Controlled sequential Monte Carlo

Jeremy Heng,
Department of Statistics, Harvard University

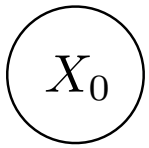
Joint work with Adrian Bishop (UTS, CSIRO), George Deligiannidis & Arnaud Doucet (Oxford)

Bayesian Computation for High-Dimensional Statistical Models
Institute for Mathematical Sciences, NUS
14 September 2018

Outline

Outline

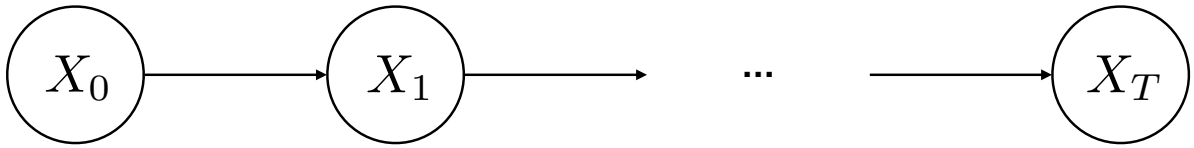
State space models



Latent Markov chain

$$X_0 \sim \mu,$$

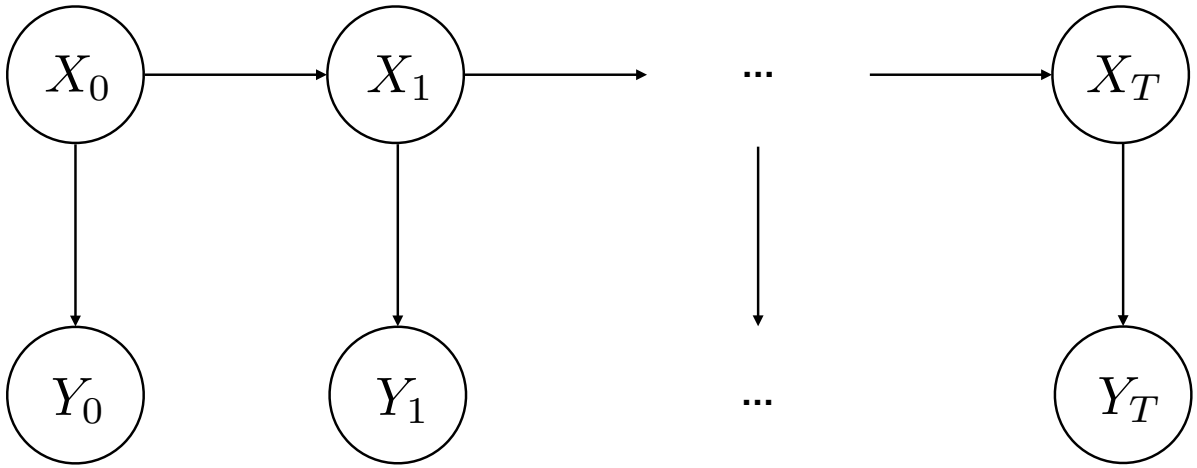
State space models



Latent Markov chain

$$X_0 \sim \mu, \quad X_t | X_{t-1} \sim f_t(X_{t-1}, \cdot), \quad t \in [1 : T]$$

State space models



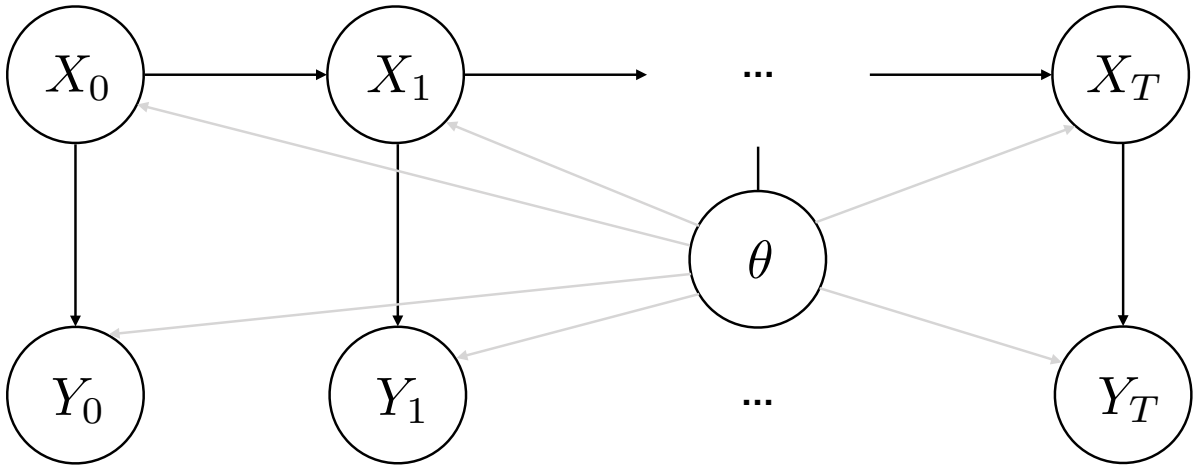
Latent Markov chain

$$X_0 \sim \mu, \quad X_t | X_{t-1} \sim f_t(X_{t-1}, \cdot), \quad t \in [1 : T]$$

Observations

$$Y_t | X_{0:T} \sim g_t(X_t, \cdot), \quad t \in [0 : T]$$

State space models



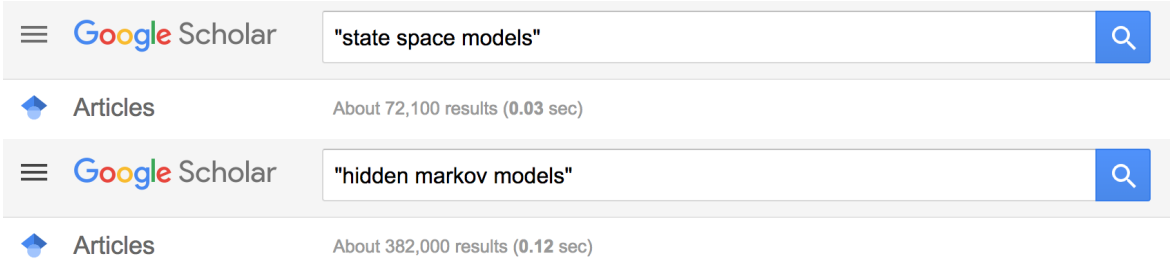
Latent Markov chain

$$X_0 \sim \mu_\theta, \quad X_t | X_{t-1} \sim f_{t,\theta}(X_{t-1}, \cdot), \quad t \in [1 : T]$$

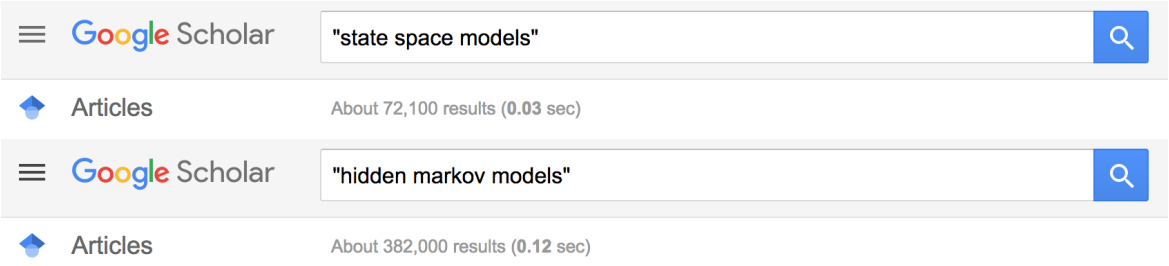
Observations

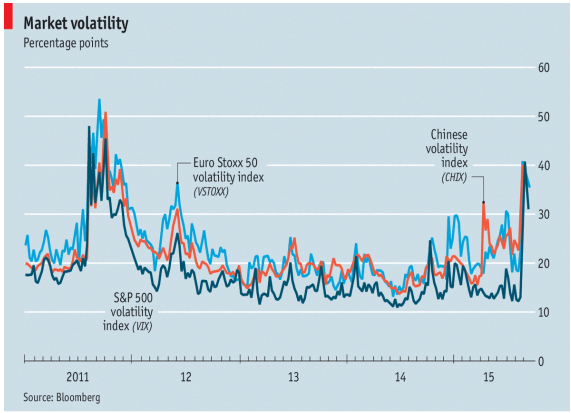
$$Y_t | X_{0:T} \sim g_{t,\theta}(X_t, \cdot), \quad t \in [0 : T]$$

State space models

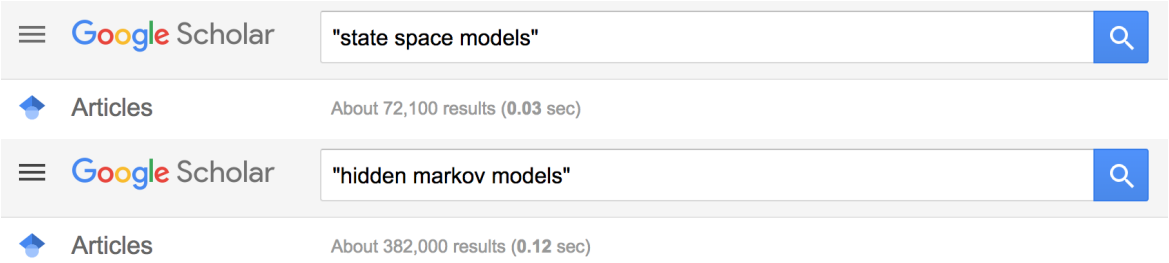


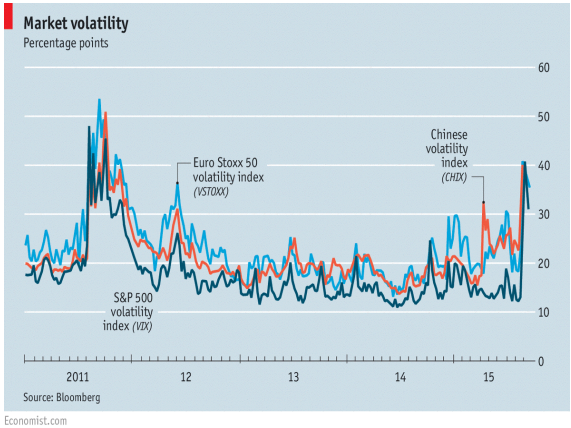
State space models



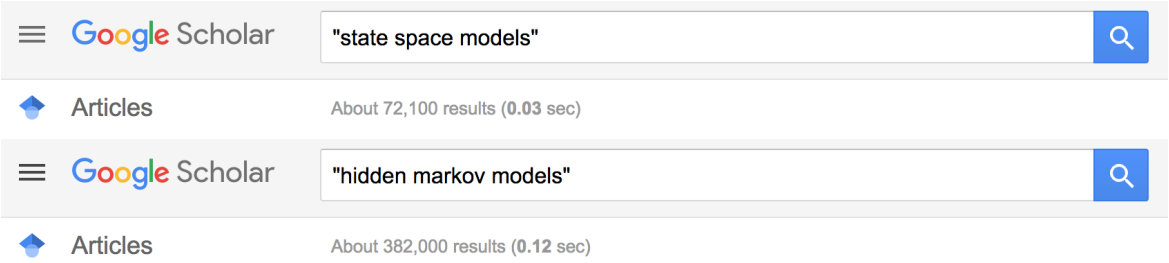


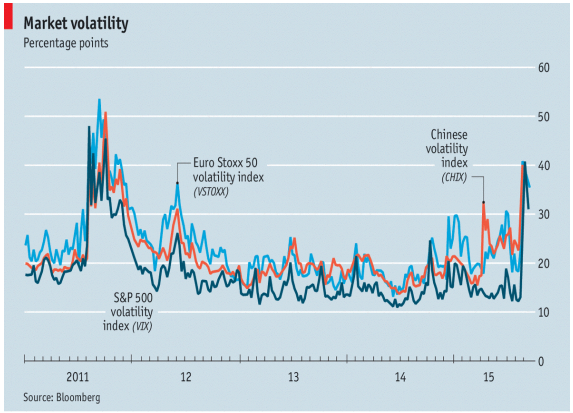
State space models



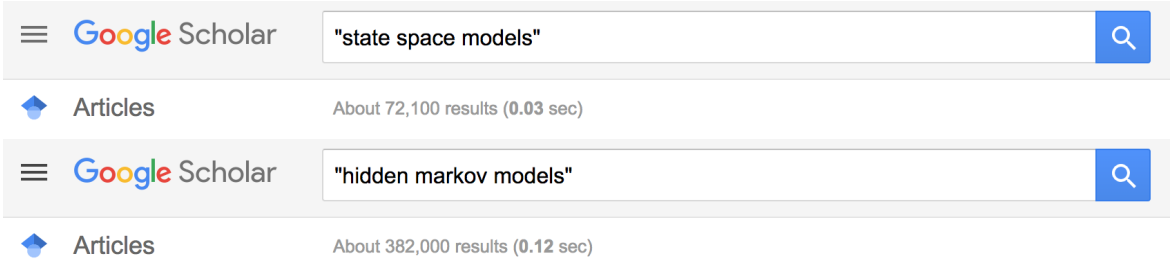


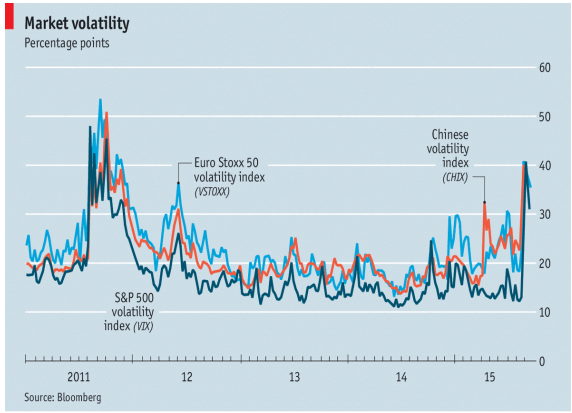
State space models

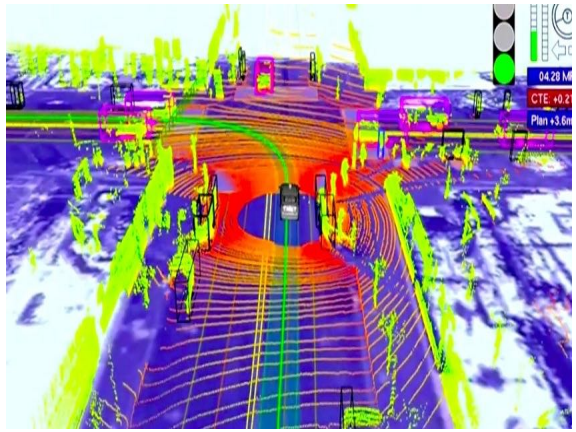




State space models





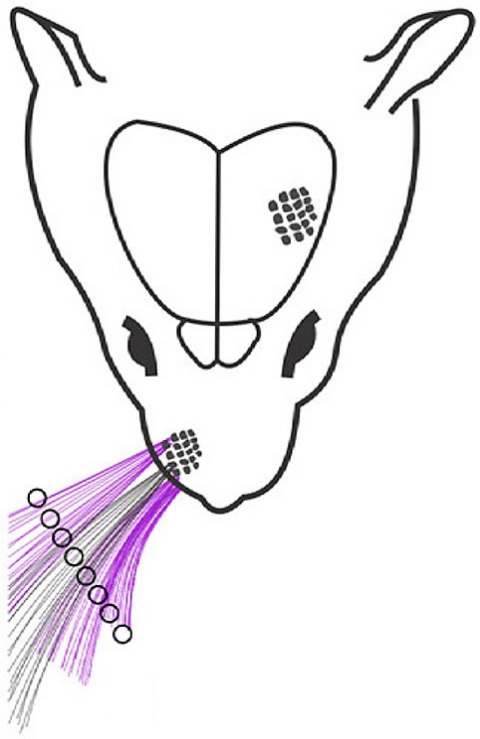


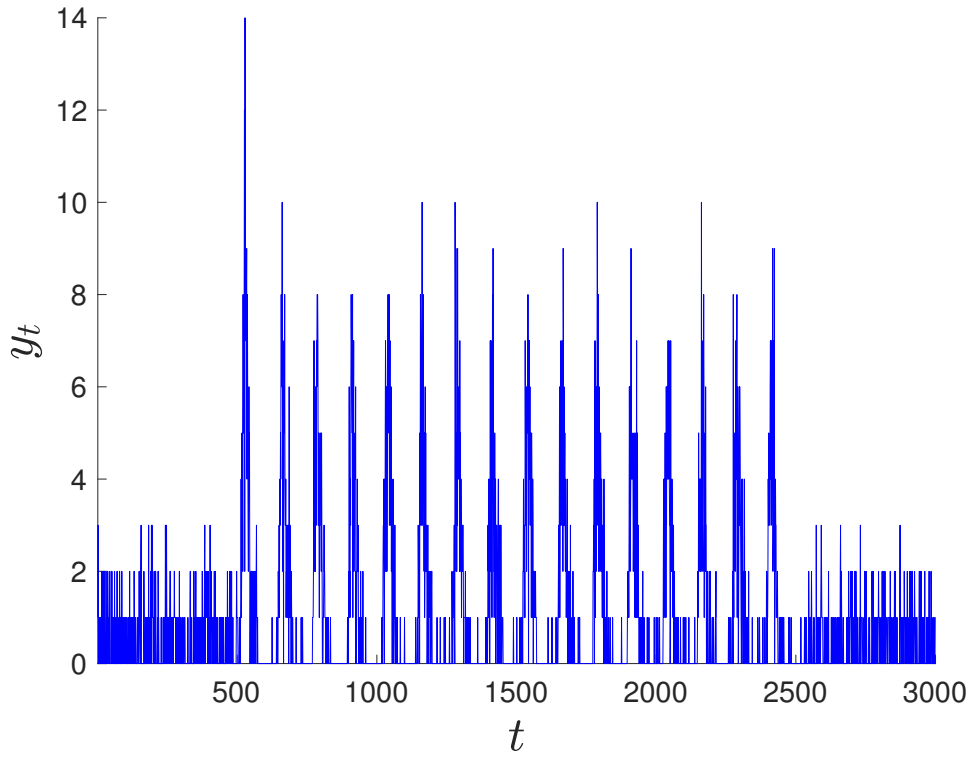
Neuroscience example

- Joint work with Demba Ba, Harvard School of Engineering

Neuroscience example

- Joint work with Demba Ba, Harvard School of Engineering
- 3000 measurements $y_t \in \{0, \ldots, 50\}$ collected from a neuroscience experiment (Temereanca et al., 2008)





Neuroscience example

- Observation model

$$Y_t | X_t \sim \text{Binomial}\left(50, \kappa(X_t)\right), \quad \kappa(u) = (1 + \exp(-u))^{-1}$$

Neuroscience example

- Observation model

$$Y_t|X_t \sim \text{Binomial}\left(50, \kappa(X_t)\right), \quad \kappa(u) = (1+\exp(-u))^{-1}$$

- Latent Markov chain

$$X_0 \sim \mathcal{N}(0,1), \quad X_t|X_{t-1} \sim \mathcal{N}(\alpha X_{t-1}, \sigma^2)$$

Neuroscience example

- Observation model

$$Y_t|X_t \sim \text{Binomial}\left(50, \kappa(X_t)\right), \quad \kappa(u) = (1+\exp(-u))^{-1}$$

- Latent Markov chain

$$X_0 \sim \mathcal{N}(0,1), \quad X_t|X_{t-1} \sim \mathcal{N}(\alpha X_{t-1}, \sigma^2)$$

- Unknown parameters

$$\theta = (\alpha, \sigma^2) \in [0,1] \times (0,\infty)$$

Objects of interest

- Online estimation: compute **filtering distributions**

$$p(x_t|y_{0:t}, \theta), \quad t \geq 0$$

Objects of interest

- Online estimation: compute **filtering distributions**

$$p(x_t|y_{0:t}, \theta), \quad t \geq 0$$

- Offline estimation: compute **smoothing distribution**

$$p(x_{0:T}|y_{0:T}, \theta), \quad T \in \mathbb{N}$$

or **marginal likelihood**

$$p(y_{0:T}|\theta) = \int_{\mathcal{X}^{T+1}} \mu_\theta(x_0) \prod_{t=1}^{T} f_{t,\theta}(x_{t-1}, x_t) \prod_{t=0}^{T} g_{t,\theta}(x_t, y_t) dx_{0:T}$$

Objects of interest

- Online estimation: compute **filtering distributions**

$$p(x_t|y_{0:t},\theta), \quad t \geq 0$$

- Offline estimation: compute **smoothing distribution**

$$p(x_{0:T}|y_{0:T},\theta), \quad T \in \mathbb{N}$$

or **marginal likelihood**

$$p(y_{0:T}|\theta) = \int_{\mathcal{X}^{T+1}} \mu_\theta(x_0) \prod_{t=1}^{T} f_{t,\theta}(x_{t-1},x_t) \prod_{t=0}^{T} g_{t,\theta}(x_t,y_t) dx_{0:T}$$

- Parameter inference

$$\arg\max_{\theta\in\Theta} p(y_{0:T}|\theta), \quad p(\theta|y_{0:T}) \propto p(\theta)p(y_{0:T}|\theta)$$

Outline

Sequential Monte Carlo

- Sequential Monte Carlo (SMC) aka bootstrap particle filter (BPF) recursively simulates an interacting particle system of size N

$$(X_t^1, \ldots, X_t^N), \quad t \in [0 : T]$$

Del Moral (2004). *Feynman-Kac formulae*.

Sequential Monte Carlo

- Sequential Monte Carlo (SMC) aka bootstrap particle filter (BPF) recursively simulates an interacting particle system of size N

$$(X_t^1, \ldots, X_t^N), \quad t \in [0 : T]$$

- Unbiased and consistent marginal likelihood estimator

$$\hat{p}(y_{0:T}|\theta) = \prod_{t=0}^{T} \left\{ \frac{1}{N} \sum_{n=1}^{N} g_{t,\theta}(X_t^n, y_t) \right\}$$

Del Moral (2004). *Feynman-Kac formulae*.

Sequential Monte Carlo

- Sequential Monte Carlo (SMC) aka bootstrap particle filter (BPF) recursively simulates an interacting particle system of size N

$$(X_t^1, \ldots, X_t^N), \quad t \in [0 : T]$$

- Unbiased and consistent marginal likelihood estimator

$$\hat{p}(y_{0:T}|\theta) = \prod_{t=0}^{T} \left\{ \frac{1}{N} \sum_{n=1}^{N} g_{t,\theta}(X_t^n, y_t) \right\}$$

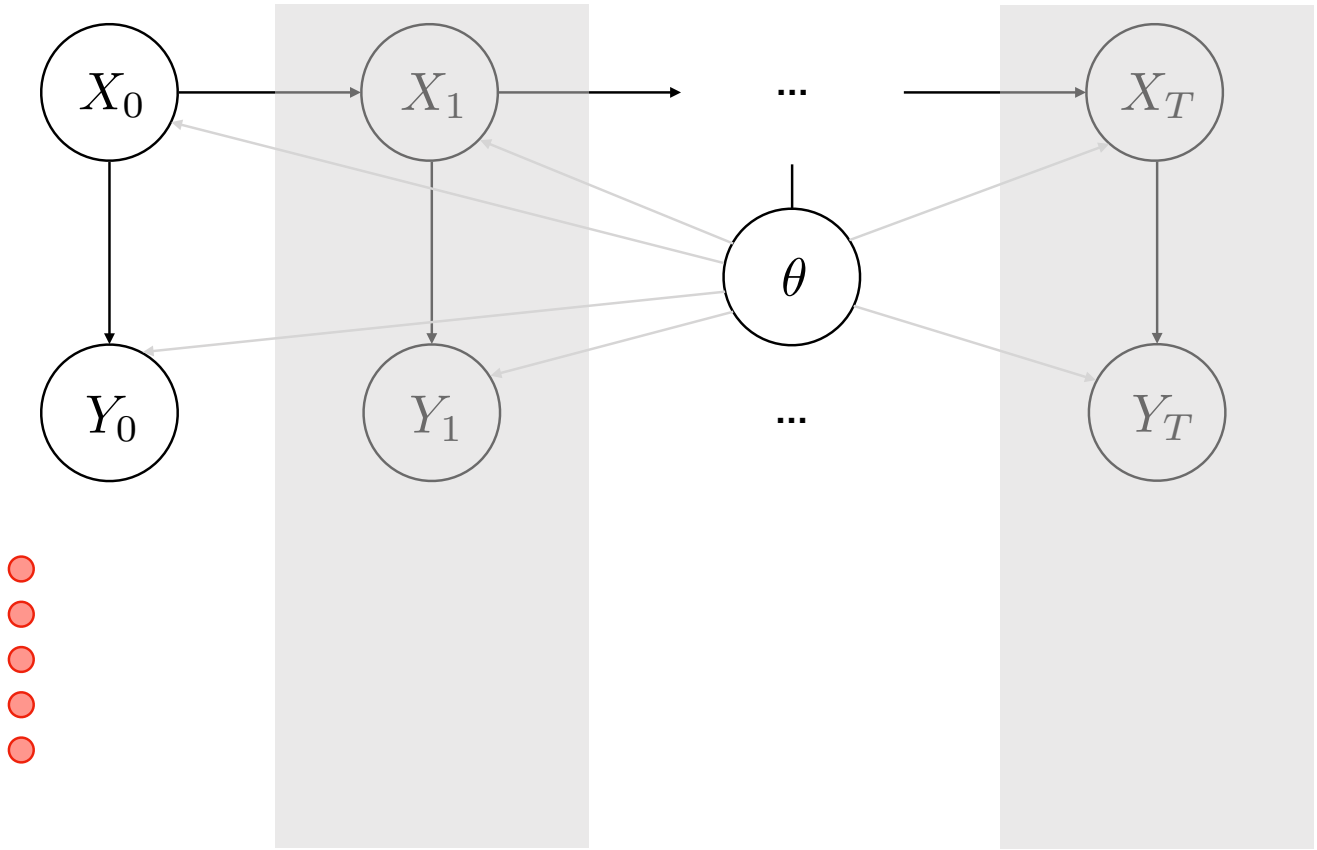
- Consistent approximation of smoothing distribution

$$\frac{1}{N} \sum_{n=1}^{N} \varphi(X_{0:T}^n) \to \int \varphi(x_{0:T}) p(x_{0:T}|y_{0:T}, \theta) dx_{0:T}$$

as $N \to \infty$

Del Moral (2004). *Feynman-Kac formulae*.

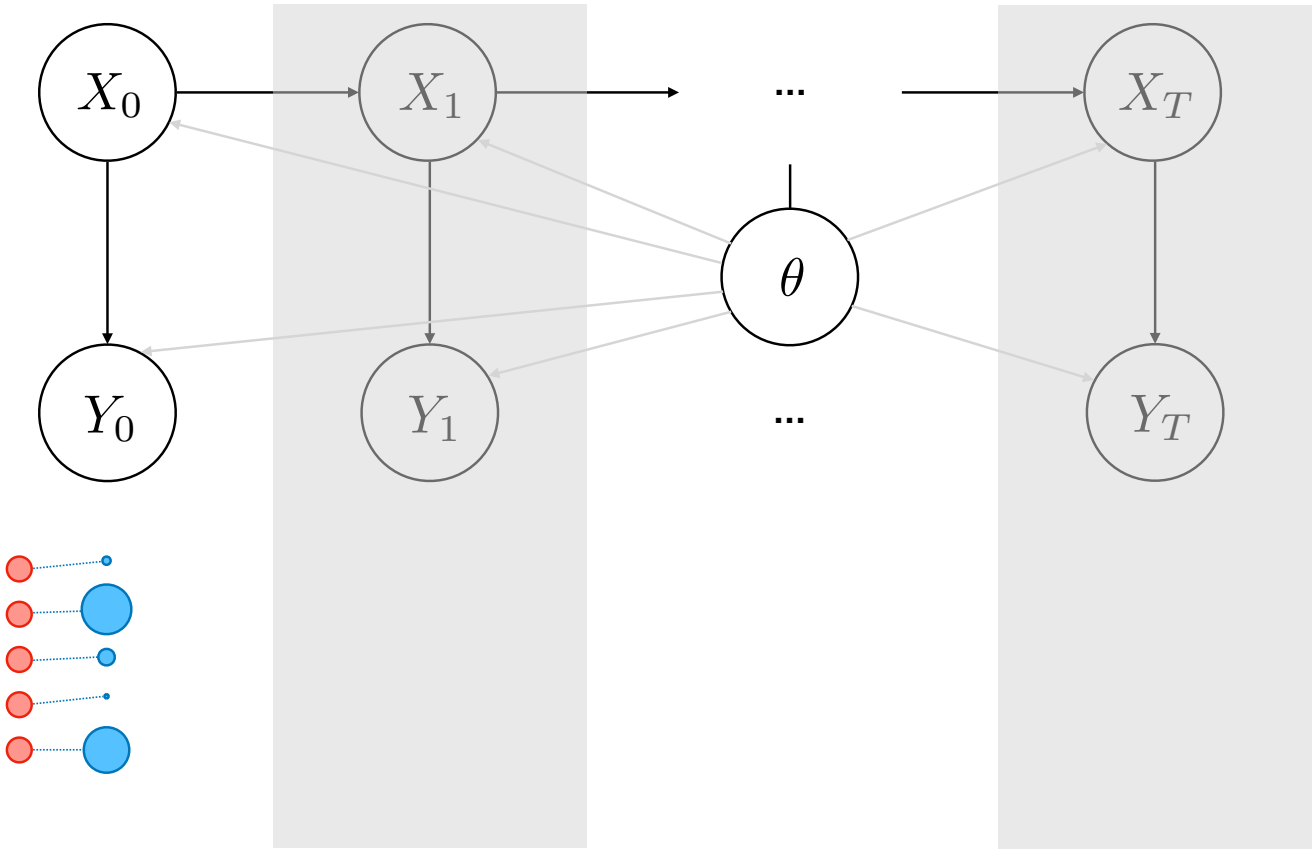
Sequential Monte Carlo



For time $t = 0$ and particle $n \in [1 : N]$

$$\text{sample } X_0^n \sim \mu_\theta$$

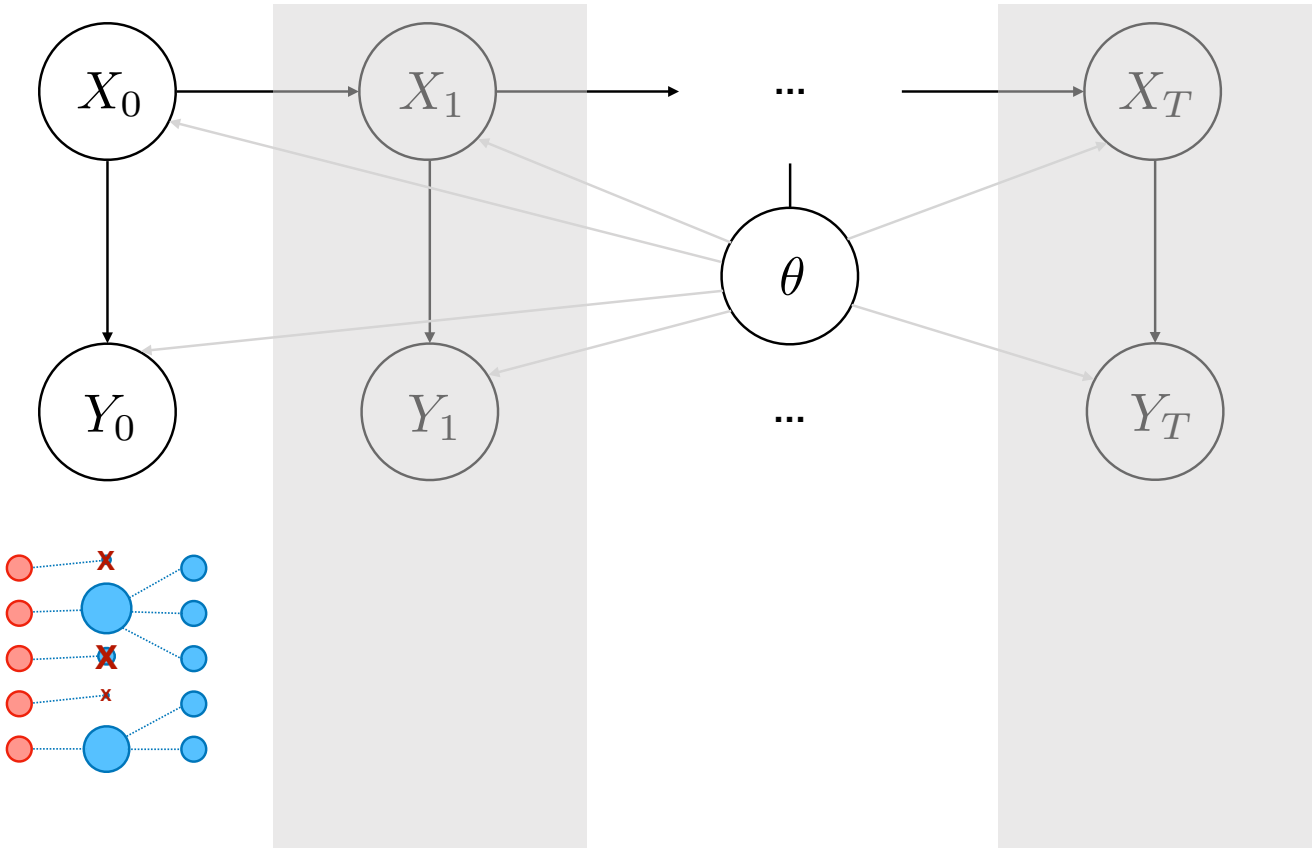
Sequential Monte Carlo



For time $t = 0$ and particle $n \in [1 : N]$

$$\text{weight } W_0^n \propto g_{0,\theta}(X_0^n, y_0)$$

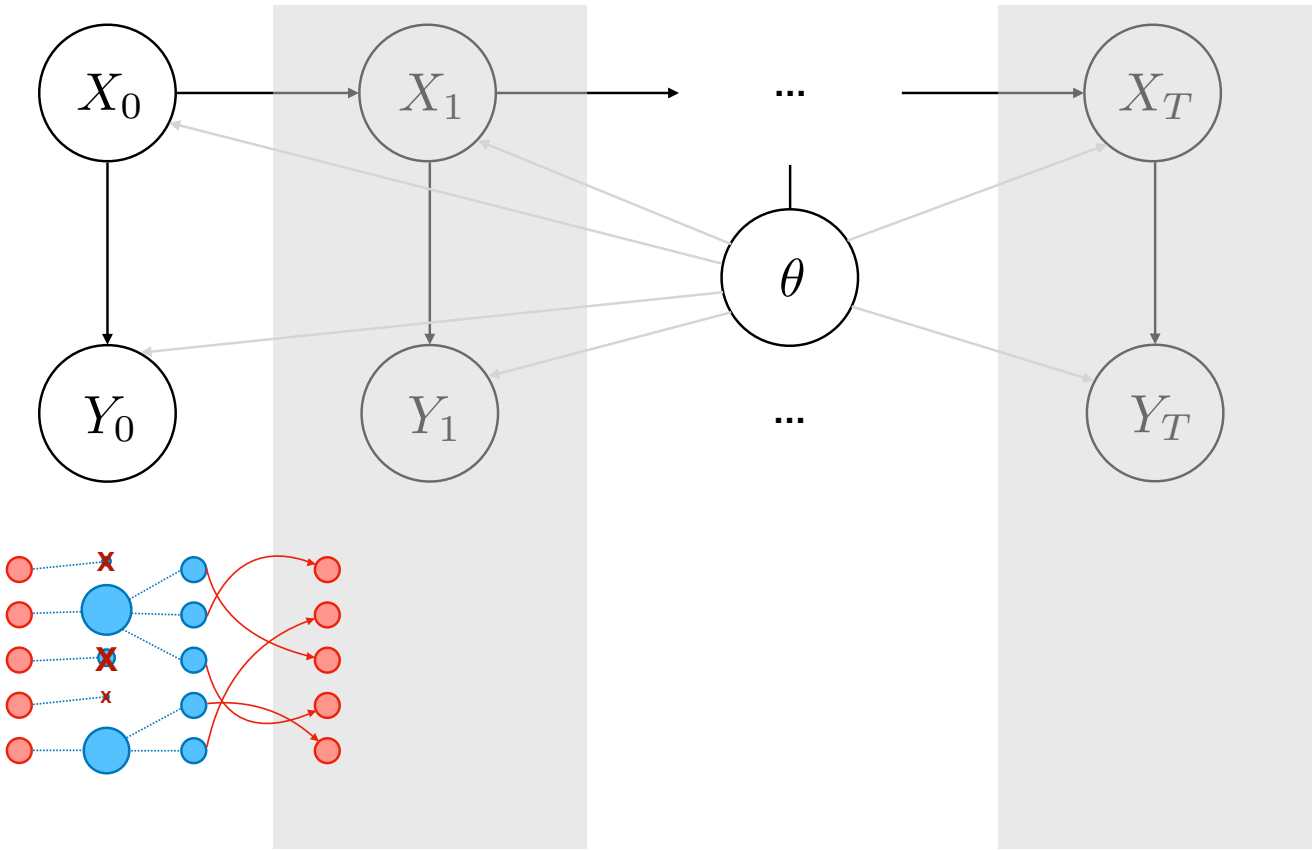
Sequential Monte Carlo



For time $t = 0$ and particle $n \in [1 : N]$

sample ancestor $A_0^n \sim \mathcal{R}\left(W_0^1, \ldots, W_0^N\right)$, resampled particle: $X_0^{A_0^n}$

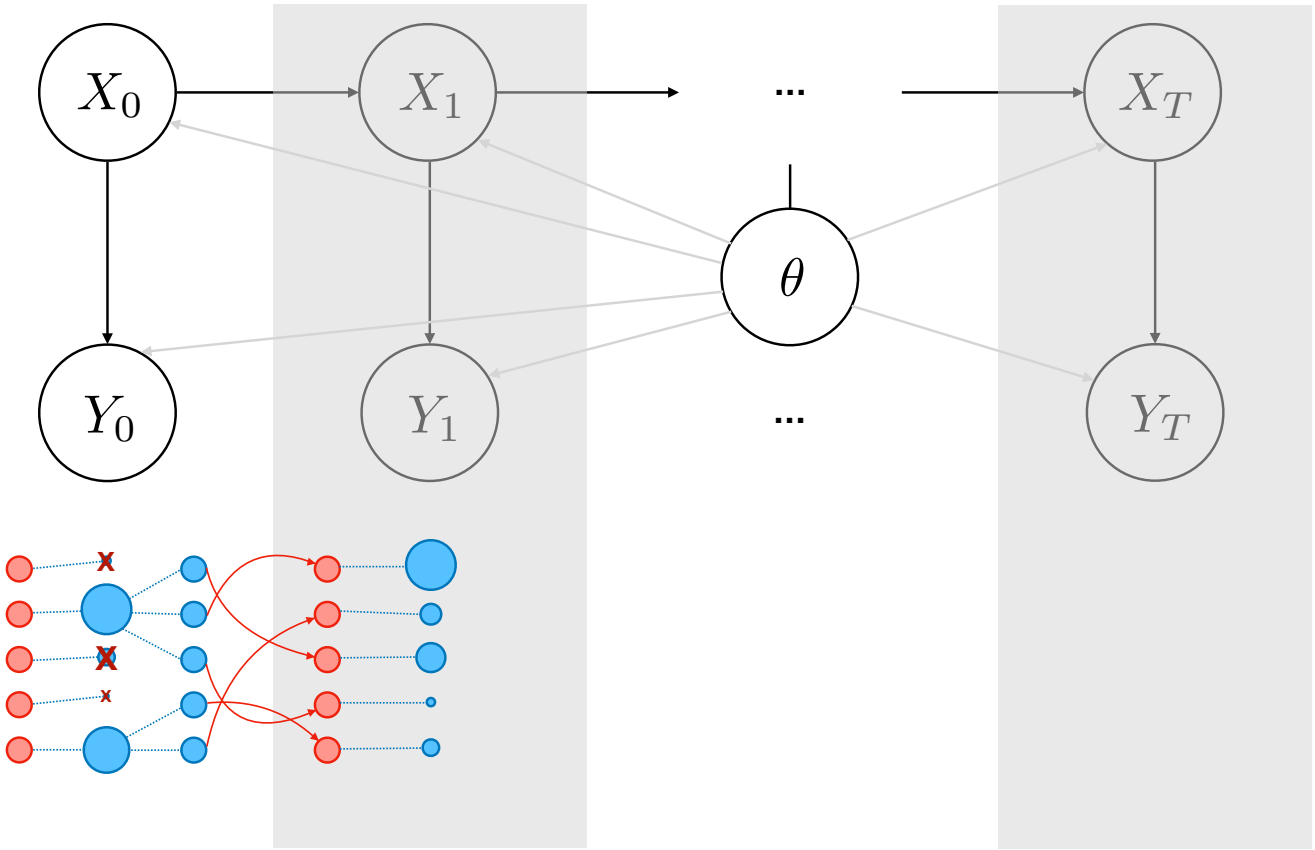
Sequential Monte Carlo



For time $t = 1$ and particle $n \in [1 : N]$

$$\text{sample } X_1^n \sim f_{1,\theta}(X_0^{A_0^n}, \cdot)$$

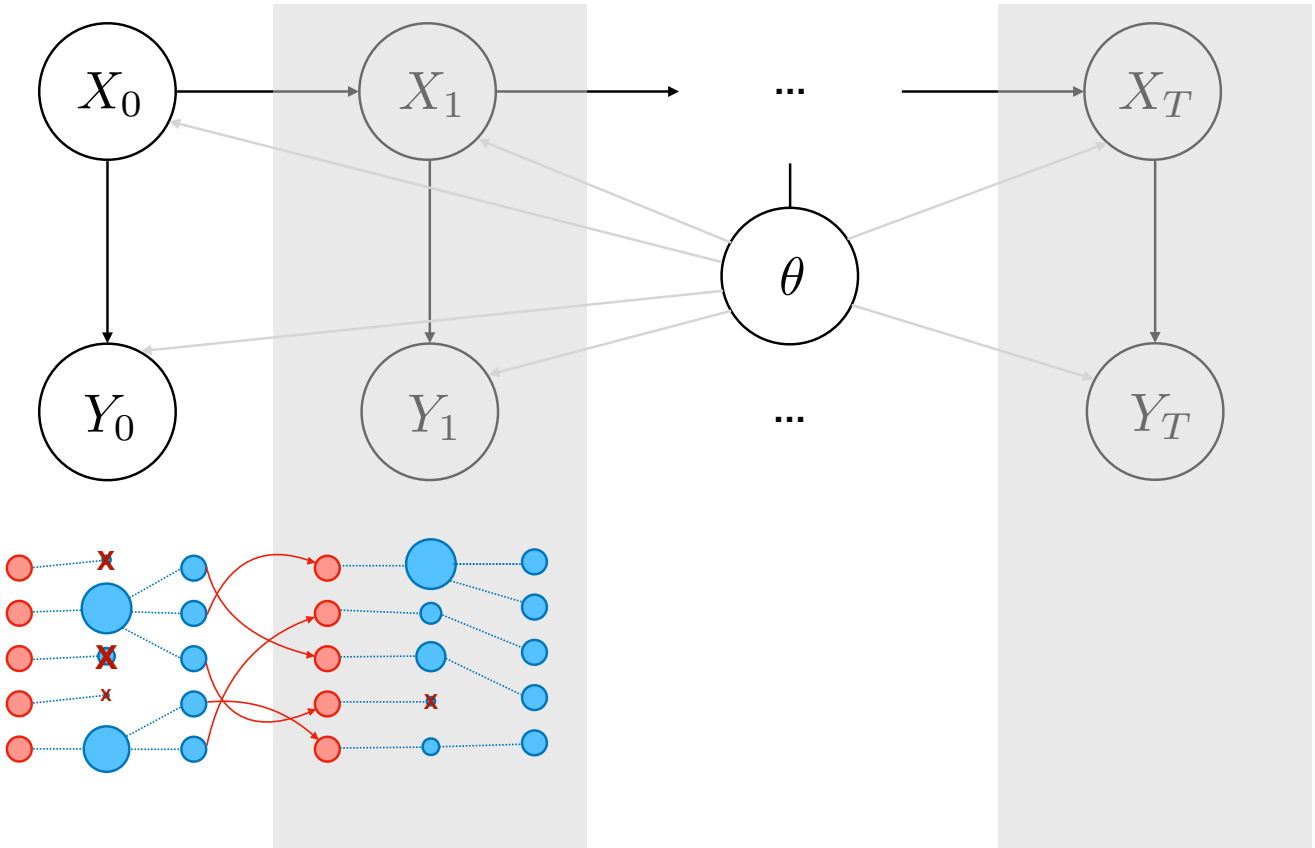
Sequential Monte Carlo



For time $t = 1$ and particle $n \in [1 : N]$

$$\text{weight } W_1^n \propto g_{1,\theta}(X_1^n, y_1)$$

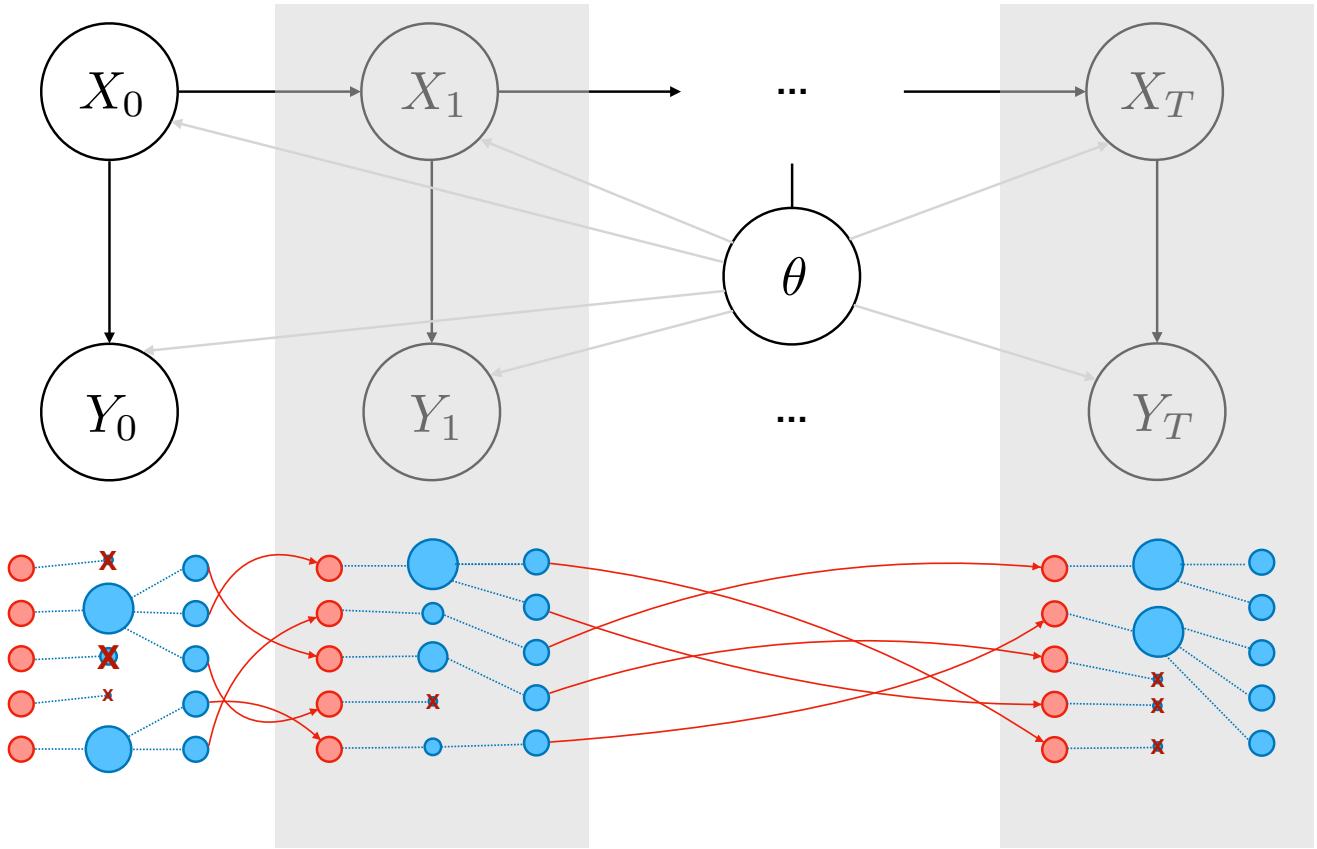
Sequential Monte Carlo



For time $t = 1$ and particle $n \in [1 : N]$

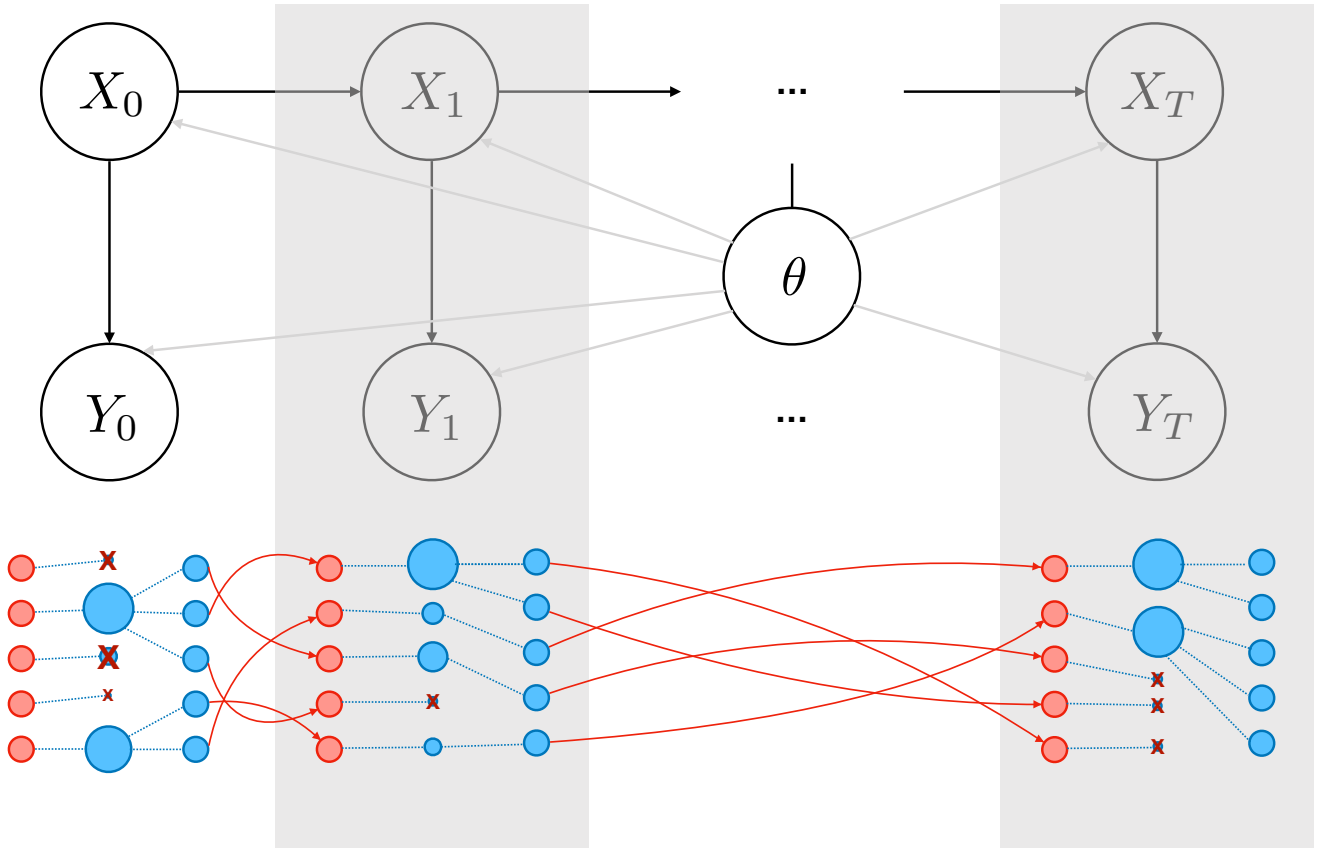
sample ancestor $A_1^n \sim \mathcal{R}\left(W_1^1, \ldots, W_1^N\right)$, resampled particle: $X_1^{A_1^n}$

Sequential Monte Carlo



Repeat for time $t \in [2 : T]$.

Sequential Monte Carlo



Repeat for time $t \in [2 : T]$. Note this is for a given θ!

Ideal Metropolis-Hastings

Cannot run Metropolis-Hastings algorithm to sample from

$$p(\theta|y_{0:T}) \propto p(\theta)p(y_{0:T}|\theta)$$

For iteration $i \geq 1$

1. Sample $\theta^* \sim q(\theta^{(i-1)}, \cdot)$
2. With probability

$$\min\left\{1, \frac{p(\theta^*)p(y_{0:T}|\theta^*)q(\theta^*, \theta^{(i-1)})}{p(\theta^{(i-1)})p(y_{0:T}|\theta^{(i-1)})q(\theta^{(i-1)}, \theta^*)}\right\}$$

set $\theta^{(i)} = \theta^*$, otherwise set $\theta^{(i)} = \theta^{(i-1)}$

Particle marginal Metropolis-Hastings (PMMH)

For iteration $i \geq 1$

1. Sample $\theta^* \sim q(\theta^{(i-1)}, \cdot)$
2. Compute $\hat{p}(y_{0:T}|\theta^*)$ with SMC
2. With probability

$$\min\left\{1, \frac{p(\theta^*)\hat{p}(y_{0:T}|\theta^*)q(\theta^*, \theta^{(i-1)})}{p(\theta^{(i-1)})\hat{p}(y_{0:T}|\theta^{(i-1)})q(\theta^{(i-1)}, \theta^*)}\right\}$$

set $\theta^{(i)} = \theta^*$ and $\hat{p}(y_{0:T}|\theta^{(i)}) = \hat{p}(y_{0:T}|\theta^*)$, otherwise set $\theta^{(i)} = \theta^{(i-1)}$ and $\hat{p}(y_{0:T}|\theta^{(i)}) = \hat{p}(y_{0:T}|\theta^{(i-1)})$

Andrieu, Doucet & Holenstein (2010). *Journal of the Royal Statistical Society: Series B*.

Particle marginal Metropolis-Hastings (PMMH)

- Exact approximation:

$$\frac{1}{m}\sum_{i=1}^{m}\varphi(\theta^{(i)}) \to \int_{\Theta}\varphi(\theta)p(\theta|y_{0:T})d\theta$$

as $m \to \infty$, for any $N \geq 1$

Particle marginal Metropolis-Hastings (PMMH)

- Exact approximation:

$$\frac{1}{m}\sum_{i=1}^{m}\varphi(\theta^{(i)}) \to \int_{\Theta}\varphi(\theta)p(\theta|y_{0:T})d\theta$$

  as $m \to \infty$, for any $N \geq 1$

- Performance depends on the variance of $\hat{p}(y_{0:T}|\theta)$

Andrieu & Vihola (2015). *The Annals of Applied Probability*.

Particle marginal Metropolis-Hastings (PMMH)

- Exact approximation:

$$\frac{1}{m}\sum_{i=1}^{m}\varphi(\theta^{(i)}) \to \int_{\Theta}\varphi(\theta)p(\theta|y_{0:T})d\theta$$

  as $m \to \infty$, for any $N \geq 1$

- Performance depends on the variance of $\hat{p}(y_{0:T}|\theta)$

  Andrieu & Vihola (2015). *The Annals of Applied Probability*.

- Account for computational cost to optimize efficiency

  Sherlock, Thiery, Roberts, & Rosenthal (2015). *The Annals of Statistics*.
  Doucet, Pitt, Deligiannidis & Kohn (2015). *Biometrika*.

Particle marginal Metropolis-Hastings (PMMH)

- Exact approximation:

$$\frac{1}{m}\sum_{i=1}^{m}\varphi(\theta^{(i)}) \to \int_{\Theta}\varphi(\theta)p(\theta|y_{0:T})d\theta$$

  as $m \to \infty$, for any $N \geq 1$

- Performance depends on the variance of $\hat{p}(y_{0:T}|\theta)$

  Andrieu & Vihola (2015). *The Annals of Applied Probability*.

- Account for computational cost to optimize efficiency

  Sherlock, Thiery, Roberts, & Rosenthal (2015). *The Annals of Statistics*.
  Doucet, Pitt, Deligiannidis & Kohn (2015). *Biometrika*.

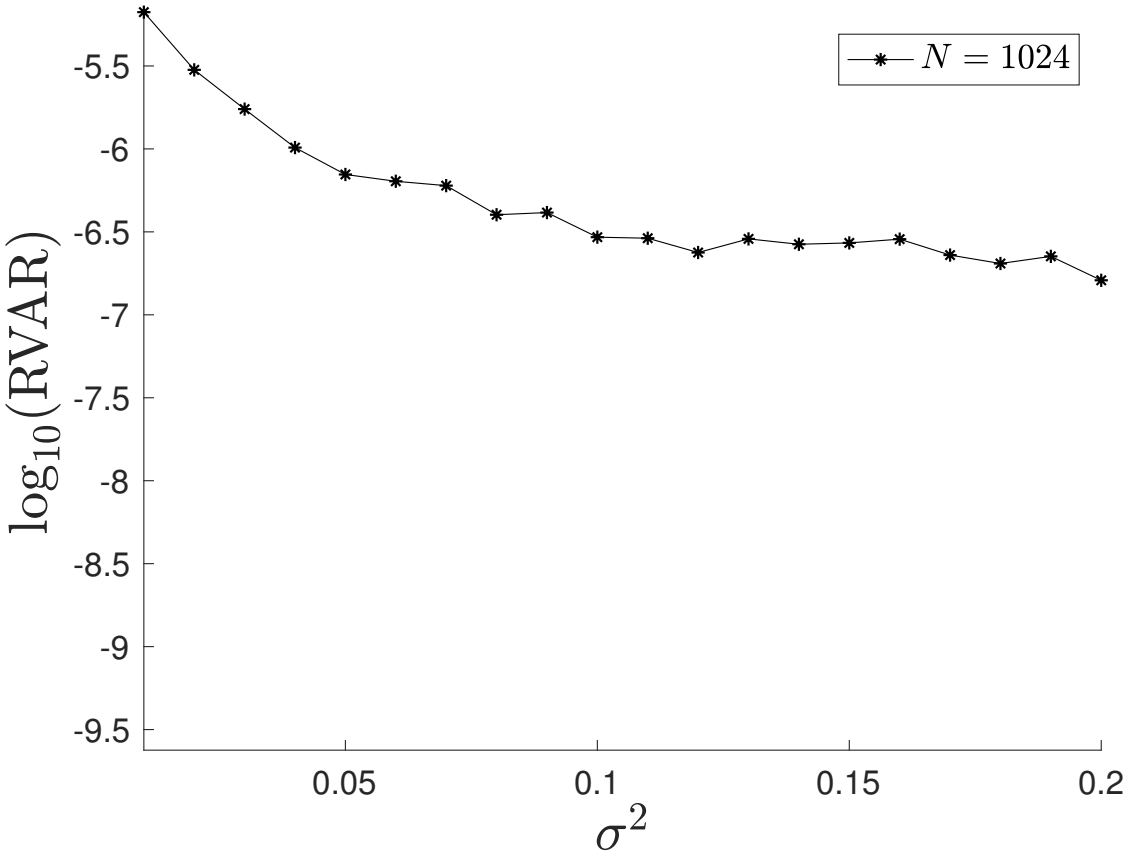
- Proposed method lowers variance of $\hat{p}(y_{0:T}|\theta)$ at fixed cost

Neuroscience example: SMC performance

Relative variance of log-marginal likelihood estimator

$$\sigma^2 \mapsto \mathrm{Var}\left[\frac{\log \hat{p}(y_{0:T}|(\alpha,\sigma^2))}{\log p(y_{0:T}|(\alpha,\sigma^2))}\right], \quad \text{fix } \alpha = 0.99$$

with $N = 1024$

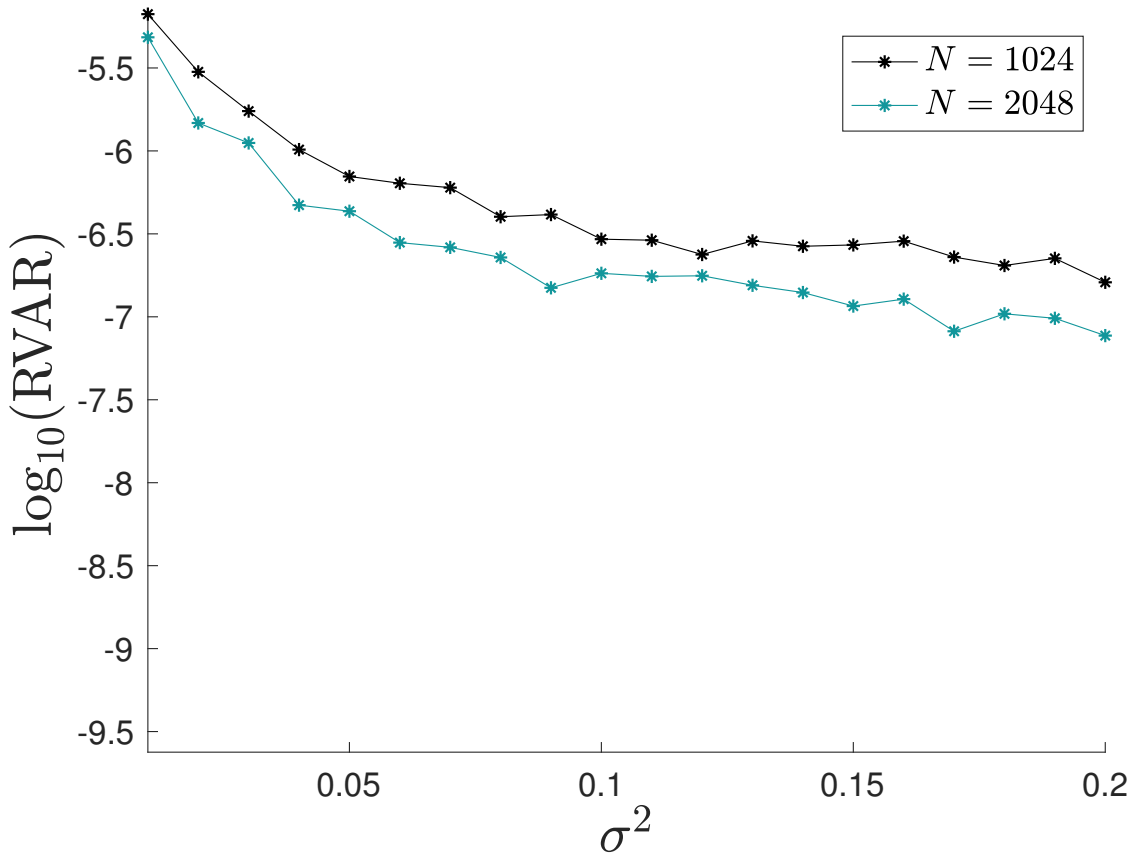


Neuroscience example: SMC performance

Relative variance of log-marginal likelihood estimator

$$\sigma^2 \mapsto \mathrm{Var}\left[\frac{\log \hat{p}(y_{0:T}|(\alpha, \sigma^2))}{\log p(y_{0:T}|(\alpha, \sigma^2))}\right], \quad \text{fix } \alpha = 0.99$$

with $N = 2048$

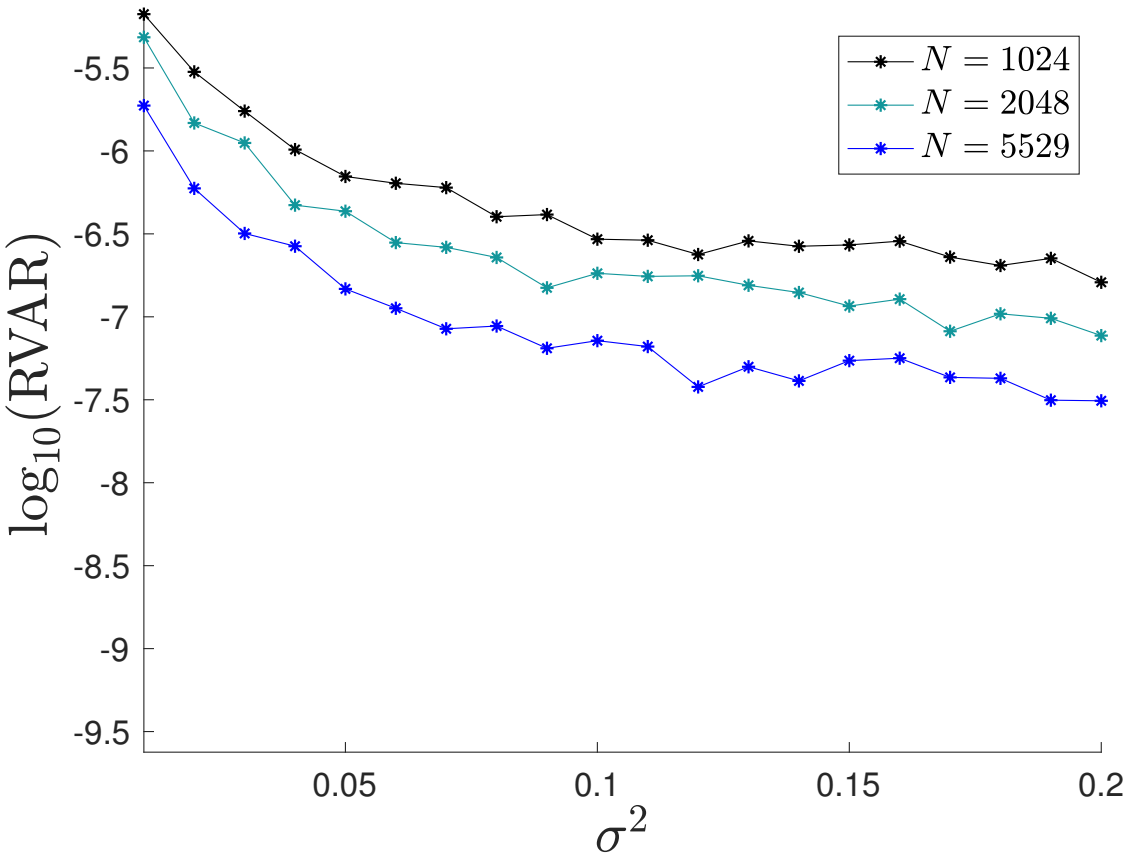


Neuroscience example: SMC performance

Relative variance of log-marginal likelihood estimator

$$\sigma^2 \mapsto \mathrm{Var}\left[\frac{\log \hat{p}(y_{0:T}|(\alpha,\sigma^2))}{\log p(y_{0:T}|(\alpha,\sigma^2))}\right], \quad \text{fix } \alpha = 0.99$$

with $N = 5529$

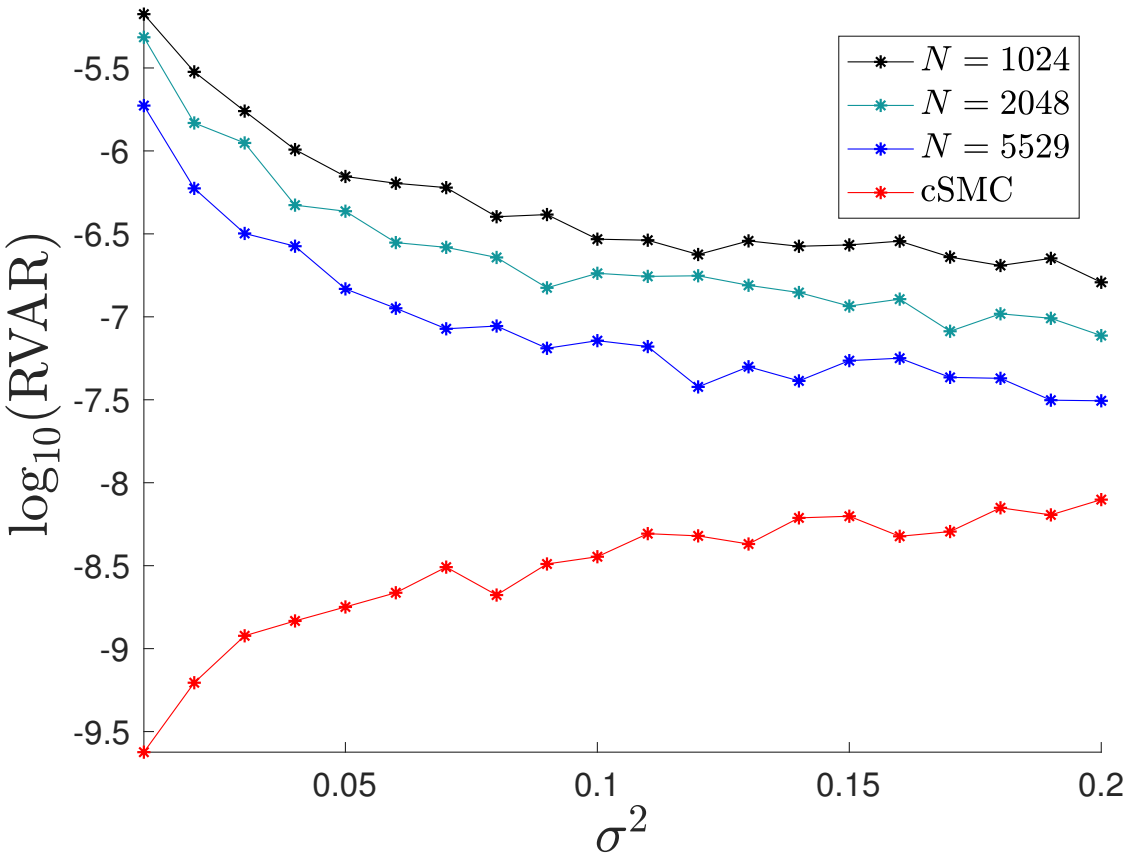


Neuroscience example: SMC performance

Relative variance of log-marginal likelihood estimator

$$\sigma^2 \mapsto \mathrm{Var}\left[\frac{\log \hat{p}(y_{0:T}|(\alpha,\sigma^2))}{\log p(y_{0:T}|(\alpha,\sigma^2))}\right], \quad \text{fix } \alpha = 0.99$$

with $N = 5529$ vs. controlled SMC

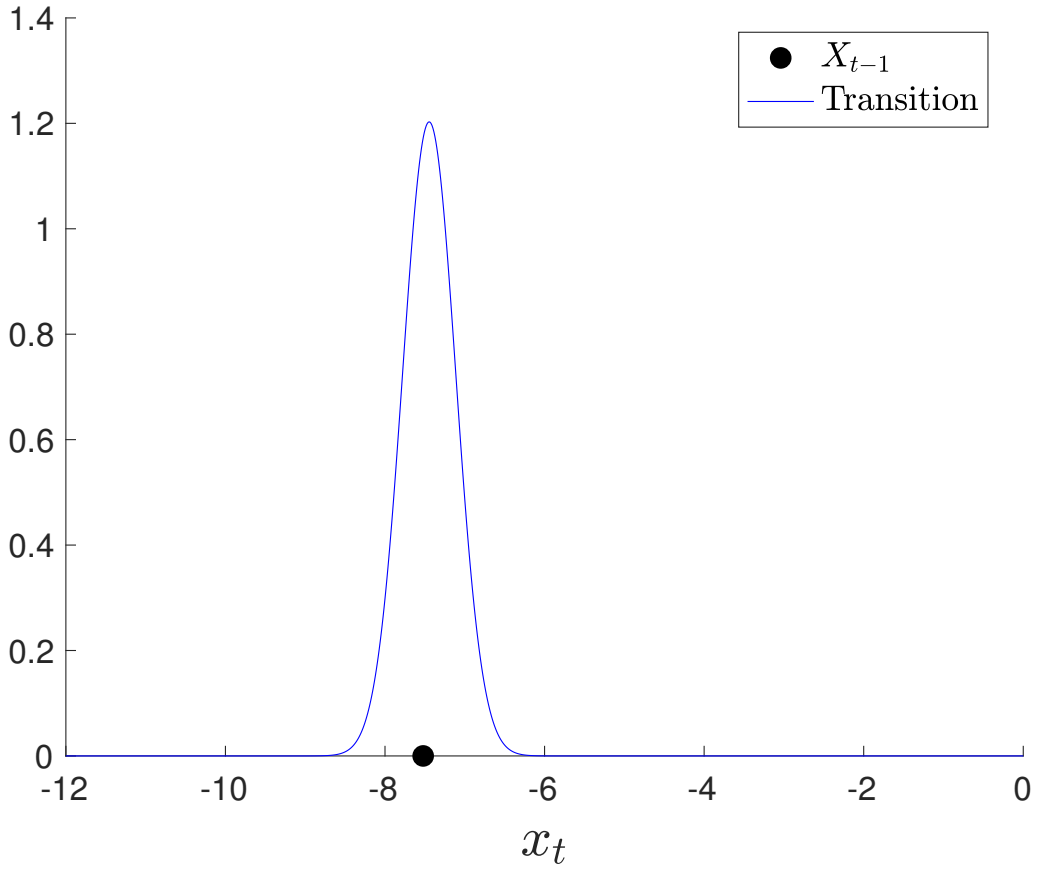


Mismatch between dynamics and observations

SMC weights samples from model dynamics

$$X_t | X_{t-1} \sim \mathcal{N}(\alpha X_{t-1}, \sigma^2)$$

without taking observations into account

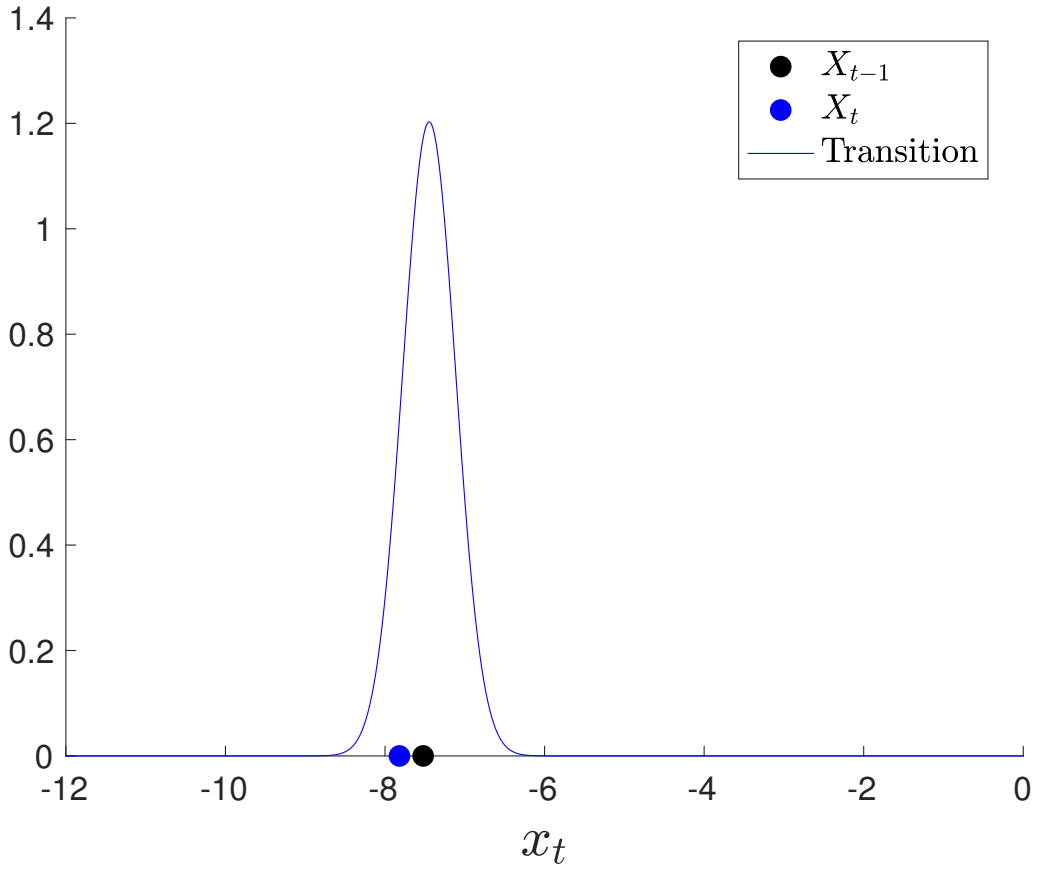


Mismatch between dynamics and observations

SMC weights samples from model dynamics

$$X_t | X_{t-1} \sim \mathcal{N}(\alpha X_{t-1}, \sigma^2)$$

without taking observations into account

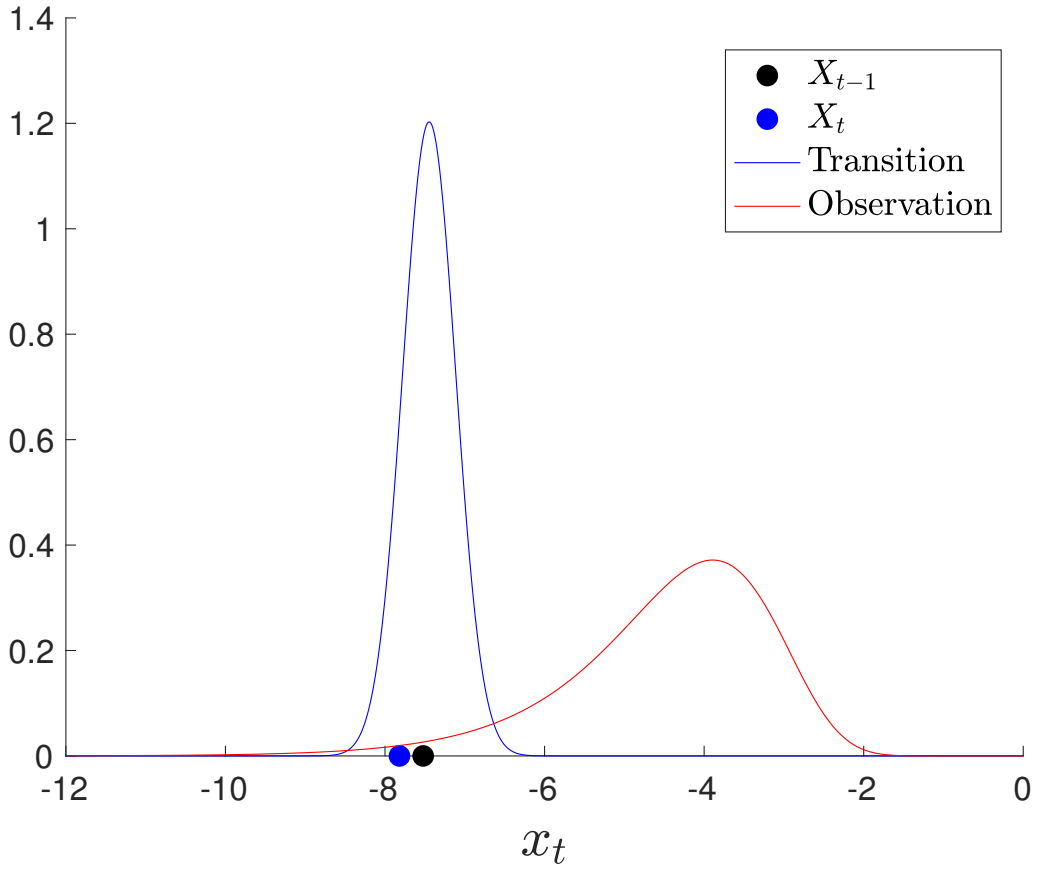


Mismatch between dynamics and observations

SMC weights samples from model dynamics

$$X_t | X_{t-1} \sim \mathcal{N}(\alpha X_{t-1}, \sigma^2)$$

without taking observations into account

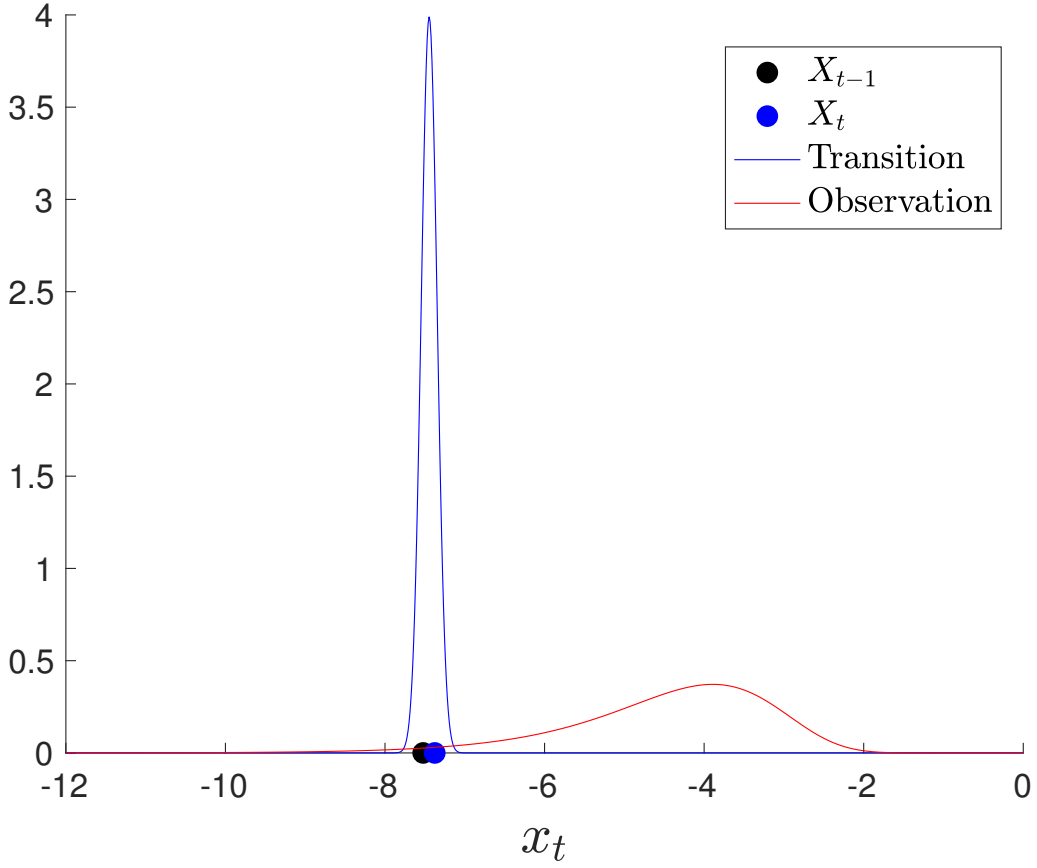


Mismatch between dynamics and observations

SMC weights samples from model dynamics

$$X_t | X_{t-1} \sim \mathcal{N}(\alpha X_{t-1}, \sigma^2)$$

without taking observations into account



Outline

Optimal dynamics

- Fix θ and suppress notational dependency

Optimal dynamics

- Fix θ and suppress notational dependency
- Sampling from smoothing distribution $p(x_{0:T}|y_{0:T})$

$$X_0 \sim p(x_0|y_{0:T}), \quad X_t|X_{t-1} \sim p(x_t|x_{t-1}, y_{t:T}), \quad t \in [1:T]$$

Optimal dynamics

- Fix θ and suppress notational dependency
- Sampling from smoothing distribution $p(x_{0:T}|y_{0:T})$

$$X_0 \sim p(x_0|y_{0:T}), \quad X_t|X_{t-1} \sim p(x_t|x_{t-1}, y_{t:T}), \quad t \in [1:T]$$

- Define **backward information filter** $\psi_t^*(x_t) = p(y_{t:T}|x_t)$, then

$$p(x_0|y_{0:T}) = \frac{\mu(x_0)\psi_0^*(x_0)}{\mu(\psi_0^*)}$$

with $\mu(\psi_0^*) = \int_{\mathcal{X}} \psi_0^*(x_0)\mu(x_0)dx_0$, and

$$p(x_t|x_{t-1}, y_{t:T}) = \frac{f_t(x_{t-1}, x_t)\psi_t^*(x_t)}{f_t(\psi_t^*)(x_{t-1})}$$

with $f_t(\psi_t^*)(x_{t-1}) = \int_{\mathcal{X}} \psi_t^*(x_t)f_t(x_{t-1}, x_t)dx_t$

Controlled state space model

- Given a **policy**

$$\psi = (\psi_0, \ldots, \psi_T)$$

  i.e. positive and bounded functions

Controlled state space model

- Given a **policy**

$$\psi = (\psi_0, \ldots, \psi_T)$$

  i.e. positive and bounded functions

- Construct ψ-**controlled dynamics**

$$X_0 \sim \mu^\psi, \quad X_t | X_{t-1} \sim f_t^\psi(X_{t-1}, \cdot), \quad t \in [1 : T]$$

  where

$$\mu^\psi(x_0) = \frac{\mu(x_0)\psi_0(x_0)}{\mu(\psi_0)}, \quad f_t^\psi(x_{t-1}, x_t) = \frac{f_t(x_{t-1}, x_t)\psi_t(x_t)}{f_t(\psi_t)(x_{t-1})}$$

Controlled state space model

- Given a **policy**

$$\psi = (\psi_0, \ldots, \psi_T)$$

  i.e. positive and bounded functions

- Construct ψ-**controlled dynamics**

$$X_0 \sim \mu^\psi, \quad X_t | X_{t-1} \sim f_t^\psi(X_{t-1}, \cdot), \quad t \in [1 : T]$$

  where

$$\mu^\psi(x_0) = \frac{\mu(x_0)\psi_0(x_0)}{\mu(\psi_0)}, \quad f_t^\psi(x_{t-1}, x_t) = \frac{f_t(x_{t-1}, x_t)\psi_t(x_t)}{f_t(\psi_t)(x_{t-1})}$$

- Introducing ψ-**controlled observation model**

$$Y_t | X_{0:T} \sim g_t^\psi(X_t, \cdot), \quad t \in [0 : T]$$

  gives a ψ-**controlled state space model**

Controlled state space model

- Define **controlled observation densities** $(g_0^\psi, \ldots, g_T^\psi)$ so that

$$p^\psi(x_{0:T}|y_{0:T}) = p(x_{0:T}|y_{0:T}), \quad p^\psi(y_{0:T}) = p(y_{0:T})$$

Controlled state space model

- Define **controlled observation densities** $(g_0^\psi, \ldots, g_T^\psi)$ so that

$$p^\psi(x_{0:T}|y_{0:T}) = p(x_{0:T}|y_{0:T}), \quad p^\psi(y_{0:T}) = p(y_{0:T})$$

- Achieved with

$$g_0^\psi(x_0, y_0) = \frac{\mu(\psi_0) g_0(x_0, y_0) f_1(\psi_1)(x_0)}{\psi_0(x_0)},$$

$$g_t^\psi(x_t, y_t) = \frac{g_t(x_t, y_t) f_{t+1}(\psi_{t+1})(x_t)}{\psi_t(x_t)}, \quad t \in [1 : T-1],$$

$$g_T^\psi(x_T, y_T) = \frac{g_T(x_T, y_T)}{\psi_T(x_T)}$$

Controlled state space model

- Define **controlled observation densities** $(g_0^\psi, \ldots, g_T^\psi)$ so that

$$p^\psi(x_{0:T}|y_{0:T}) = p(x_{0:T}|y_{0:T}), \quad p^\psi(y_{0:T}) = p(y_{0:T})$$

- Achieved with

$$g_0^\psi(x_0, y_0) = \frac{\mu(\psi_0) g_0(x_0, y_0) f_1(\psi_1)(x_0)}{\psi_0(x_0)},$$

$$g_t^\psi(x_t, y_t) = \frac{g_t(x_t, y_t) f_{t+1}(\psi_{t+1})(x_t)}{\psi_t(x_t)}, \quad t \in [1 : T-1],$$

$$g_T^\psi(x_T, y_T) = \frac{g_T(x_T, y_T)}{\psi_T(x_T)}$$

- Requirements on policy ψ
  - Evaluating g_t^ψ tractable

Controlled state space model

- Define **controlled observation densities** $(g_0^\psi, \ldots, g_T^\psi)$ so that

$$p^\psi(x_{0:T}|y_{0:T}) = p(x_{0:T}|y_{0:T}), \quad p^\psi(y_{0:T}) = p(y_{0:T})$$

- Achieved with

$$g_0^\psi(x_0, y_0) = \frac{\mu(\psi_0) g_0(x_0, y_0) f_1(\psi_1)(x_0)}{\psi_0(x_0)},$$

$$g_t^\psi(x_t, y_t) = \frac{g_t(x_t, y_t) f_{t+1}(\psi_{t+1})(x_t)}{\psi_t(x_t)}, \quad t \in [1 : T-1],$$

$$g_T^\psi(x_T, y_T) = \frac{g_T(x_T, y_T)}{\psi_T(x_T)}$$

- Requirements on policy ψ
  - Evaluating g_t^ψ tractable
  - Sampling μ^ψ and f_t^ψ feasible

Neuroscience example

- Gaussian policy for neuroscience example

$$\psi_t(x_t) = \exp\left(-a_t x_t^2 - b_t x_t - c_t\right), \quad (a_t, b_t, c_t) \in \mathbb{R}^3$$

Neuroscience example

- Gaussian policy for neuroscience example

$$\psi_t(x_t) = \exp\left(-a_t x_t^2 - b_t x_t - c_t\right), \quad (a_t, b_t, c_t) \in \mathbb{R}^3$$

- Both requirements satisfied since

$$\mu^{\psi} = \mathcal{N}(-k_0 b_0, k_0), \quad f_t^{\psi}(x_{t-1}, \cdot) = \mathcal{N}(k_t\{\alpha\sigma^{-2} x_{t-1} - b_t\}, k_t)$$

with $k_0 = (1 + 2a_0)^{-1}$ and $k_t = (\sigma^{-2} + 2a_t)^{-1}$

Controlled SMC

- Construct ψ-**controlled SMC** as SMC applied to ψ-controlled state space model

$$X_0 \sim \mu^\psi, \quad X_t | X_{t-1} \sim f_t^\psi(X_{t-1}, \cdot), \quad t \in [1 : T]$$
$$Y_t | X_{0:T} \sim g_t^\psi(X_t, \cdot), \quad t \in [0 : T]$$

Controlled SMC

- Construct ψ-**controlled SMC** as SMC applied to ψ-controlled state space model

$$X_0 \sim \mu^\psi, \quad X_t | X_{t-1} \sim f_t^\psi(X_{t-1}, \cdot), \quad t \in [1 : T]$$
$$Y_t | X_{0:T} \sim g_t^\psi(X_t, \cdot), \quad t \in [0 : T]$$

- Unbiased and consistent marginal likelihood estimator

$$\hat{p}^\psi(y_{0:T}) = \prod_{t=0}^{T} \left\{ \frac{1}{N} \sum_{n=1}^{N} g_t^\psi(X_t^n, y_t) \right\}$$

Controlled SMC

- Construct ψ-**controlled SMC** as SMC applied to ψ-controlled state space model

$$X_0 \sim \mu^\psi, \quad X_t | X_{t-1} \sim f_t^\psi(X_{t-1}, \cdot), \quad t \in [1:T]$$
$$Y_t | X_{0:T} \sim g_t^\psi(X_t, \cdot), \quad t \in [0:T]$$

- Unbiased and consistent marginal likelihood estimator

$$\hat{p}^\psi(y_{0:T}) = \prod_{t=0}^{T} \left\{ \frac{1}{N} \sum_{n=1}^{N} g_t^\psi(X_t^n, y_t) \right\}$$

- Consistent approximation of smoothing distribution

$$\frac{1}{N} \sum_{n=1}^{N} \varphi(X_{0:T}^n) \to \int \varphi(x_{0:T}) p(x_{0:T} | y_{0:T}) dx_{0:T}$$

as $N \to \infty$

Optimal policy

- Policy $\psi_t^*(x_t) = p(y_{t:T}|x_t)$ is optimal since ψ^*-controlled SMC gives

Optimal policy

- Policy $\psi_t^*(x_t) = p(y_{t:T}|x_t)$ is optimal since ψ^*-controlled SMC gives
- ψ^*-controlled SMC gives **independent samples** from smoothing distribution

$$X_{0:T}^n \sim p(x_{0:T}|y_{0:T}), \quad n \in [1:N],$$

and **zero variance** estimator of marginal likelihood for any $N \geq 1$

$$\hat{p}^{\psi^*}(y_{0:T}) = p(y_{0:T})$$

Optimal policy

- Policy $\psi_t^*(x_t) = p(y_{t:T}|x_t)$ is optimal since ψ^*-controlled SMC gives
- ψ^*-controlled SMC gives **independent samples** from smoothing distribution

$$X_{0:T}^n \sim p(x_{0:T}|y_{0:T}), \quad n \in [1:N],$$

and **zero variance** estimator of marginal likelihood for any $N \geq 1$

$$\hat{p}^{\psi^*}(y_{0:T}) = p(y_{0:T})$$

- (Proposition 1) Optimal policy satisfies **backward recursion**

$$\psi_T^*(x_T) = g_T(x_T, y_T),$$
$$\psi_t^*(x_t) = g_t(x_t, y_t) f_{t+1}(\psi_{t+1}^*)(x_t), \quad t \in [T-1:0]$$

Optimal policy

- Policy $\psi_t^*(x_t) = p(y_{t:T}|x_t)$ is optimal since ψ^*-controlled SMC gives
- ψ^*-controlled SMC gives **independent samples** from smoothing distribution

$$X_{0:T}^n \sim p(x_{0:T}|y_{0:T}), \quad n \in [1:N],$$

and **zero variance** estimator of marginal likelihood for any $N \geq 1$

$$\hat{p}^{\psi^*}(y_{0:T}) = p(y_{0:T})$$

- (Proposition 1) Optimal policy satisfies **backward recursion**

$$\psi_T^*(x_T) = g_T(x_T, y_T),$$
$$\psi_t^*(x_t) = g_t(x_t, y_t) f_{t+1}(\psi_{t+1}^*)(x_t), \quad t \in [T-1:0]$$

- Backward recursion typically intractable but can be approximated

Connection to optimal control

- $V_t^* = -\log \psi_t^*$ are the optimal **value** functions of **Kullback-Leibler** control problem

$$\inf_{\psi \in \Psi} \mathrm{KL}\left(p^{\psi}(x_{0:T}) \,\middle|\, p(x_{0:T}|y_{0:T}) \right)$$

Connection to optimal control

- $V_t^* = -\log \psi_t^*$ are the optimal **value** functions of **Kullback-Leibler** control problem

$$\inf_{\psi \in \Psi} \mathrm{KL}\left(p^{\psi}(x_{0:T}) \,\middle|\, p(x_{0:T}|y_{0:T}) \right)$$

- Connection useful for **methodology** and **analysis**

Bertsekas & Tsitsiklis (1996). *Neuro-dynamic programming*.
Tsitsiklis & Van Roy (2001). *IEEE Transactions on Neural Networks*.

Connection to optimal control

- $V_t^* = -\log \psi_t^*$ are the optimal **value** functions of **Kullback-Leibler** control problem

$$\inf_{\psi \in \Psi} \mathrm{KL}\left(p^{\psi}(x_{0:T}) \,\middle|\, p(x_{0:T}|y_{0:T}) \right)$$

- Connection useful for **methodology** and **analysis**

Bertsekas & Tsitsiklis (1996). *Neuro-dynamic programming*.
Tsitsiklis & Van Roy (2001). *IEEE Transactions on Neural Networks*.

- Methods to approximate backward recursion are known as **approximate dynamic programming** (ADP) for finite horizon control problems

Approximate dynamic programming

- First run standard SMC to get $(X_0^n, \ldots, X_T^n), n \in [1 : N]$

Approximate dynamic programming

- First run standard SMC to get $(X_0^n, \ldots, X_T^n), n \in [1:N]$
- For time T, approximate

$$\psi_T^*(x_T) = g_T(x_T, y_T)$$

by **least squares**

$$\hat{\psi}_T = \arg\min_{\xi \in \mathcal{F}} \sum_{n=1}^{N} \{\log \xi(X_T^n) - \log g_T(X_T^n, y_T)\}^2$$

Approximate dynamic programming

- First run standard SMC to get $(X_0^n, \ldots, X_T^n), n \in [1:N]$
- For time T, approximate

$$\psi_T^*(x_T) = g_T(x_T, y_T)$$

by **least squares**

$$\hat{\psi}_T = \arg\min_{\xi \in \mathcal{F}} \sum_{n=1}^{N} \{\log \xi(X_T^n) - \log g_T(X_T^n, y_T)\}^2$$

- For $t \in [T-1:0]$, approximate

$$\psi_t^*(x_t) = g_t(x_t, y_t) f_{t+1}(\psi_{t+1}^*)(x_t)$$

by **least squares** and $\psi_{t+1}^* \approx \hat{\psi}_{t+1}$

$$\hat{\psi}_t = \arg\min_{\xi \in \mathcal{F}} \sum_{n=1}^{N} \left\{\log \xi(X_t^n) - \log g_t(X_t^n, y_t) - \log f_{t+1}(\hat{\psi}_{t+1})(X_t^n)\right\}^2$$

Guarniero, Johansen & Lee (2017). *The iterated auxiliary particle filter.*

Approximate dynamic programming

- (Proposition 3) Error bounds

$$\mathbb{E}\|\hat{\psi}_t - \psi_t^*\| \leq \sum_{s=t}^{T} C_{t-1,s-1} e_s^N$$

where $C_{t,s}$ are **stability constants** and e_t^N are **least squares errors**

Approximate dynamic programming

- (Proposition 3) Error bounds

$$\mathbb{E}\|\hat{\psi}_t - \psi_t^*\| \leq \sum_{s=t}^{T} C_{t-1,s-1} e_s^N$$

where $C_{t,s}$ are **stability constants** and e_t^N are **least squares errors**

- (Theorem 1) As $N \to \infty$, $\hat{\psi}$ converges to **idealized ADP**

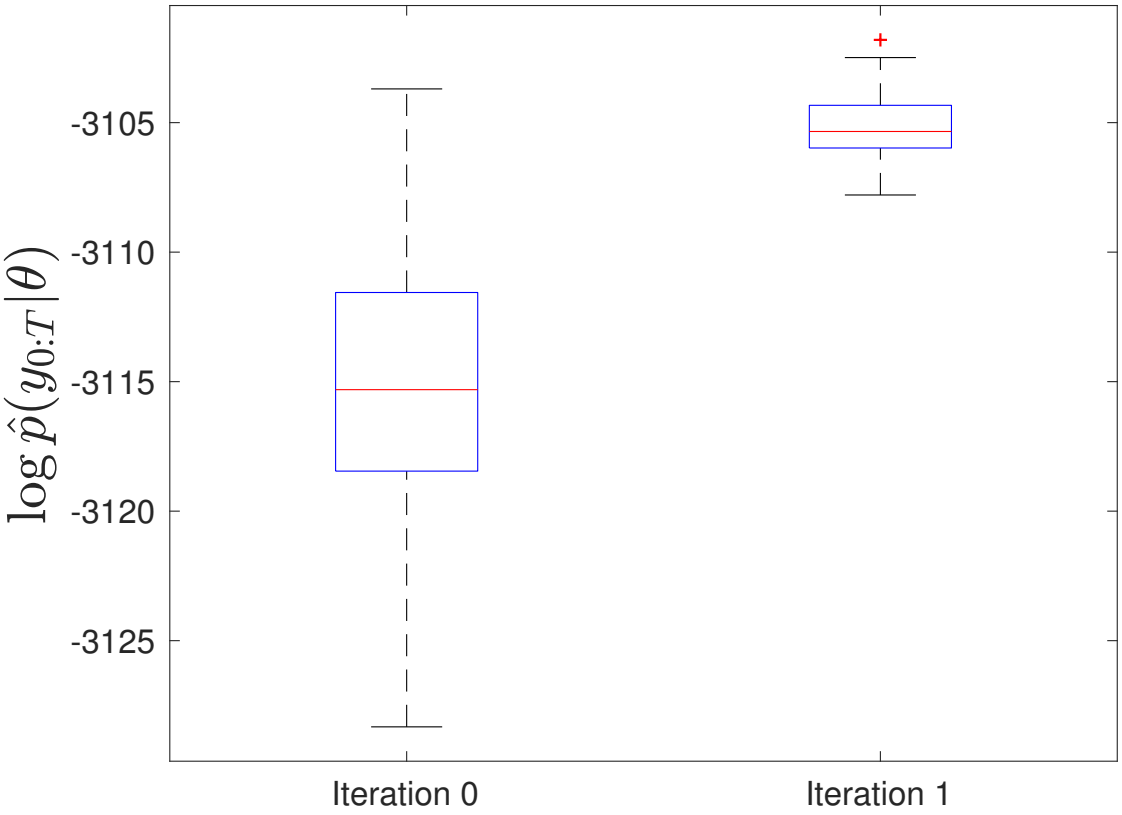
$$\tilde{\psi}_T = \arg\min_{\xi \in \mathcal{F}} \mathbb{E}\left[\{\log \xi(X_T) - \log g_T(X_T, y_T)\}^2\right],$$

$$\tilde{\psi}_t = \arg\min_{\xi \in \mathcal{F}} \mathbb{E}\left[\left\{\log \xi(X_t) - \log g_t(X_t, y_t) - \log f_{t+1}(\tilde{\psi}_{t+1})(X_t)\right\}^2\right]$$

Neuroscience example: controlled SMC

Marginal likelihood estimates of $\hat{\psi}$-controlled SMC with $N = 128$ ($\alpha = 0.99, \sigma^2 = 0.11$)

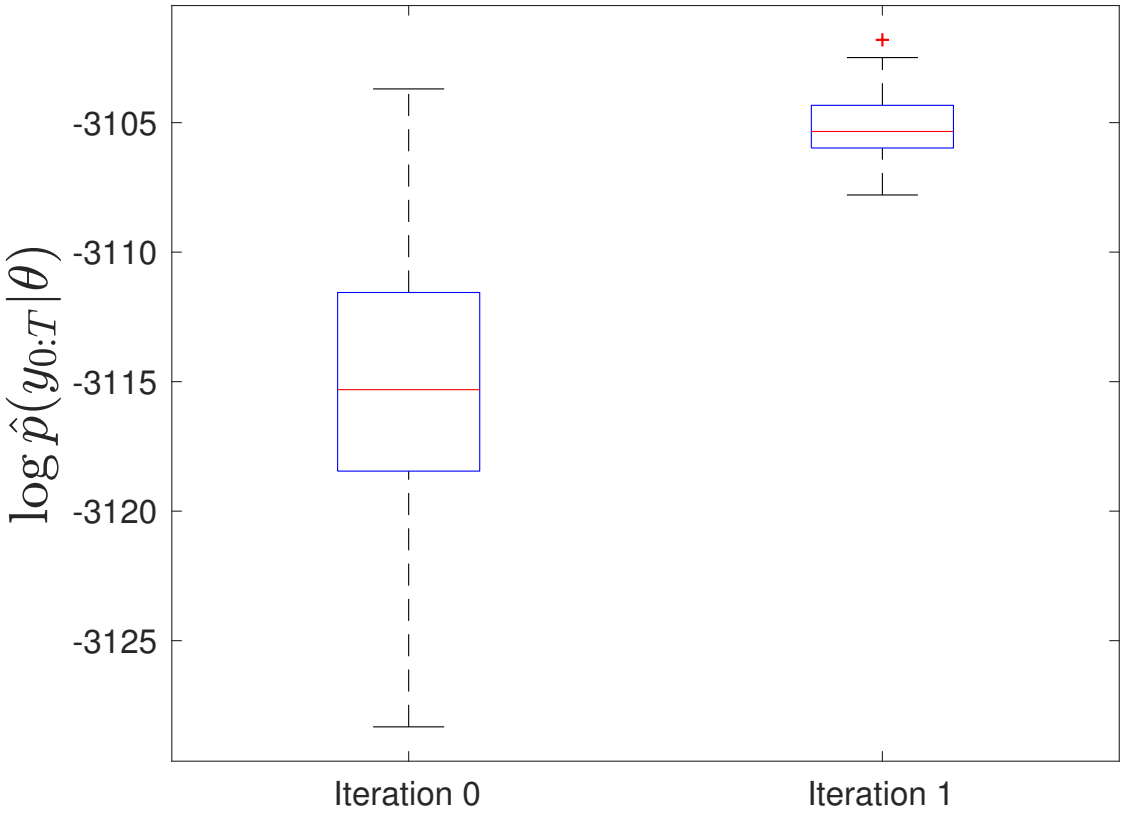
Variance reduction $\approx$ 22 times



Neuroscience example: controlled SMC

Marginal likelihood estimates of $\hat{\psi}$-controlled SMC with $N = 128$ ($\alpha = 0.99, \sigma^2 = 0.11$)

Variance reduction $\approx$ 22 times



We can do better!

Policy refinement

- **Current policy** $\hat{\psi}$ defines the dynamics

$$X_0 \sim \mu^{\hat{\psi}}, \quad X_t | X_{t-1} \sim f_t^{\hat{\psi}}(X_{t-1}, \cdot), \quad t \in [1 : T]$$

Policy refinement

- **Current policy** $\hat{\psi}$ defines the dynamics

$$X_0 \sim \mu^{\hat{\psi}}, \quad X_t | X_{t-1} \sim f_t^{\hat{\psi}}(X_{t-1}, \cdot), \quad t \in [1:T]$$

- Further control these dynamics with policy $\phi = (\phi_0, \ldots \phi_T)$

$$X_0 \sim \left(\mu^{\hat{\psi}}\right)^{\phi}, \quad X_t | X_{t-1} \sim \left(f_t^{\hat{\psi}}\right)^{\phi}(X_{t-1}, \cdot), \quad t \in [1:T]$$

Policy refinement

- **Current policy** $\hat{\psi}$ defines the dynamics

$$X_0 \sim \mu^{\hat{\psi}}, \quad X_t | X_{t-1} \sim f_t^{\hat{\psi}}(X_{t-1}, \cdot), \quad t \in [1:T]$$

- Further control these dynamics with policy $\phi = (\phi_0, \ldots \phi_T)$

$$X_0 \sim \left(\mu^{\hat{\psi}}\right)^{\phi}, \quad X_t | X_{t-1} \sim \left(f_t^{\hat{\psi}}\right)^{\phi}(X_{t-1}, \cdot), \quad t \in [1:T]$$

- Equivalent to controlling model dynamics μ and f_t with policy

$$\hat{\psi} \cdot \phi = (\hat{\psi}_0 \cdot \phi_0, \ldots, \hat{\psi}_T \cdot \phi_T)$$

Policy refinement

- (Proposition 1) **Optimal refinement** of ϕ^* current policy $\hat{\psi}$

$$\phi_T^*(x_T) = g_T^{\hat{\psi}}(x_T, y_T),$$
$$\phi_t^*(x_t) = g_t^{\hat{\psi}}(x_t, y_t) f_{t+1}^{\hat{\psi}}(\phi_{t+1}^*)(x_t), \quad t \in [T-1:0]$$

Policy refinement

- (Proposition 1) **Optimal refinement** of ϕ^* current policy $\hat{\psi}$

$$\phi_T^*(x_T) = g_T^{\hat{\psi}}(x_T, y_T),$$
$$\phi_t^*(x_t) = g_t^{\hat{\psi}}(x_t, y_t) f_{t+1}^{\hat{\psi}}(\phi_{t+1}^*)(x_t), \quad t \in [T-1:0]$$

- Optimal policy $\psi^* = \hat{\psi} \cdot \phi^*$

Policy refinement

- (Proposition 1) **Optimal refinement** of ϕ^* current policy $\hat{\psi}$

$$\phi_T^*(x_T) = g_T^{\hat{\psi}}(x_T, y_T),$$
$$\phi_t^*(x_t) = g_t^{\hat{\psi}}(x_t, y_t) f_{t+1}^{\hat{\psi}}(\phi_{t+1}^*)(x_t), \quad t \in [T-1:0]$$

- Optimal policy $\psi^* = \hat{\psi} \cdot \phi^*$
- Approximate backward recursion to obtain $\hat{\phi} \approx \phi^*$
  - using particles from $\hat{\psi}$-controlled SMC
  - same function class $\mathcal{F}$

Policy refinement

- (Proposition 1) **Optimal refinement** of ϕ^* current policy $\hat{\psi}$

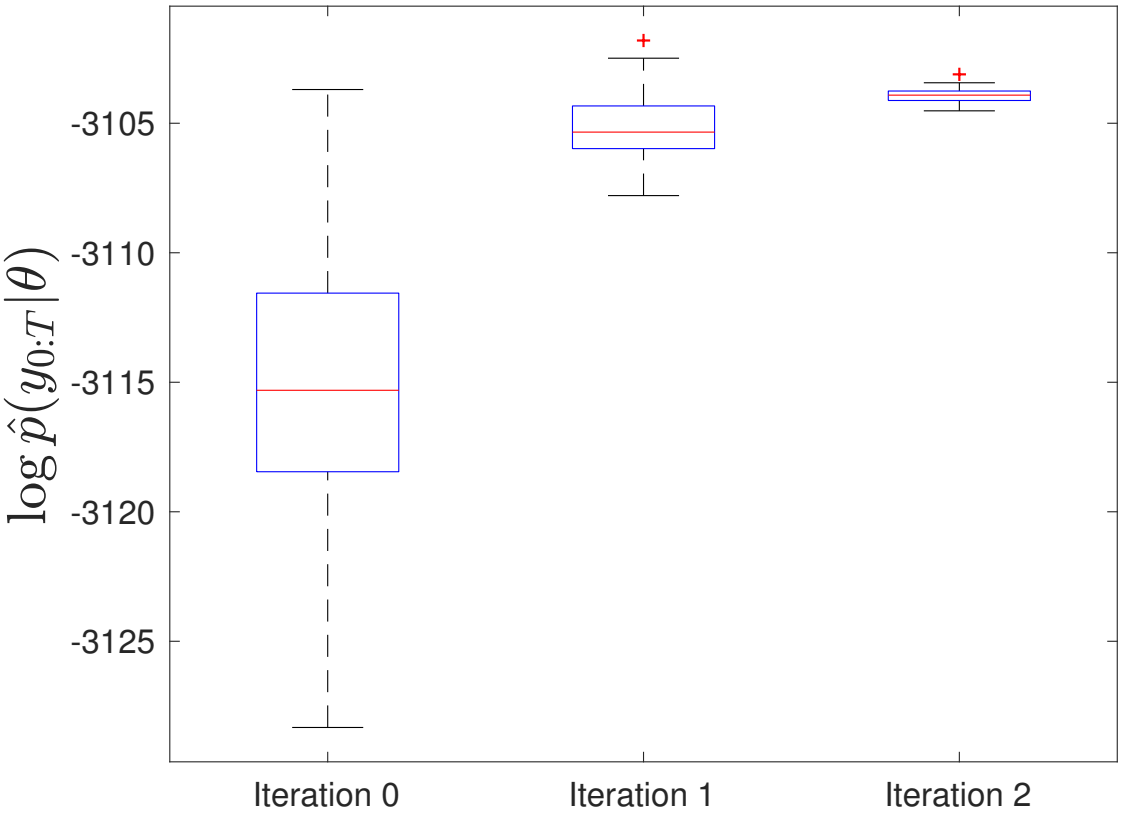
$$\phi_T^*(x_T) = g_T^{\hat{\psi}}(x_T, y_T),$$
$$\phi_t^*(x_t) = g_t^{\hat{\psi}}(x_t, y_t) f_{t+1}^{\hat{\psi}}(\phi_{t+1}^*)(x_t), \quad t \in [T-1:0]$$

- Optimal policy $\psi^* = \hat{\psi} \cdot \phi^*$
- Approximate backward recursion to obtain $\hat{\phi} \approx \phi^*$
  - using particles from $\hat{\psi}$-controlled SMC
  - same function class $\mathcal{F}$
- Run controlled SMC with **refined policy** $\hat{\psi} \cdot \hat{\phi}$

Neuroscience example: controlled SMC

Marginal likelihood estimates of controlled SMC iteration 2 with $N = 128$ ($\alpha = 0.99, \sigma^2 = 0.11$)

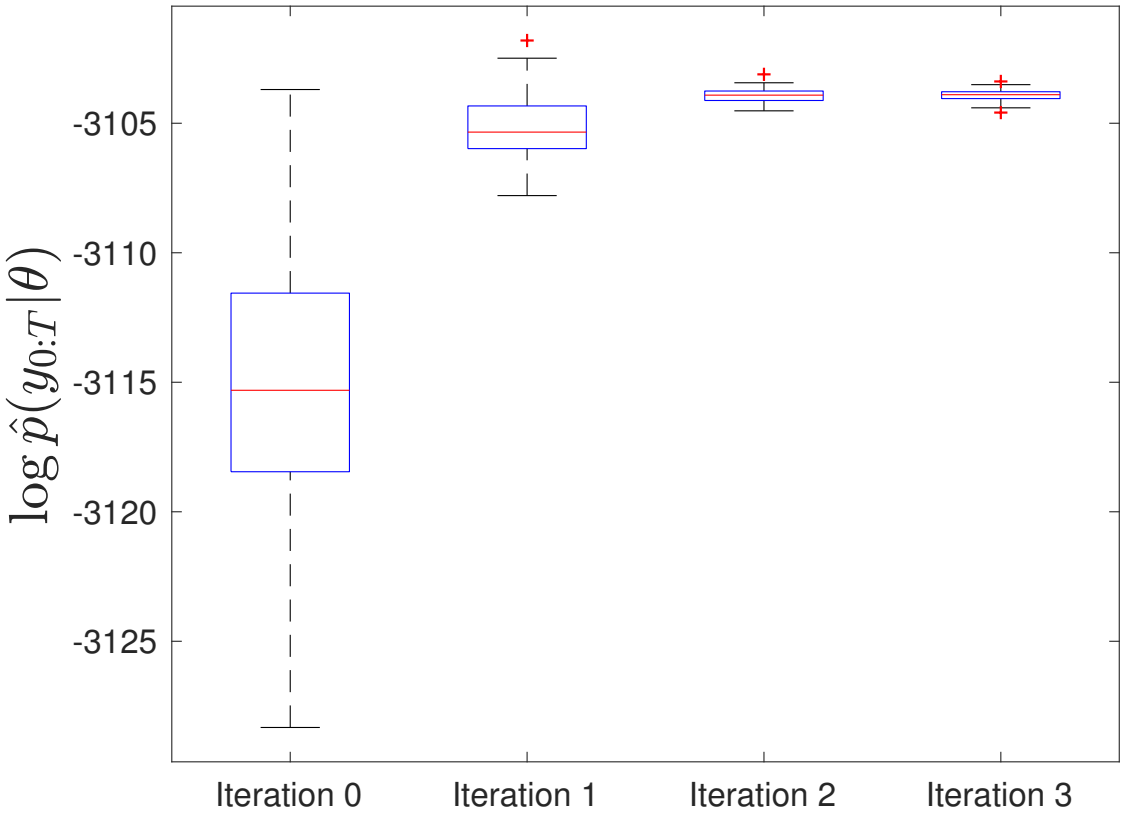
Further variance reduction $\approx$ 24 times



Neuroscience example: controlled SMC

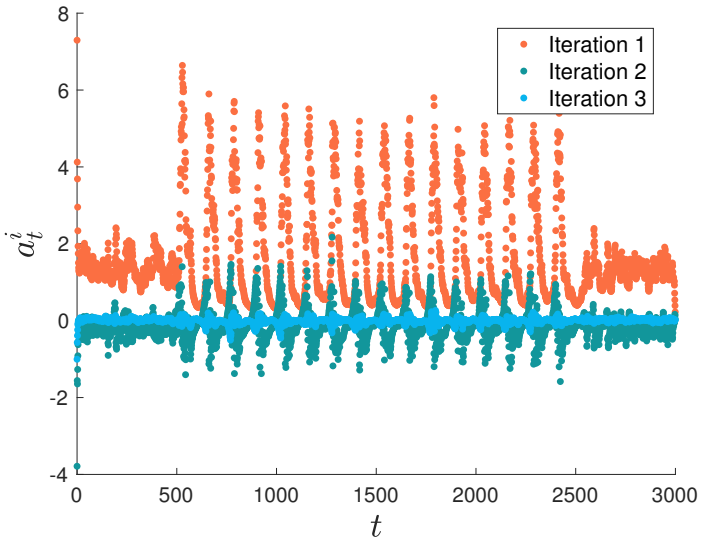
Marginal likelihood estimates of controlled SMC iteration 3 with $N = 128$ ($\alpha = 0.99, \sigma^2 = 0.11$)

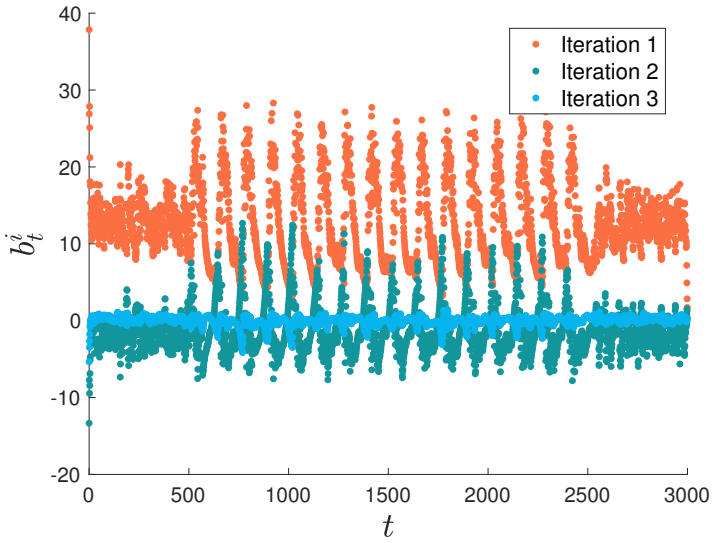
Further variance reduction $\approx$ 1.3 times



Neuroscience example: controlled SMC

Coefficients (a_t^i, b_t^i) of Gaussian approximation estimated at iteration $i \geq 1$





Effect of policy refinement

- **Residual** from ADP when fitting $\hat{\psi}$

$$\varepsilon_t(x_t) = \log \hat{\psi}_t(x_t) - \log g(x_t, y_t) - \log f_{t+1}(\hat{\psi}_{t+1})(x_t)$$

Effect of policy refinement

- **Residual** from ADP when fitting $\hat{\psi}$

$$\varepsilon_t(x_t) = \log \hat{\psi}_t(x_t) - \log g(x_t, y_t) - \log f_{t+1}(\hat{\psi}_{t+1})(x_t)$$

- Performance of $\hat{\psi}$-controlled SMC related to $\|\varepsilon_t\|$

Effect of policy refinement

- **Residual** from ADP when fitting $\hat{\psi}$

$$\varepsilon_t(x_t) = \log \hat{\psi}_t(x_t) - \log g(x_t, y_t) - \log f_{t+1}(\hat{\psi}_{t+1})(x_t)$$

- Performance of $\hat{\psi}$-controlled SMC related to $\|\varepsilon_t\|$
- Next ADP refinement **re-fits residual** (like L^2-boosting)

$$\hat{\phi}_t = \arg\min_{\xi \in \mathcal{F}} \sum_{n=1}^{N} \left\{ \log \xi(X_t^n) - \varepsilon_t(X_t^n) - \log f_{t+1}^{\hat{\psi}}(\hat{\phi}_{t+1})(X_t^n) \right\}^2$$

Bühlmann & Yu (2003). *Journal of the American Statistical Association*.

Effect of policy refinement

- **Residual** from ADP when fitting $\hat{\psi}$

$$\varepsilon_t(x_t) = \log \hat{\psi}_t(x_t) - \log g(x_t, y_t) - \log f_{t+1}(\hat{\psi}_{t+1})(x_t)$$

- Performance of $\hat{\psi}$-controlled SMC related to $\|\varepsilon_t\|$
- Next ADP refinement **re-fits residual** (like L^2-boosting)

$$\hat{\phi}_t = \arg\min_{\xi \in \mathcal{F}} \sum_{n=1}^{N} \left\{ \log \xi(X_t^n) - \varepsilon_t(X_t^n) - \log f_{t+1}^{\hat{\psi}}(\hat{\phi}_{t+1})(X_t^n) \right\}^2$$

Bühlmann & Yu (2003). *Journal of the American Statistical Association*.

Effect of policy refinement

- **Residual** from ADP when fitting $\hat{\psi}$

$$\varepsilon_t(x_t) = \log \hat{\psi}_t(x_t) - \log g(x_t, y_t) - \log f_{t+1}(\hat{\psi}_{t+1})(x_t)$$

- Performance of $\hat{\psi}$-controlled SMC related to $\|\varepsilon_t\|$
- Next ADP refinement **re-fits residual** (like L^2-boosting)

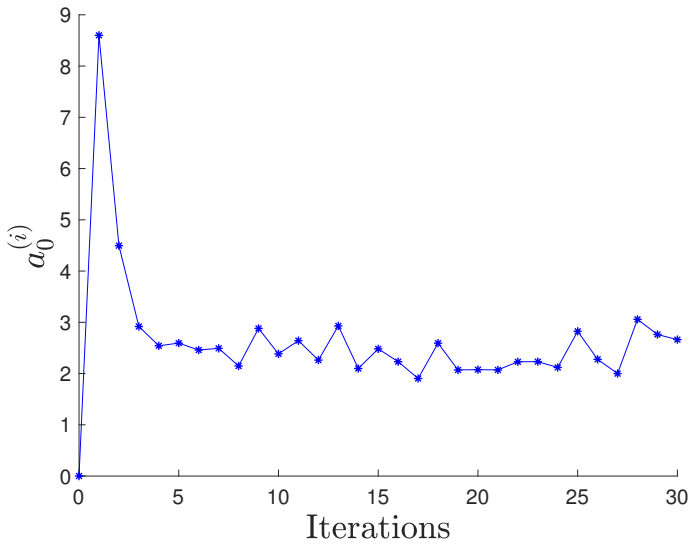
$$\hat{\phi}_t = \arg\min_{\xi \in \mathcal{F}} \sum_{n=1}^{N} \left\{ \log \xi(X_t^n) - \varepsilon_t(X_t^n) - \log f_{t+1}^{\hat{\psi}}(\hat{\phi}_{t+1})(X_t^n) \right\}^2$$

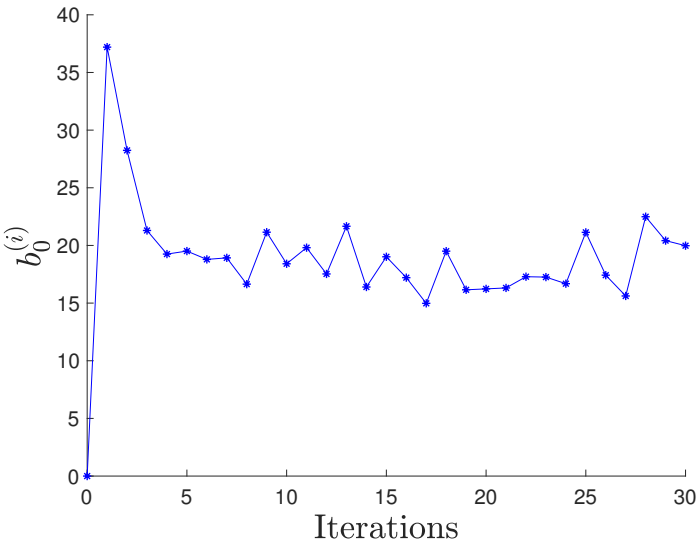
Bühlmann & Yu (2003). *Journal of the American Statistical Association*.

This explains previous plots!

Effect of policy refinement

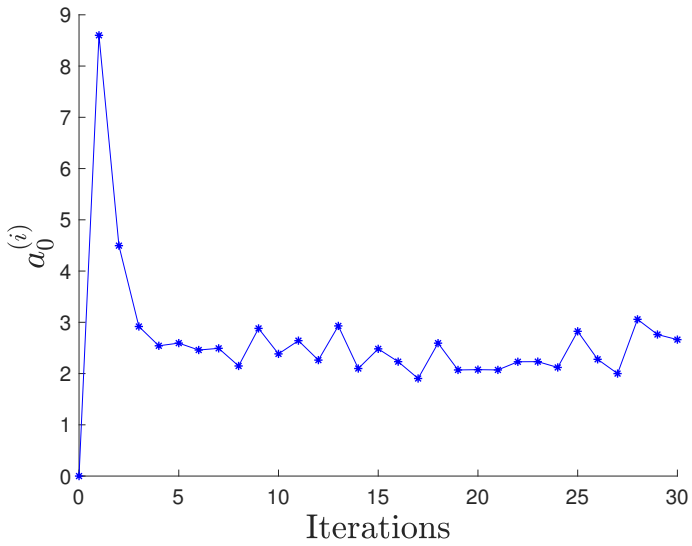
Coefficients of policy at time 0 over 30 iterations

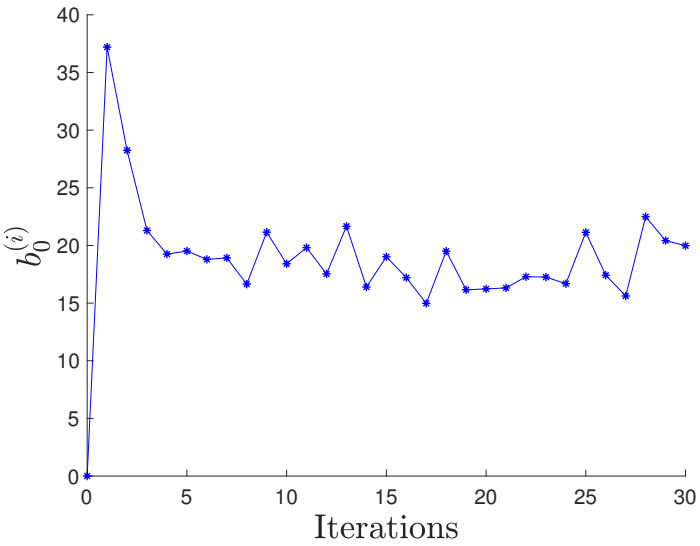




Effect of policy refinement

Coefficients of policy at time 0 over 30 iterations



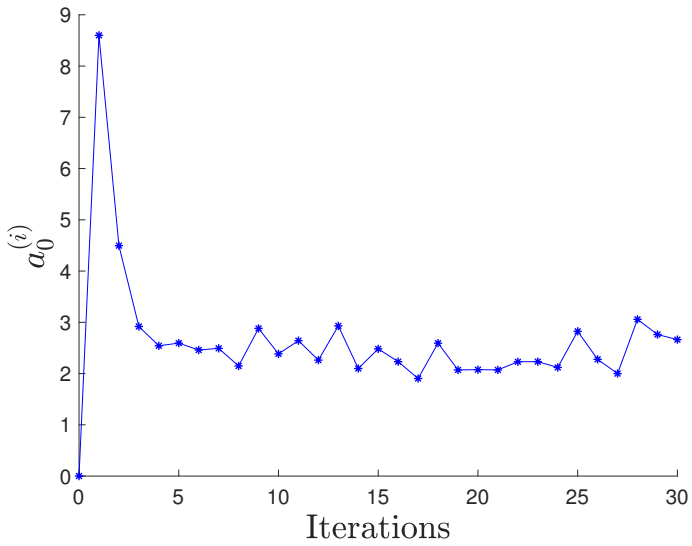


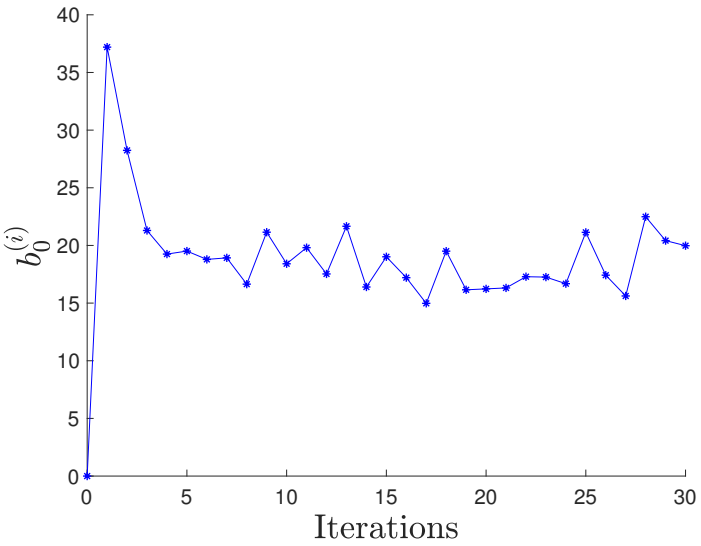
(Theorem 2) Under regularity conditions

- Policy refinement generates a **Markov chain** on **policy space**

Effect of policy refinement

Coefficients of policy at time 0 over 30 iterations



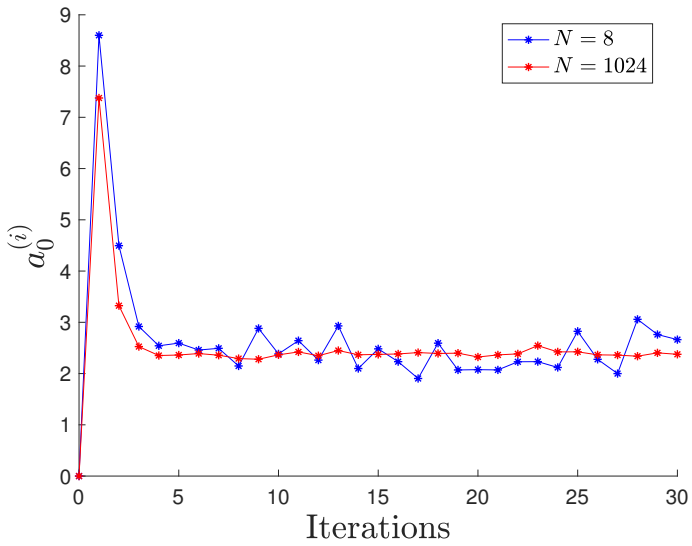


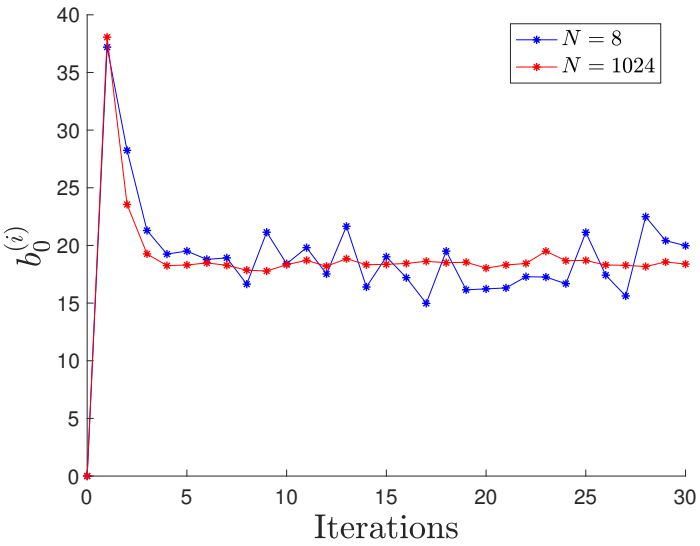
(Theorem 2) Under regularity conditions

- Policy refinement generates a **Markov chain** on **policy space**
- Converges to unique **stationary distribution**

Effect of policy refinement

Coefficients of policy at time 0 over 30 iterations





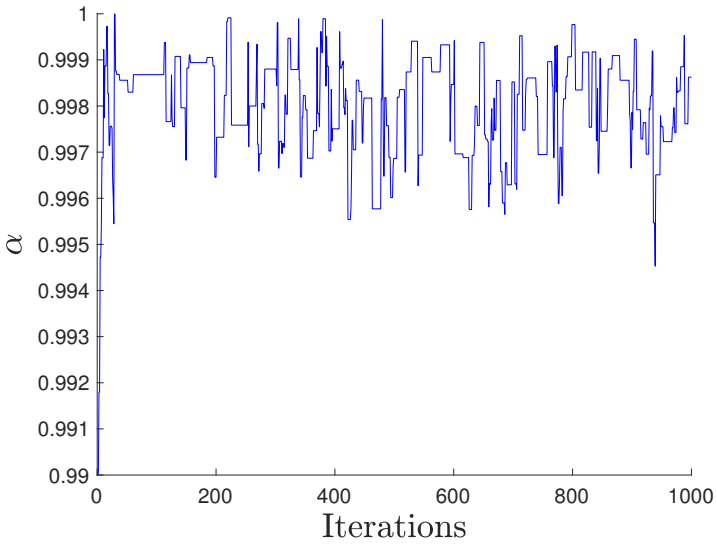
(Theorem 2) Under regularity conditions

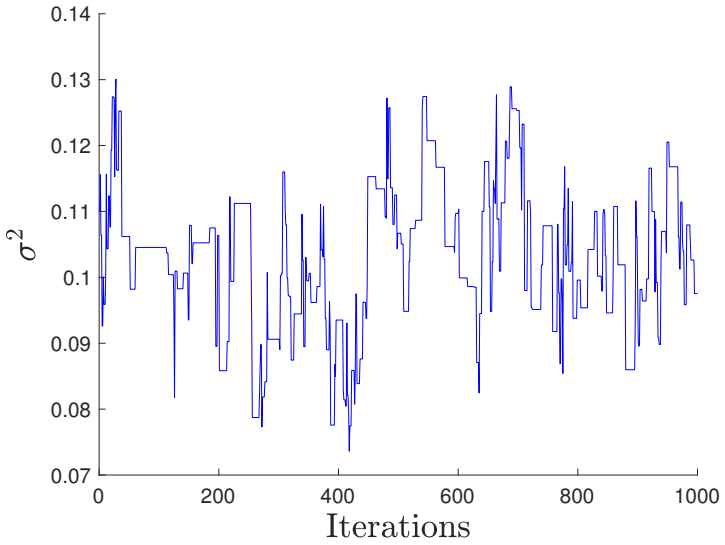
- Policy refinement generates a **Markov chain** on **policy space**
- Converges to unique **stationary distribution**
- Characterization of stationary distribution as $N \to \infty$

Outline

Neuroscience example: PMMH performance

Trace plots of particle marginal Metropolis-Hastings chain





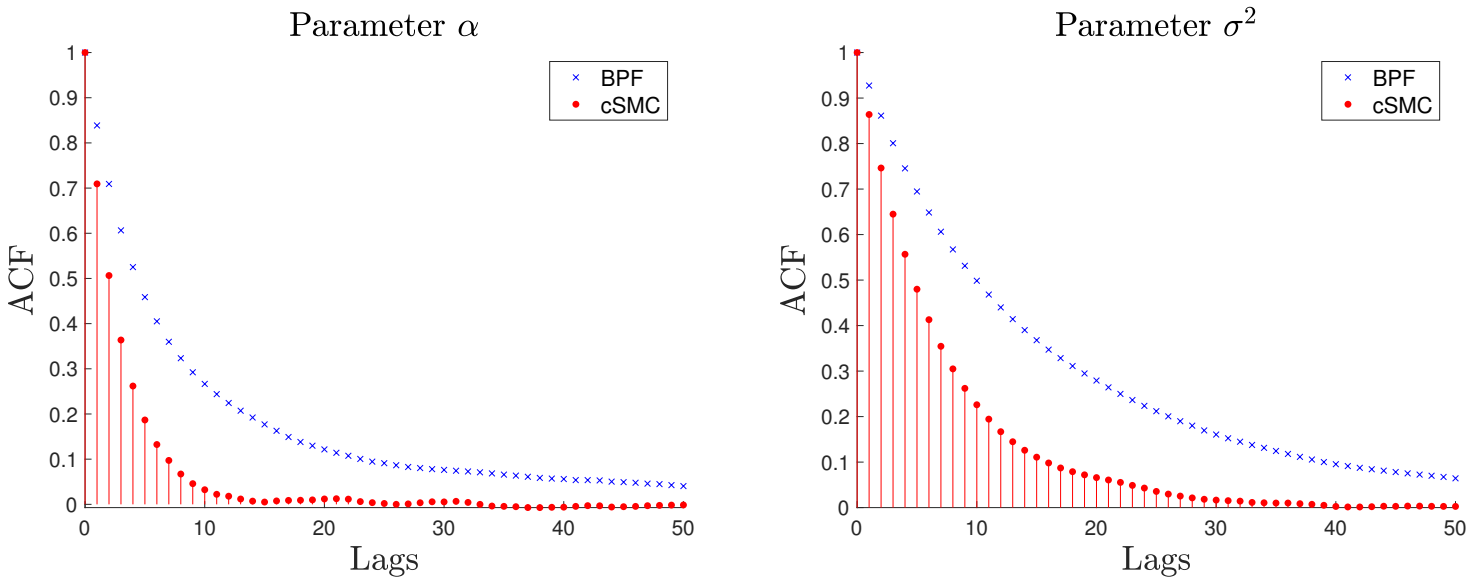
BPF: $N = 5529$

cSMC: $N = 128$, 3 refinements

Each iteration takes 2-3 seconds

Neuroscience example: PMMH

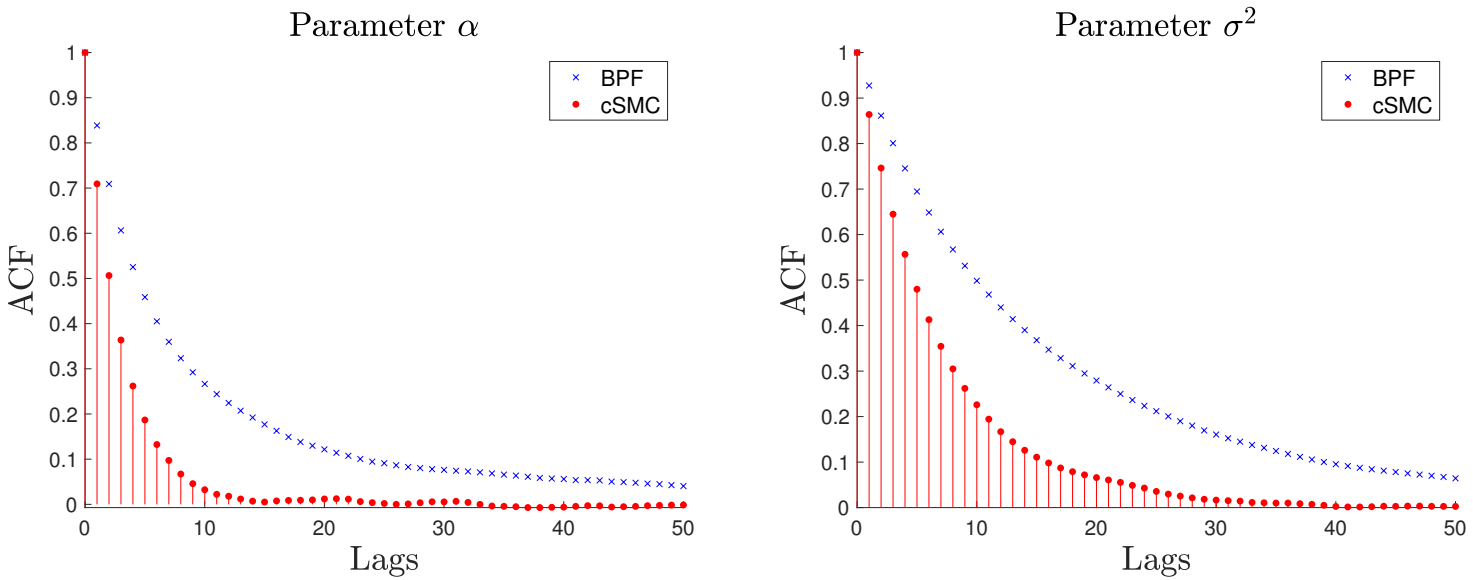
Autocorrelation function of particle marginal Metropolis-Hastings chain



100,000 iterations with BPF (3 days)
$\approx$ 20,000 iterations with cSMC (1/2 day)

Neuroscience example: PMMH

Autocorrelation function of particle marginal Metropolis-Hastings chain



100,000 iterations with BPF (3 days)

$\approx$ 20,000 iterations with cSMC (1/2 day)

$\approx$ 2,000 iterations with cSMC + parallel computation (1.5 hours)

Middleton, Deligiannidis, Doucet & Jacob (2018). *Unbiased Markov chain Monte Carlo for intractable target distributions*.

Outline

Static models

- Extension to **static models**

$$\pi_t(\theta) \propto p(\theta)p(y|\theta)^{\lambda_t}$$

where $0 = \lambda_0 < \cdots < \lambda_T = 1$

Static models

- Extension to **static models**

$$\pi_t(\theta) \propto p(\theta)p(y|\theta)^{\lambda_t}$$

  where $0 = \lambda_0 < \cdots < \lambda_T = 1$
- **SMC samplers** introduces potential

$$G_t(\theta_{t-1}, \theta_t) = \frac{\pi_t(\theta_t)L_{t-1}(\theta_t, \theta_{t-1})}{\pi_{t-1}(\theta_{t-1})M_t(\theta_{t-1}, \theta_t)}$$

  Del Moral, Doucet & Jasra (2006). *JRSSB*.

Static models

- Extension to **static models**

$$\pi_t(\theta) \propto p(\theta)p(y|\theta)^{\lambda_t}$$

  where $0 = \lambda_0 < \cdots < \lambda_T = 1$

- **SMC samplers** introduces potential

$$G_t(\theta_{t-1}, \theta_t) = \frac{\pi_t(\theta_t)L_{t-1}(\theta_t, \theta_{t-1})}{\pi_{t-1}(\theta_{t-1})M_t(\theta_{t-1}, \theta_t)}$$

  Del Moral, Doucet & Jasra (2006). *JRSSB*.

- Annealed importance sampling

M_t is π_t-invariant, L_{t-1} is reversal of $M_t \Longrightarrow G_t(\theta_{t-1}) = \frac{\pi_t}{\pi_{t-1}}(\theta_{t-1})$

Jarzynski (1997); Neal (2001); Chopin (2004).

Static models

- Extension to **static models**

$$\pi_t(\theta) \propto p(\theta)p(y|\theta)^{\lambda_t}$$

  where $0 = \lambda_0 < \cdots < \lambda_T = 1$
- **SMC samplers** introduces potential

$$G_t(\theta_{t-1}, \theta_t) = \frac{\pi_t(\theta_t)L_{t-1}(\theta_t, \theta_{t-1})}{\pi_{t-1}(\theta_{t-1})M_t(\theta_{t-1}, \theta_t)}$$

  Del Moral, Doucet & Jasra (2006). *JRSSB*.
- Annealed importance sampling

M_t is π_t-invariant, L_{t-1} is reversal of $M_t \Longrightarrow G_t(\theta_{t-1}) = \frac{\pi_t}{\pi_{t-1}}(\theta_{t-1})$

  Jarzynski (1997); Neal (2001); Chopin (2004).
- We consider M_t as unadjusted Langevin algorithm (ULA) and $L_{t-1}(\theta_t, \theta_{t-1}) = M_t(\theta_t, \theta_{t-1})$

Static models

- Optimally controlled SMC gives **independent** samples from $p(\theta|y)$ and a **zero variance** estimator of $p(y)$

Static models

- Optimally controlled SMC gives **independent** samples from $p(\theta|y)$ and a **zero variance** estimator of $p(y)$

- Policy for Cox point process model

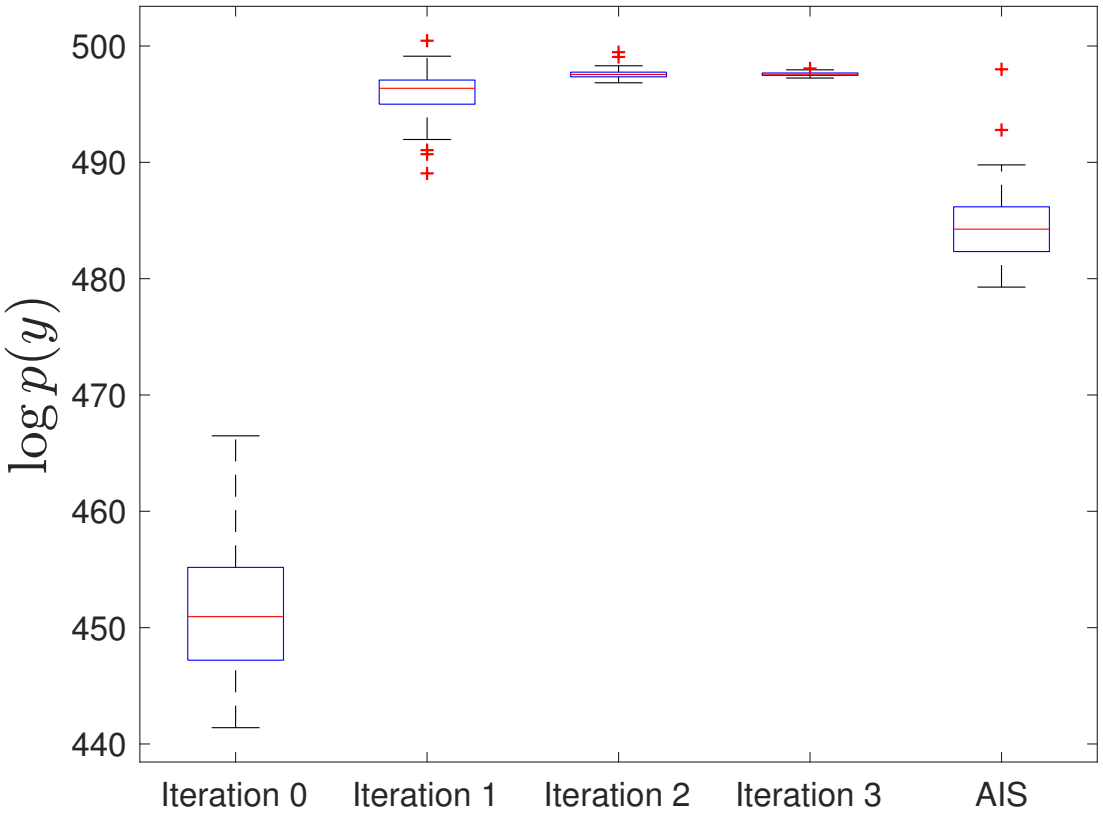
$$\psi_t(\theta_{t-1}, \theta_t) = \exp\left\{-\theta_t^T A_t \theta_t - \theta_t^T b_t - c_t + (\lambda_t - \lambda_{t-1}) \log p(y|\theta_{t-1})\right\}$$

for $A_t \in \mathbb{R}^{d \times d}$ diagonal, $b_t \in \mathbb{R}^d$, $c_t \in \mathbb{R}$

Static models

Model evidence estimates of Cox point process model in 900 dimensions

Variance reduction $\approx$ 370 times compared to AIS



Concluding remarks

- Extensions:
  - Online filtering
  - Relax requirements on policies

Concluding remarks

- Extensions:
  - Online filtering
  - Relax requirements on policies

- Controlled sequential Monte Carlo.
  Heng, Bishop, Deligiannidis & Doucet. arXiv:1708.08396.

Concluding remarks

- Extensions:
  - Online filtering
  - Relax requirements on policies

- Controlled sequential Monte Carlo.
  Heng, Bishop, Deligiannidis & Doucet. arXiv:1708.08396.

- MATLAB code:
  `https://github.com/jeremyhengjm/controlledSMC`