

# Asymptotic Genealogies of Sequential Monte Carlo Algorithms

**Suzie Brown**

University of Warwick, U.K.

with Paul Jenkins, Adam Johansen & Jere Koskela

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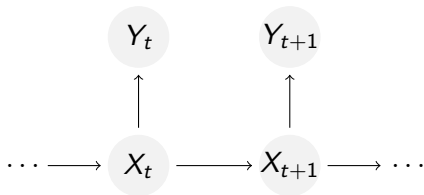
# Outline

1. Sequential Monte Carlo
2. Resampling & Genealogies
3. Results
4. Examples

# Sequential Monte Carlo

- ▶ Monte Carlo = approximating probability distributions via sampling
- ▶ Sequence of probability distributions
- ▶ Dimension of distributions increases along the sequence
- ▶ Strong dependence between consecutive distributions

# State space models

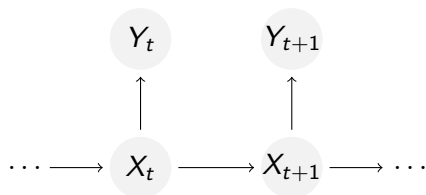


$$X_0 \sim \mu(\cdot)$$

$$X_{t+1} \mid X_t$$

$$Y_t \mid X_t$$

# State space models



$$X_0 \sim \mu(\cdot)$$

$$X_{t+1} \mid X_t$$

$$Y_t \mid X_t$$

Inference problems ( $s < t$ ):

$$p(x_t \mid y_{1:s}) \quad \text{"prediction"}$$

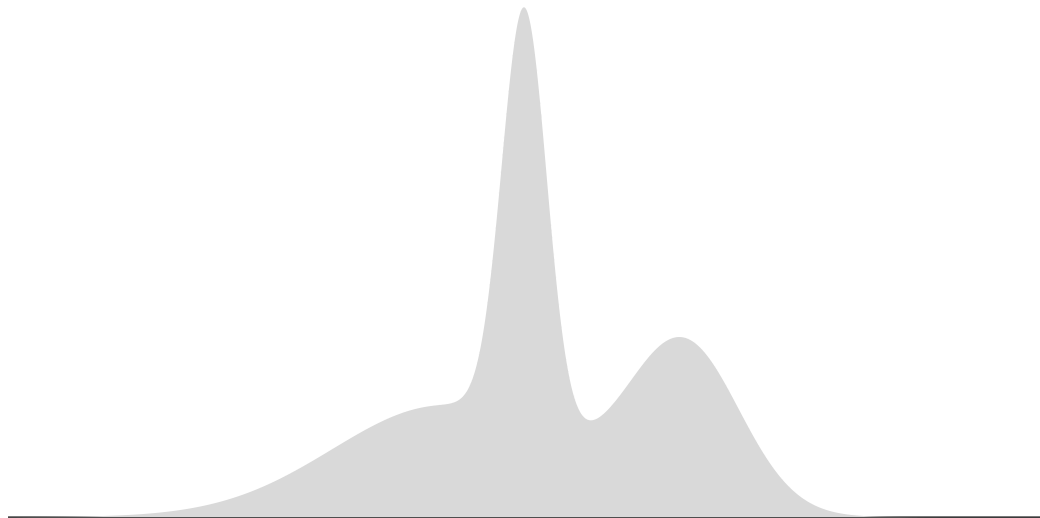
$$p(x_t \mid y_{1:t}) \quad \text{"filtering"}$$

$$p(x_s \mid y_{1:t}) \quad \text{"smoothing"}$$

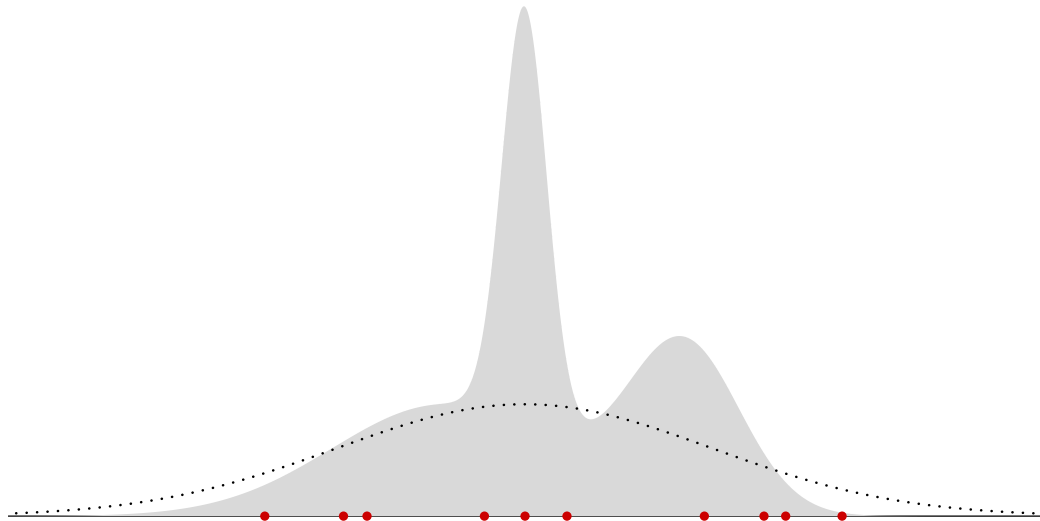
# State space models

- ▶ **Kalman filter** and **Rauch-Tung-Striebel smoother** give exact solutions, but only for linear Gaussian models
- ▶ **Markov chain Monte Carlo** fails due to high dimension and high correlation between dimensions
- ▶ **Sequential Monte Carlo** has computational complexity that is linear in  $t$ , and can update posteriors on-line

# Importance sampling

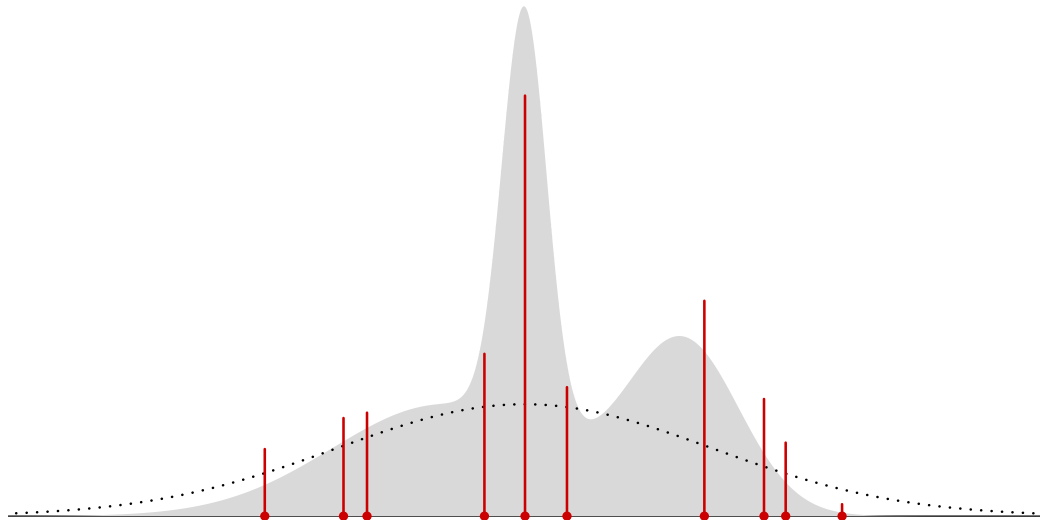


# Importance sampling





# Importance sampling

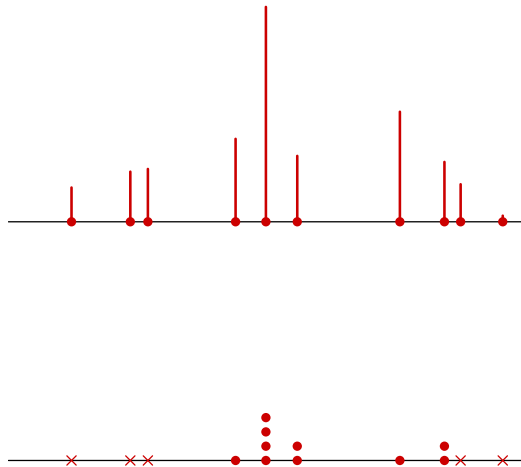


# Sequential importance sampling

- ▶ Idea: use weighted samples from one time step to construct a proposal for the next step
- ▶ Multiplying weights over time causes *weight degeneracy*
- ▶ Can avoid this problem by resampling

# Resampling

Stochastically map continuous weights  $(w_t^{(1)}, \dots, w_t^{(N)})$  to discrete offspring counts  $(\nu_t^{(1)}, \dots, \nu_t^{(N)})$

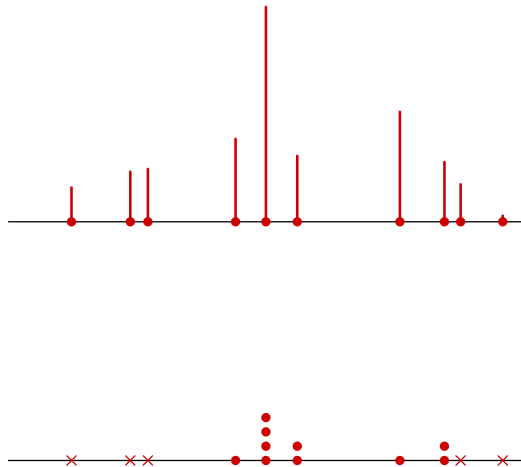


# Resampling

Stochastically map continuous weights  $(w_t^{(1)}, \dots, w_t^{(N)})$  to discrete offspring counts  $(\nu_t^{(1)}, \dots, \nu_t^{(N)})$

Properties:

- ▶ Number of particles constant  
 $\sum_{i=1}^N \nu_t^{(i)} = N$
- ▶ Equal weights after resampling  
 $w_{t+}^{(i)} = 1/N$
- ▶ Unbiased  
 $\mathbb{E}[\nu_t^{(i)} | w_t^{(1:N)}] = N w_t^{(i)}$



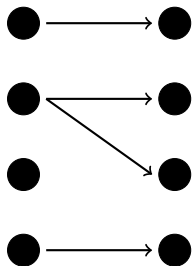
# Sequential Monte Carlo

Initialise by sampling  $N$  particles from  $\mu(\cdot)$ .

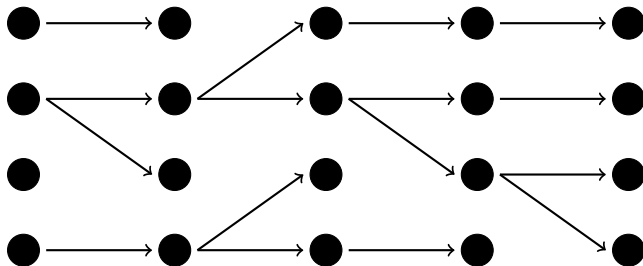
Iterate these steps:

1. **Mutate** particles via Markov transition kernel  $M_t$
2. **Weight** particles by potential function  $g_t$
3. **Resample** particles in proportion to their weights

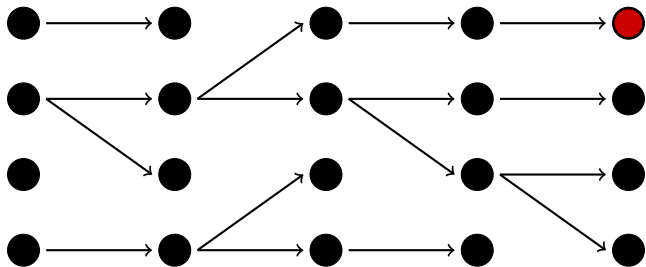
## Resampling induces a genealogy



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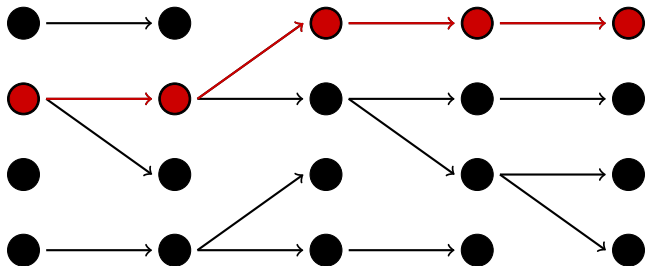


## Resampling induces a genealogy

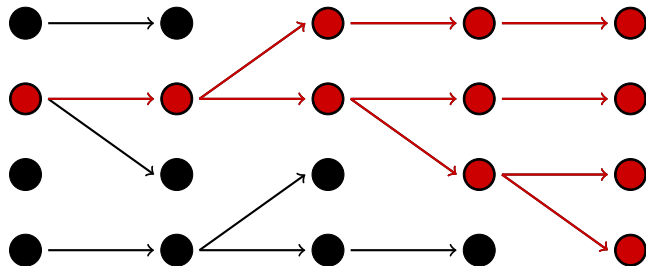




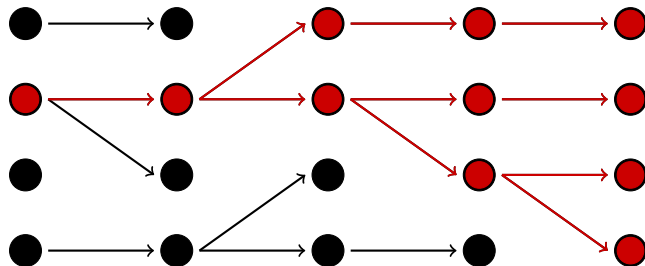
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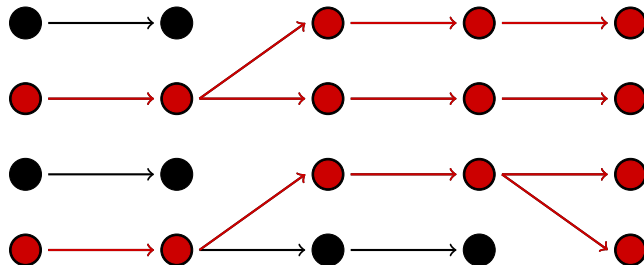


**Ancestral degeneracy:** for  $t \ll T$ , few distinct samples are available

## Mitigating ancestral degeneracy

Resample less often?

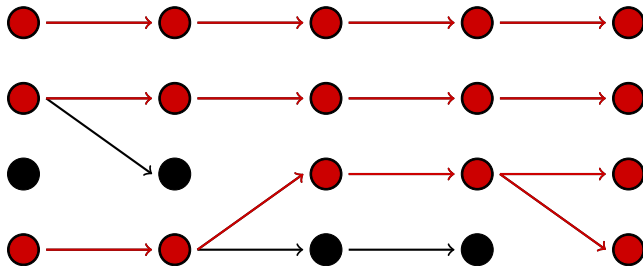
**Adaptive resampling:** only resample when effective sample size falls below some threshold.



## Mitigating ancestral degeneracy

Resample more cleverly?

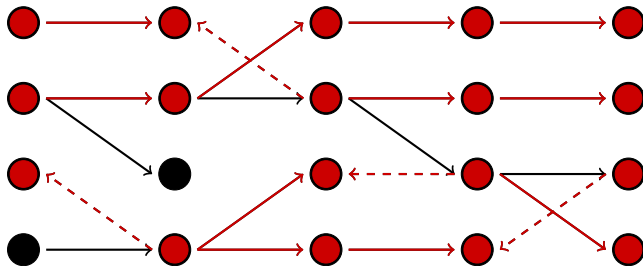
**Low-variance resampling:** resample in a way that reduces the extra randomness added by the resampling step.



## Mitigating ancestral degeneracy

Make use of killed samples?

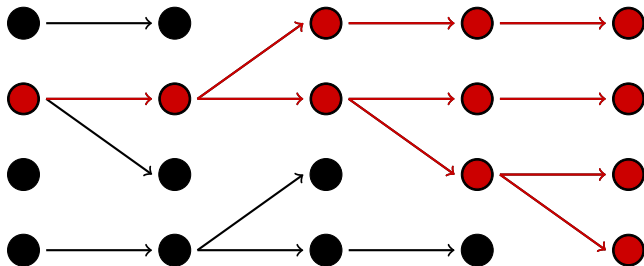
**Backward simulation:** use a backward pass to sample new ancestors for the terminal particles.



# Analysing genealogies

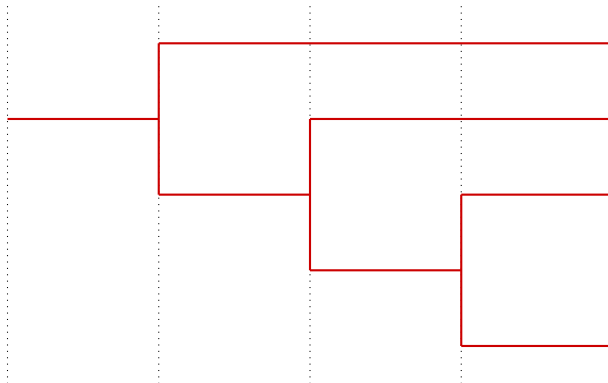
- ▶ How many particles should I use to maintain  $k$  distinct trajectories across time horizon  $T$ ?
- ▶ How big a lag can I use in fixed-lag smoothing?
- ▶ How reliable is my smoothing estimator?
- ▶ How do resampling schemes compare?

# Encoding genealogies





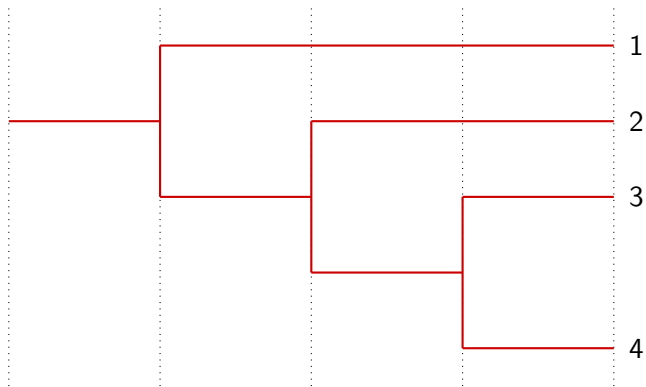
# Encoding genealogies



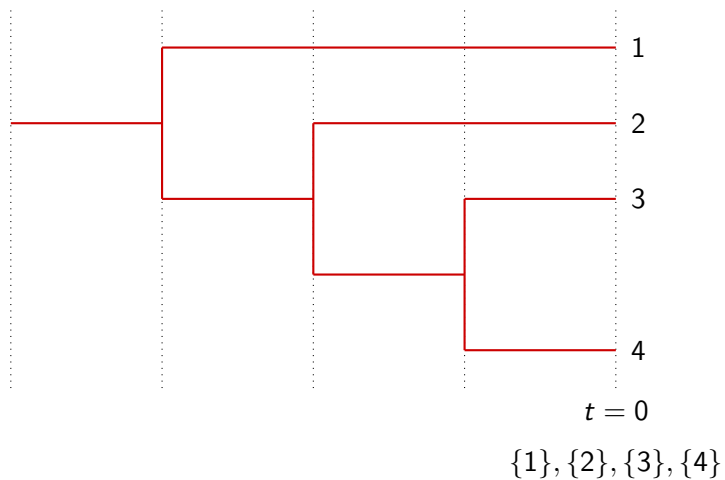
# Encoding genealogies

- ▶ Label time in reverse
- ▶ Population of  $N$  particles;  $N \rightarrow \infty$
- ▶ Sample  $n \leq N$  terminal particles at random
- ▶ Describe genealogy by stochastic process  $(G_t^{(n,N)})_{t \in \mathbb{N}_0}$  on space of partitions of  $\{1, \dots, n\}$
- ▶ Elements  $i, j$  are in the same block of the partition  $G_t^{(n,N)}$  iff particles  $i$  and  $j$  share a common ancestor at time  $t$
- ▶ Initially  $G_0^{(n,N)} = \{\{1\}, \dots, \{n\}\}$
- ▶ The only possible non-identity transitions are those that merge blocks
- ▶ The trivial partition  $\{\{1, \dots, n\}\}$  is an absorbing state

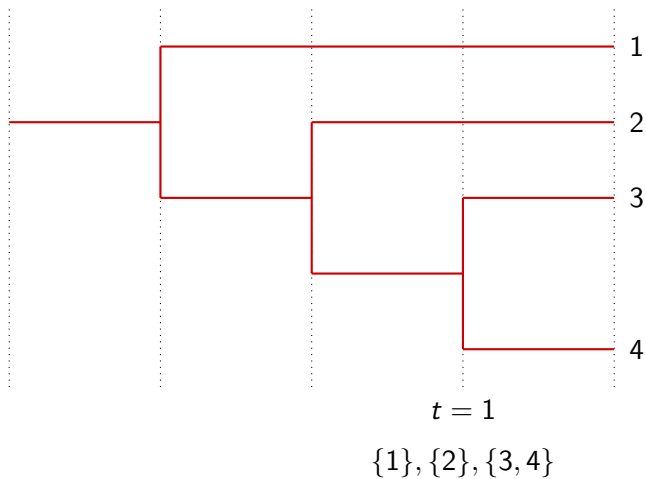
## Encoding genealogies



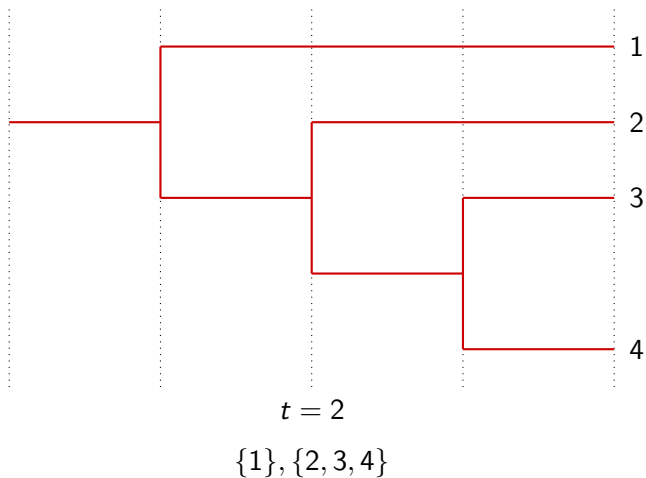
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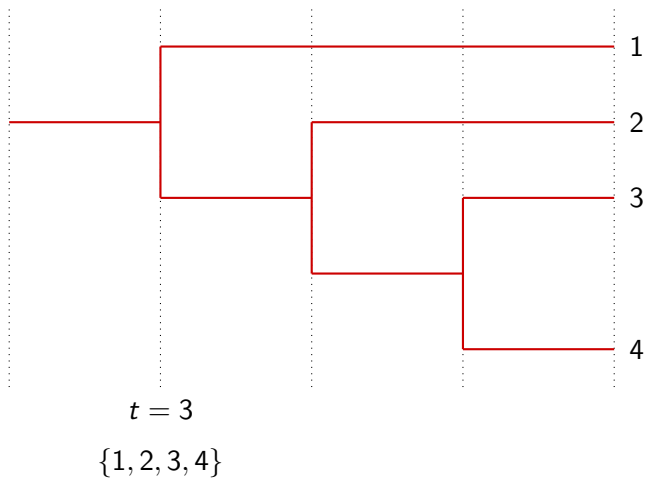
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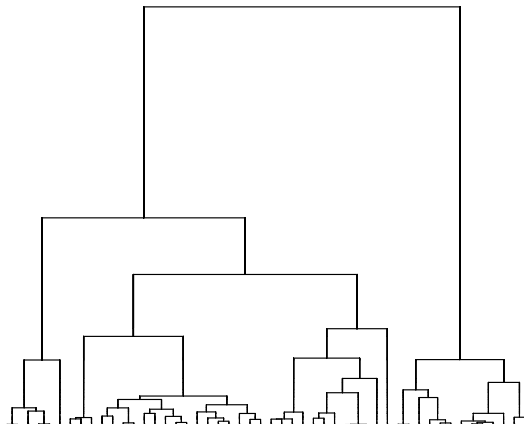


# Encoding genealogies



# Kingman's $n$ -coalescent<sup>1</sup>

- ▶ Continuous-time Markov chain on the space of partitions of  $\{1, \dots, n\}$
- ▶ Single pair mergers only
- ▶ Each pair merges independently at rate 1 (total merge rate  $\binom{k}{2}$  while there are  $k$  distinct lineages)



<sup>1</sup>JFC Kingman, *Stochastic Processes & their Applications*, 1982.



## Time scale

Pair merger probability conditional on  $(\nu_t^{(1)}, \dots, \nu_t^{(N)})$ :

$$c_N(t) = \frac{1}{(N)_2} \sum_{i=1}^N (\nu_t^{(i)})_2$$

Rescale time by inverse:

$$\tau_N(t) := \inf \left\{ s \geq 1 : \sum_{r=1}^s c_N(r) \geq t \right\}$$

# Main theorem<sup>2</sup>

Conditions:

- ▶ Parent-offspring assignments are uniform given offspring counts
- ▶ Time scale does not explode (i.e.  $\mathbb{P}[\tau_N(t) = \infty] = 0$  for all finite  $t$ )
- ▶ There exists a sequence  $(b_N)$  such that  $\lim_{N \rightarrow \infty} b_N = 0$  and

$$\frac{1}{(N)_3} \sum_{i=1}^N \mathbb{E}_t[(\nu_t^{(i)})_3] \leq b_N \frac{1}{(N)_2} \sum_{i=1}^N \mathbb{E}_t[(\nu_t^{(i)})_2]$$

Then the time-rescaled genealogies  $\left(G_{\tau_N(t)}^{(n,N)}\right)_{t \geq 0}$  converge weakly to Kingman's  $n$ -coalescent as  $N \rightarrow \infty$ .

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<sup>2</sup>S Brown, PA Jenkins, AM Johansen, J Koskela, *Electronic Journal of Probability*, 2021.

# Examples

- ▶ Multinomial resampling
- ▶ Stochastic rounding
- ▶ (Conditional SMC with multinomial resampling)

# Multinomial resampling

Resample from a Categorical distribution, so offspring counts are Multinomial:

$$(\nu_t^{(1)}, \dots, \nu_t^{(N)}) \sim \text{Multinomial} \left( N, (w_t^{(1)}, \dots, w_t^{(N)}) \right)$$

Suppose the transition kernels  $M_t$  admit densities  $m_t$ , and  $\forall x, x'$ ,

$$\frac{1}{a} \leq g_t(x, x') \leq a \quad \varepsilon h(x') \leq m_t(x, x') \leq \frac{1}{\varepsilon} h(x')$$

for constants  $0 < \varepsilon \leq 1 \leq a < \infty$ , and probability distribution  $h(\cdot)$ .

Then the rescaled genealogies converge to the  $n$ -coalescent.<sup>3</sup>

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<sup>3</sup>J Koskela, PA Jenkins, AM Johansen, D Spanò. *Annals of Statistics*, 2020.

# Stochastic rounding

$\mathbf{Y} : \mathbb{R}_+^N \rightarrow \mathbb{N}^N$  is a *stochastic rounding* of  $\mathbf{X}$  if for  $i = 1, \dots, N$

$$Y_i \mid X_i = \begin{cases} \lfloor X_i \rfloor & \text{with probability } 1 - X_i + \lfloor X_i \rfloor \\ \lfloor X_i \rfloor + 1 & \text{with probability } X_i - \lfloor X_i \rfloor \end{cases}$$

- ▶ Take  $X_i = Nw_t^{(i)}$  and  $Y_i = \nu_t^{(i)}$
- ▶ By construction  $\mathbb{E}[Y_i \mid \mathbf{X}] = X_i$
- ▶ Require further constraint  $Y_1 + \dots + Y_N = N$
- ▶ **Examples:** systematic resampling, residual-stratified resampling

# Stochastic rounding

Resample using any stochastic rounding procedure.

Suppose the transition kernels  $M_t$  admit densities  $m_t$ , and  $\forall x, x'$ ,

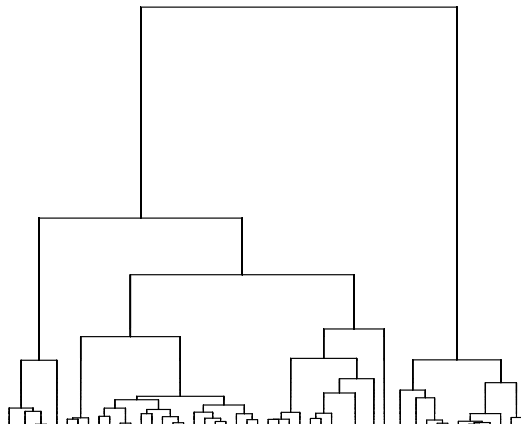
$$\frac{1}{a} \leq g_t(x, x') \leq a \quad \varepsilon \leq m_t(x, x') \leq \frac{1}{\varepsilon}$$

for constants  $0 < \varepsilon \leq 1 \leq a < \infty$ .

Then the rescaled genealogies converge to the  $n$ -coalescent.

# Quantities of interest

- ▶ Time to MRCA: first time when there is only one distinct lineage
- ▶  $t_k$ : for how long are there exactly  $k$  distinct lineages
- ▶ Total branch length: storage cost



# Comparing resampling schemes

- ▶ The expected time scale is the same for every stochastic rounding scheme
- ▶ Coalescence is faster for multinomial resampling than for stochastic rounding



## Mitigating ancestral degeneracy, revisited

- ▶ **Adaptive resampling**: should slow down the time-scale on which the coalescent is recovered (it may have some other effect)
- ▶ **Low-variance resampling**: stochastic rounding schemes have minimal variance
- ▶ **Backward simulation**: the backward-in-time process is not a pure coalescent, and is not induced by resampling

## In conclusion...

- ▶ Genealogies can help us to analyse performance of SMC algorithms which suffer ancestral degeneracy
- ▶ We have simple conditions under which these genealogies converge to Kingman's  $n$ -coalescent
- ▶ These conditions are verified for some important classes of SMC algorithms

# Open questions

- ▶ Other resampling schemes (stratified, residual-multinomial, ...)
- ▶ Effect of adaptive resampling
- ▶ Estimating the time scale  $\tau_N$  a priori (since it depends on observed offspring counts)
- ▶ Finite- $N$  behaviour

Thank you!

# Conditional SMC

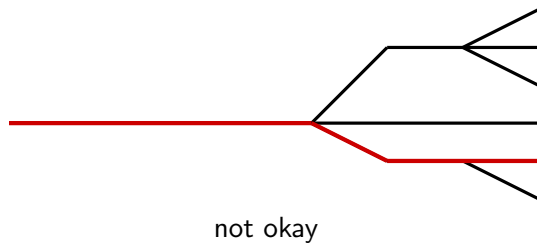
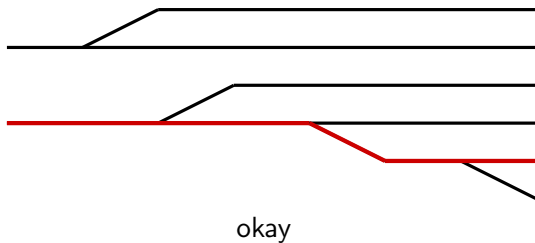
A particle Gibbs<sup>4</sup> scenario...

- ▶ Want to target  $p(\theta, x_{0:T} \mid y_{0:T})$
- ▶ Gibbs sampler: alternate samples from  
 $p(\theta \mid x_{0:T}, y_{0:T})$  (easy) and  
 $p(x_{0:T} \mid \theta, y_{0:T})$  (using SMC)
- ▶ Standard SMC updates don't target the correct distribution
- ▶ Use SMC updates that are *conditioned* on the previous  $X_{0:T}$  trajectory (states and ancestors)
- ▶ Resampling must deterministically propagate this “immortal lineage”

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<sup>4</sup>C Andrieu, A Doucet, R Holenstein. *Journal of the Royal Statistical Society B*, 2010.

# Conditional SMC



# Conditional SMC

Consider a conditional SMC algorithm with multinomial resampling.

Assume

$$\frac{1}{a} \leq g_t(x, x') \leq a \quad \varepsilon h(x') \leq m_t(x, x') \leq \frac{1}{\varepsilon} h(x').$$

Then the rescaled genealogies converge to the  $n$ -coalescent.