum_{i=1}^N w_t^i p(\mathbf{x}_{t+1} | \mathbf{x}_t^i)$$

- Combined:

$$\begin{aligned} p(\mathbf{x}_t | \mathbf{x}_{t+1}, \mathbf{y}_{1:t}) &\approx \frac{\sum_{i=1}^N w_t^i p(\mathbf{x}_{t+1} | \mathbf{x}_t^i) \delta_{\mathbf{x}_t^i}(\mathbf{x}_t)}{\sum_{i=1}^N w_t^i p(\mathbf{x}_{t+1} | \mathbf{x}_t^i)} \\ &= \sum_{i=1}^N \tilde{w}_t^i p(\mathbf{x}_{t+1} | \mathbf{x}_t^i) \delta_{\mathbf{x}_t^i}(\mathbf{x}_t) \quad \tilde{w}_t^i = w_t^i p(\mathbf{x}_{t+1} | \mathbf{x}_t^i) \end{aligned}$$

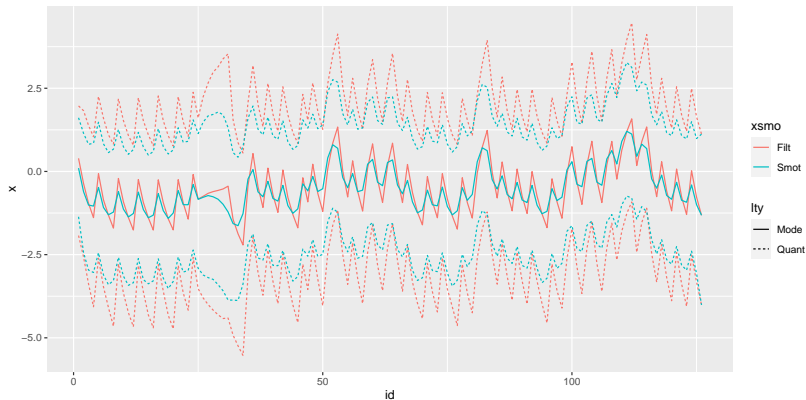
Smoothing algorithm

Algorithm 5 Particle smoother

- 1: Put $\tilde{w}_T^i = w_T^i, i = 1, \dots, N$
 - 2: Sample $\{B_T^1, \dots, B_T^N\}$ from $\{1, \dots, N\}$ with probabilities $\{\tilde{w}_T^i\}$. ▷ Initialization
 - 3: **for** $t = T - 1, T - 2, \dots, 1$ **do** ▷ Backwards smoothing
 - 4: Calculate $\tilde{w}_t^i = w_t^i \cdot p(\mathbf{x}_{t+1}^{B_{t+1}^i} | \mathbf{x}_t^i)$ for $i = 1, \dots, N$.
 - 5: Sample $\{B_t^1, \dots, B_t^N\}$ from $\{1, \dots, N\}$ with probabilities $\{\tilde{w}_t^i\}$.
 - 6: **end for**
-

- Approximation: $p(\mathbf{x}_t | \mathbf{y}_{1:T}) \approx \sum_{i=1}^N \tilde{w}_t^i \delta_{\mathbf{x}_t^{B_t^i}}(\mathbf{x}_t)$
- Several other smoother algorithms

Lemmings - smoothing results



A Case study - Covid-19

Case study - Covid-19

See separate file

SMC and parameter estimation

SMC and parameter estimation

- Assume

$$\mathbf{x}_t \sim p(\mathbf{x}_t | \mathbf{x}_{t-1}; \theta)$$

$$y_t \sim p(y_t | \mathbf{x}_t; \theta)$$

SMC and parameter estimation

- Assume

$$\mathbf{x}_t \sim p(\mathbf{x}_t | \mathbf{x}_{t-1}; \theta)$$

$$y_t \sim p(y_t | \mathbf{x}_t; \theta)$$

- Aim now: Simultaneous inference on θ

- Two main approaches:

- Maximum likelihood:** $\hat{\theta}_{ML} = \arg \max_{\theta} L(\theta)$

- Bayesian approach:** $p(\theta | \mathbf{y}_{1:T}) \propto p(\theta) p(\mathbf{y}_{1:T} | \theta) = p(\theta) L(\theta)$

- Important property of SMC: Unbiased estimate of marginal likelihood

$$L_t(\theta) = p(\mathbf{y}_{1:T} | \theta):$$

$$\hat{L}_T(\theta) = \prod_{t=1}^T \left(\frac{1}{N} \sum_{i=1}^N w_t^i \right)$$

- Two main classes of methods

- Offline** methods

- Online** methods

SMC and Bayesian parameter estimation

- Assume

$$\mathbf{x}_1 \sim p(\mathbf{x}_1; \theta)$$

$$\mathbf{x}_t \sim p(\mathbf{x}_t | \mathbf{x}_{t-1}; \theta)$$

$$Y_t \sim p(\mathbf{y}_t | \mathbf{x}_t; \theta)$$

$$\theta \sim p(\theta)$$

- Aim now: Simulate from $p(\mathbf{x}_t, \theta | \mathbf{y}_{1:t})$
- Several approaches
 - Direct use of SMC
 - Introducing dynamics in θ
 - Using sufficient statistics
 - Particle MCMC

SMC and maximum likelihood

- Interested in **maximizing**

$$L_t(\theta) = p(\mathbf{y}_{1:t}|\theta) = \int_{\mathbf{x}_{1:t}} p(\mathbf{y}_{1:t}|\mathbf{x}_{1:t}; \theta)p(\mathbf{x}_{1:t}|\theta)d\mathbf{x}_{1:t}.$$

SMC and maximum likelihood

- Interested in **maximizing**

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- Main **problem**: Calculation of the likelihood function
(and possibly the **score function** in order to do optimization)

SMC and maximum likelihood

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$$L_t(\theta) = p(\mathbf{y}_{1:t}|\theta) = \int_{\mathbf{x}_{1:t}} p(\mathbf{y}_{1:t}|\mathbf{x}_{1:t}; \theta)p(\mathbf{x}_{1:t}|\theta)d\mathbf{x}_{1:t}.$$

- Main **problem**: Calculation of the likelihood function
(and possibly the **score function** in order to do optimization)
- Main **approach**: Use that

$$L(\theta) = p(\mathbf{y}_{1:T}|\theta) = p(\mathbf{y}_1|\theta) \prod_{t=2}^T p(\mathbf{y}_s|\mathbf{y}_{1:s-1}; \theta) \approx \prod_{t=1}^T \left(\frac{1}{N} \sum_{i=1}^N w_t^i \right)$$

- Poyiadjis et al. (2011)**: Algorithms for calculating the score function and information (matrix) recursively
- Can be used for gradient descent methods

Particle MCMC

- Andrieu et al. (2010)
- Ideal MCMC ($p(\theta|\mathbf{y}) \propto p(\theta)L(\theta)$):
 - 1 Sample $\theta^* \sim g(\theta^*|\theta)$
 - 2 Calculate M-H ratio $r = \frac{p(\theta^*)L(\theta^*)g(\theta|\theta^*)}{p(\theta)L(\theta)g(\theta^*|\theta)}$
 - 3 Accept θ^* with prob $\min\{1, r\}$

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 - 3 Accept θ^* with prob $\min\{1, r\}$
- Pseudo-Marginal algorithm:
 - 1 Sample $\theta^* \sim g(\theta^*|\theta)$
 - 2 Calculate $\hat{L}(\theta^*)$
 - 3 Calculate M-H ratio $\hat{r} = \frac{\pi(\theta^*)p(\theta|\theta^*)}{\pi(\theta)p(\theta^*|\theta)}$
 - 4 Accept θ^* with prob $\min\{1, \hat{r}\}$
- **Particle MCMC**: Use SMC to calculate $\hat{L}(\theta^*)$

Direct use of SMC

- Assume at time $t - 1$ the existence of a properly weighted sample $\{(\mathbf{x}_{t-1}^i, \theta^i, w_{t-1}^i)\}$ with respect to $p(\mathbf{x}_{t-1}, \theta | \mathbf{y}_{1:t-1})$.
- We have

$$\begin{aligned} p(\mathbf{x}_t, \theta | \mathbf{y}_{1:t-1}) &= \int_{\mathbf{x}_{t-1}} p(\mathbf{x}_t | \mathbf{x}_{t-1}, \theta) p(\mathbf{x}_{t-1}, \theta | \mathbf{y}_{1:t-1}) d\mathbf{x}_{t-1} \\ &\approx \sum_{i=1}^N w_{t-1}^i p(\mathbf{x}_t | \mathbf{x}_{t-1}^i, \theta^i) \delta_{\theta}(\theta^i) \end{aligned}$$

and

$$p(\mathbf{x}_t, \theta | \mathbf{y}_{1:t}) \approx c \cdot \sum_{i=1}^N w_{t-1}^i p(\mathbf{x}_t | \mathbf{x}_{t-1}^i, \theta^i) \delta_{\theta^i}(\theta) p(\mathbf{y}_t | \mathbf{x}_t, \theta^i)$$

- Updated samples $\{(\theta^i, \mathbf{x}_t^i, w_t^i)\}$:
 - 1 Simulate $\mathbf{x}_t^i \sim p(\mathbf{x}_t | \mathbf{x}_{t-1}^i, \theta^i)$
 - 2 Update the weights by $w_t^i \propto w_{t-1}^i p(\mathbf{y}_t | \mathbf{x}_t^i, \theta^i)$
- The sample $\{\theta^i\}$ **do not change** over time.
- With resampling, this will lead to **degeneracy**

Direct use of SMC - properly weighted?

- Proposal:

$$\theta^i \sim g(\theta) \mathbf{x}_s^i \sim p(\mathbf{x}_s | \mathbf{x}_{s-1}^i, \theta^i), \quad s = 1, \dots, t$$

- Weights at time $t = 1$:

$$w_1^i = \frac{p(\theta^i)p(\mathbf{x}_1^i|\theta^i)p(\mathbf{y}_1|\mathbf{x}_1^i, \theta^i)}{g(\theta)p(\mathbf{x}_1^i|\theta^i)} = \frac{p(\theta^i)p(\mathbf{y}_1|\mathbf{x}_1^i, \theta^i)}{g(\theta)}$$

giving properly weighted samples at time 1.

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giving properly weighted samples at time 1.

- At time t :

$$\begin{aligned} w_t^i &= \frac{p(\theta^i)p(\mathbf{x}_1^i|\theta^i)p(\mathbf{y}_1|\mathbf{x}_1^i, \theta^i) \prod_{s=2}^t p(\mathbf{x}_s^i|\mathbf{x}_{s-1}^i, \theta^i)p(\mathbf{y}_s|\mathbf{x}_s^i, \theta^i)}{g(\theta)p(\mathbf{x}_1^i|\theta^i) \prod_{s=2}^t p(\mathbf{x}_s^i|\mathbf{x}_{s-1}^i, \theta^i)} \\ &= \frac{p(\theta^i)p(\mathbf{x}_1^i|\theta^i)p(\mathbf{y}_1|\mathbf{x}_1^i, \theta^i) \prod_{s=2}^t p(\mathbf{y}_s|\mathbf{x}_s^i, \theta^i)}{g(\theta)p(\mathbf{x}_1^i|\theta^i)} \\ &= \frac{p(\theta^i)p(\mathbf{x}_1^i|\theta^i)p(\mathbf{y}_1|\mathbf{x}_1^i, \theta^i) \prod_{s=2}^{t-1} p(\mathbf{y}_s|\mathbf{x}_s^i, \theta^i)}{g(\theta)p(\mathbf{x}_1^i|\theta^i)} p(\mathbf{y}_t|\mathbf{x}_t^i, \theta^i) \\ &= w_{t-1}^i p(\mathbf{y}_t|\mathbf{x}_t^i, \theta^i) \end{aligned}$$

Direct use of SMC - properly weighted?

- Proposal:

$$\theta^i \sim g(\theta) \mathbf{x}_s^i \sim p(\mathbf{x}_s | \mathbf{x}_{s-1}^i, \theta^i), \quad s = 1, \dots, t$$

- Weights at time $t = 1$:

$$w_1^i = \frac{p(\theta^i)p(\mathbf{x}_1^i|\theta^i)p(\mathbf{y}_1|\mathbf{x}_1^i, \theta^i)}{g(\theta)p(\mathbf{x}_1^i|\theta^i)} = \frac{p(\theta^i)p(\mathbf{y}_1|\mathbf{x}_1^i, \theta^i)}{g(\theta)}$$

giving properly weighted samples at time 1.

- At time t :

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- Main problem: Now we need to resample $(\theta, \mathbf{x}_{1:t})$.
Will result in degeneracy when $p(\theta, \mathbf{x}_t|\mathbf{y}_{1:t})$ is of interest.

Lemmings data

- Interested in the dynamics of the lemmings populations
- From church books: Binary records on **lemmings years** or not.

Lemmings data

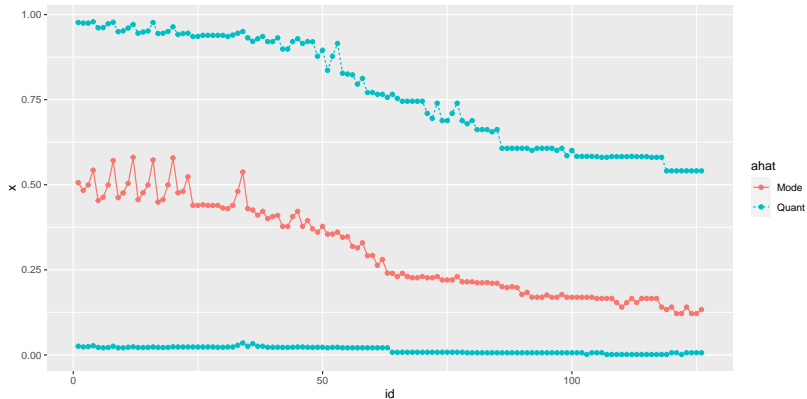
- Interested in the dynamics of the lemmings populations
- From church books: Binary records on **lemmings years** or not.
- Define $\mathbf{x}_t = \log(N_t)$, N_t population size at year t
- Model

$$\mathbf{x}_t = a\mathbf{x}_{t-1} + \varepsilon_t, \quad \varepsilon_t \sim N(0, \sigma^2)$$

$$\mathbf{y}_t \sim \text{Binom}\left(1, \frac{\exp(\mathbf{x}_t)}{1 + \exp(\mathbf{x}_t)}\right)$$

- Of interest: $p(\mathbf{x}_t | \mathbf{y}_{1:t})$, $p(a | \mathbf{y}_{1:t})$
- `SMC_lin_bin.R`, `SMC_lemmings_parest_direct.R`

Results - Lemmings



Introducing dynamics in θ

- **Liu and West (2001)**: Assume θ is (slowly) changing with time:

$$\theta_t = \theta_{t-1} + \zeta_t, \quad \zeta_t \sim N(0, q)$$

- Focus on $p(\mathbf{x}_t, \theta_t | \mathbf{y}_{1:t})$.
- Assume a weighted sample $\{(\mathbf{x}_{t-1}^i, \theta_{t-1}^i, w_{t-1}^i)\}$

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$$\begin{aligned} p(\mathbf{x}_t, \theta_t | \mathbf{y}_{1:t-1}) &= \int_{\mathbf{x}_{t-1}} p(\mathbf{x}_t | \mathbf{x}_{t-1}, \theta_t) p(\theta_t | \theta_{t-1}) p(\mathbf{x}_{t-1}, \theta_{t-1} | \mathbf{y}_{1:t-1}) d\mathbf{x}_{t-1} d\theta_{t-1} \\ &\approx \sum_{i=1}^N w_{t-1}^i p(\mathbf{x}_t | \mathbf{x}_{t-1}^i, \theta_t) p(\theta_t | \theta_{t-1}^i) \\ p(\mathbf{x}_t, \theta_t | \mathbf{y}_{1:t}) &\approx c \cdot \sum_{i=1}^N w_{t-1}^i p(\mathbf{x}_t | \mathbf{x}_{t-1}^i, \theta_t) p(\theta_t | \theta_{t-1}^i) p(\mathbf{y}_t | \mathbf{x}_t, \theta_t). \end{aligned}$$

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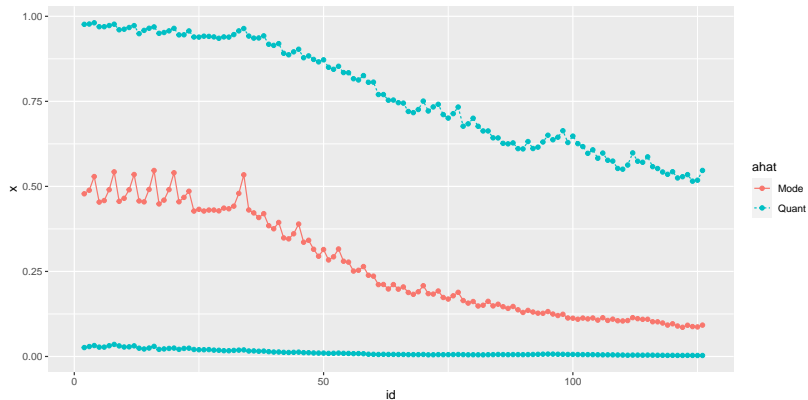
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- Update samples to $\{(\theta_t^i, \mathbf{x}_t^i, w_t^i)\}$ by
 - 1 Simulate $\theta_t^i \sim p(\theta_t | \theta_{t-1}^i)$,
 - 2 Simulate $\mathbf{x}_t^i \sim p(\mathbf{x}_t | \mathbf{x}_{t-1}^i, \theta_t^i)$
 - 3 Update the weights by $w_t^i \propto w_{t-1}^i p(\mathbf{y}_t | \mathbf{x}_t^i, \theta_t^i)$.
- SMC_lemmings_parest_dyn.R

Results - Lemmings



Dynamics in θ - continued

- New values $\{\theta_t^i\}$ are generated at each time point

Dynamics in θ - continued

- New values $\{\theta_t^i\}$ are generated at each time point
- Main problem: Introduce extra variability in θ_t .
- Consequence: Estimation of θ_t mainly based on most **recent** observations
- The model

$$\theta_t = \theta_{t-1} + \zeta_t, \quad \zeta_t \sim N(0, q)$$

might be reasonable

- New problem: Estimate the **static** parameter q .
- `SMC_lin_bin_parest_dyn.R`

Sufficient statistics

- Example:

$$\mathbf{x}_t = a\mathbf{x}_{t-1} + \varepsilon_t, \quad \varepsilon_t \sim N(0, \sigma^2), \quad \sigma \text{ known for simplicity}$$

- The distribution $p(\mathbf{y}_t|\mathbf{x}_t)$ can be arbitrary (but not depending on θ).
- $\theta = a$ needs to be estimated. Assume a prior $a \sim N(\mu_a, \sigma_a^2)$.

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- Can be shown:

$$p(a|\mathbf{x}_{1:t}) = N(\mu_{a|t}, \sigma_{a|t}^2)$$

where

$$\mu_{a|t} = \frac{\sigma_a^2 \sum_{s=2}^t \mathbf{x}_s \mathbf{x}_{s-1} + \sigma^2 \mu_a}{\sigma_a^2 \sum_{s=2}^t \mathbf{x}_{s-1}^2 + \sigma^2}; \quad \sigma_{a|t}^2 = \frac{\sigma^2 \sigma_a^2}{\sigma_a^2 \sum_{s=2}^t \mathbf{x}_{s-1}^2 + \sigma^2}.$$

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- Main point: Given $\mathbf{x}_{1:t}$, the distribution of a (and simulation) is simple.
- $p(a|\mathbf{x}_{1:t})$ only depend on $S_{t,1} = \sum_{s=2}^t \mathbf{x}_s \mathbf{x}_{s-1}$ and $S_{t,2} = \sum_{s=2}^t \mathbf{x}_{s-1}^2$
- Both terms can be **recursively updated** through

$$S_{t,1} = S_{t-1,1} + \mathbf{x}_t \mathbf{x}_{t-1}, \quad S_{t,2} = S_{t-1,2} + \mathbf{x}_{t-1}^2.$$

SMC and sufficient statistics

- Assume $p(\mathbf{y}_t|\mathbf{x}_t)$ do not depend on θ .
- Assume $p(\theta|\mathbf{x}_{1:t}) = p(\theta|S_t)$, S_t sufficient statistic.
- Assume $S_t = h(S_{t-1}, \mathbf{x}_{t-1}, \mathbf{x}_t)$

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- Fearnhead (2002) and Storvik (2002): Focus on $p(\mathbf{x}_t, S_t|\mathbf{y}_{1:t})$, not $p(\mathbf{x}_t, \theta|\mathbf{y}_{1:t})$.

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- Assume a properly weighted sample $\{(\mathbf{x}_{t-1}^i, S_{t-1}^i, w_{t-1}^i), i = 1, \dots, N\}$ with respect to $p(\mathbf{x}_{t-1}, S_{t-1}|\mathbf{y}_{1:t-1})$
- Similar recursions as before:

$$\begin{aligned} p(\mathbf{x}_t, S_t|\mathbf{y}_{1:t-1}) &= \int_{\mathbf{x}_{t-1}} p(\mathbf{x}_t, S_t|\mathbf{x}_{t-1}, S_{t-1})p(\mathbf{x}_{t-1}, S_{t-1}|\mathbf{y}_{1:t-1})d\mathbf{x}_{t-1}dS_{t-1} \\ &\approx \sum_{i=1}^N w_{t-1}^i p(\mathbf{x}_t, S_t|\mathbf{x}_{t-1}^i, S_{t-1}^i) \\ p(\mathbf{x}_t, S_t|\mathbf{y}_{1:t}) &\approx c \cdot \sum_{i=1}^N w_{t-1}^i p(\mathbf{x}_t, S_t|\mathbf{x}_{t-1}^i, S_{t-1}^i)p(\mathbf{y}_t|\mathbf{x}_t). \end{aligned}$$

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- Simulation from $p(\mathbf{x}_t, S_t|\mathbf{x}_{t-1}^i, S_{t-1}^i)$ (possible proposal function)
 - 1 Simulate $\theta^i \sim p(\theta|\mathbf{x}_{t-1}^i, S_{t-1}^i) = p(\theta|S_{t-1}^i)$.
 - 2 Simulate $\mathbf{x}_t^i \sim p(\mathbf{x}_t|\mathbf{x}_{t-1}^i, \theta^i)$.
 - 3 Put $S_t^i = h(S_{t-1}^i, \mathbf{x}_{t-1}^i, \mathbf{x}_t^i)$.

Algorithm (Storvik filter)

Algorithm 6 SMC with parameter updating

- 1: Simulate $\theta^i \sim p(\theta)$ for $i = 1, \dots, N$. ▷ Initialization
 - 2: Simulate $\mathbf{x}_1^i \sim p(\mathbf{x}_1 | \theta^i)$ for $i = 1, \dots, N$.
 - 3: Put weights $w_1^i = p(\mathbf{y}_1 | \mathbf{x}_1^i)$.
 - 4: Put $S_1^i = 0$ for $i = 1, \dots, N$.
 - 5: **for** $t = 2, 3, \dots$ **do** ▷ Sequential Monte Carlo
 - 6: Simulate $\theta^i \sim p(\theta | S_{t-1}^i)$ for $i = 1, \dots, N$.
 - 7: Simulate $\mathbf{x}_t^i \sim p(\mathbf{x}_t | \mathbf{x}_{t-1}^i, \theta^i)$ for $i = 1, \dots, N$.
 - 8: Put weights $w_t^i = w_{t-1}^i p(\mathbf{y}_t | \mathbf{x}_t^i)$.
 - 9: Put $S_t^i = h(S_{t-1}^i, \mathbf{x}_{t-1}^i, \mathbf{x}_t^i)$.
 - 10: **if** \hat{N}_{eff} is small **then** ▷ Resampling
 - 11: Resample (\mathbf{x}_t^i, S_t^i) with probabilities proportional to w_t^i .
 - 12: Put $w_t^i = 1/N$.
 - 13: **end if**
 - 14: **end for**
-

SMC_lin_bin_parest_suff.R

Offline methods

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- Can **reduce** noise at **later** time points
- Gives a good approximation to $\pi_t(\mathbf{x}_t)$
- Does **not** give a good approximation to $\pi_t(\mathbf{x}_{1:t})$ or $\pi(\mathbf{x}_1)$!
- `SMC_cosnorm.R`

Hidden Markov models - state space models

- Assume

$$\mathbf{x}_1 \sim p(\mathbf{x}_1)$$

$$\mathbf{x}_t \sim p(\mathbf{x}_t | \mathbf{x}_{t-1})$$

$$\mathbf{x}_t \sim p(\mathbf{y}_t | \mathbf{x}_t)$$

- $\{\mathbf{y}_t\}$ observed, $\{\mathbf{x}_t\}$ **hidden**
- Aim:** $p(\mathbf{x}_{1:t} | \mathbf{y}_{1:t})$ or $p(\mathbf{x}_t | \mathbf{y}_{1:t})$
- Recursive relationship:

$$\begin{aligned} p(\mathbf{x}_{1:t} | \mathbf{y}_{1:t}) &= \frac{p(\mathbf{x}_{1:t}, \mathbf{y}_t | \mathbf{y}_{1:t-1})}{p(\mathbf{y}_t | \mathbf{y}_{1:t-1})} \\ &= \frac{p(\mathbf{x}_{1:t-1} | \mathbf{y}_{1:t-1}) p(\mathbf{x}_t | \mathbf{x}_{t-1}) p(\mathbf{y}_t | \mathbf{x}_t)}{p(\mathbf{y}_t | \mathbf{y}_{1:t-1})} \\ &\propto p(\mathbf{x}_{1:t-1} | \mathbf{y}_{1:t-1}) p(\mathbf{x}_t | \mathbf{x}_{t-1}) p(\mathbf{y}_t | \mathbf{x}_t) \end{aligned}$$

SMC and hidden Markov models

- Assume $g_t(\mathbf{x}_t|\mathbf{x}_{t-1}) = p(\mathbf{x}_t|\mathbf{x}_{t-1})$

$$\begin{aligned}w_t &= \frac{p(\mathbf{x}_{1:t}|\mathbf{y}_{1:t})}{g(\mathbf{x}_{1:t})} \\&\propto \frac{p(\mathbf{x}_{1:t-1}|\mathbf{y}_{1:t-1})p(\mathbf{x}_t|\mathbf{x}_{t-1})p(\mathbf{y}_t|\mathbf{x}_t)}{\rho_{\mathbf{x}_1}(\mathbf{x}_1) \prod_{s=2}^t p(\mathbf{x}_s|\mathbf{x}_{s-1})} \\&= \frac{p(\mathbf{x}_{1:t-1}|\mathbf{y}_{1:t-1})}{g(\mathbf{x}_{1:t-1})} \frac{p(\mathbf{x}_t|\mathbf{x}_{t-1})p(\mathbf{y}_t|\mathbf{x}_t)}{\rho(\mathbf{x}_t|\mathbf{x}_{t-1})} \\&= w_{t-1}p(\mathbf{y}_t|\mathbf{x}_t)\end{aligned}$$

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 &= \frac{p(\mathbf{x}_{1:t-1}|\mathbf{y}_{1:t-1})}{g(\mathbf{x}_{1:t-1})} \frac{p(\mathbf{x}_t|\mathbf{x}_{t-1})p(\mathbf{y}_t|\mathbf{x}_t)}{\rho(\mathbf{x}_t|\mathbf{x}_{t-1})} \\
 &= w_{t-1}p(\mathbf{y}_t|\mathbf{x}_t)
 \end{aligned}$$

- Algorithm**

- 1 Sample $\mathbf{x}_1^i \sim p_{\mathbf{x}_1}(\cdot), i = 1, \dots, N$.
- 2 Let $w_1^i = p(\mathbf{y}_1|\mathbf{x}_1^i)$, normalize to $w_1^i = w_1^i / \sum_j w_1^j$. Set $t = 2$
- 3 Sample $\mathbf{x}_t^i|\mathbf{x}_{t-1}^i \sim p(\mathbf{x}_t|\mathbf{x}_{t-1}^i), i = 1, \dots, N$.
- 4 Append \mathbf{x}_t^i to $\mathbf{x}_{1:t-1}^i$, obtaining \mathbf{x}_t^i
- 5 Let $w_t^i = w_{t-1}^i p(\mathbf{y}_t|\mathbf{x}_t^i)$, **normalize** to $w_t^i = w_t^i / \sum_j w_t^j$.
- 6 If \hat{N}_{eff} is small, perform resampling
- 7 Increment t and return to step 3

Terrain navigation

- Assume movement model for airplane

$$\mathbf{x}_t = \mathbf{x}_{t-1} + \mathbf{d}_t + \boldsymbol{\varepsilon}_t$$

\mathbf{d}_t = Drift of plane measured by internal navigation system (assumed known)

$$\boldsymbol{\varepsilon}_t = \mathbf{R}_t^T \mathbf{Z}_t$$

$$\mathbf{R}_t = \frac{1}{\mathbf{x}_{1,t-1}^2 + \mathbf{x}_{2,t-1}^2} \begin{pmatrix} -\mathbf{x}_{1,t-1} & \mathbf{x}_{2,t-1} \\ -\mathbf{x}_{2,t-1} & -\mathbf{x}_{1,t-1} \end{pmatrix}$$

$$\mathbf{Z}_t \sim N_2 \left(\mathbf{0}, q^2 \begin{pmatrix} 1 & 0 \\ 0 & k^2 \end{pmatrix} \right)$$

$$q = 400, k = 0.5$$

$$Y_t = m(\mathbf{x}_t) + \delta_t$$

$m(\mathbf{x}_t)$ = Elevation at point \mathbf{x}_t

- Example_6_7.R

SMC and particle filters

- SMC with resampling usually called **particle filters**
- Some mix/confusion about terminology, mainly the same!
- **Bootstrap filter**: SMC for hidden Markov models with
 $g(\mathbf{x}_t|\mathbf{x}_{t-1}) = p(\mathbf{x}_t|\mathbf{x}_{t-1})$

Example optimal resampling

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- Sample \mathbf{D} from $\text{Multinom}(1 : N, 1, (\frac{0.1}{0.3}, \frac{0.0}{0.3}, \frac{0.05}{0.3}, \frac{0.15}{0.3}, \frac{0.0}{0.3}))$
e.g $\mathbf{D} = (1, 0, 0, 0, 0)$

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e.g $\mathbf{D} = (1, 0, 0, 0, 0)$
- Put $\mathbf{N} = \tilde{\mathbf{N}} + \mathbf{D} = (2, 2, 0, 0, 1)$