

Asymptotic genealogies of sequential Monte Carlo algorithms

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4 December 2020

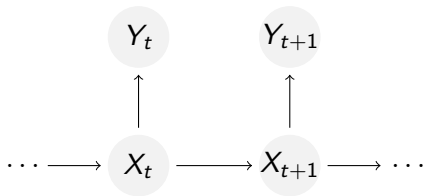
Outline

1. Sequential Monte Carlo
2. ...

Sequential Monte Carlo

- ▶ Monte Carlo = approximating probability distributions via sampling
- ▶ Want to sample from a sequence of probability distributions
- ▶ Dimension of distributions increases along the sequence
- ▶ Strong dependence between consecutive distributions

State space models

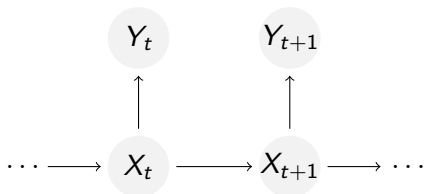


$$X_0 \sim \mu(\cdot)$$

$$X_{t+1} \mid (X_t = x_t) \sim f_t(\cdot \mid x_t)$$

$$Y_t \mid (X_t = x_t) \sim g_t(\cdot \mid x_t)$$

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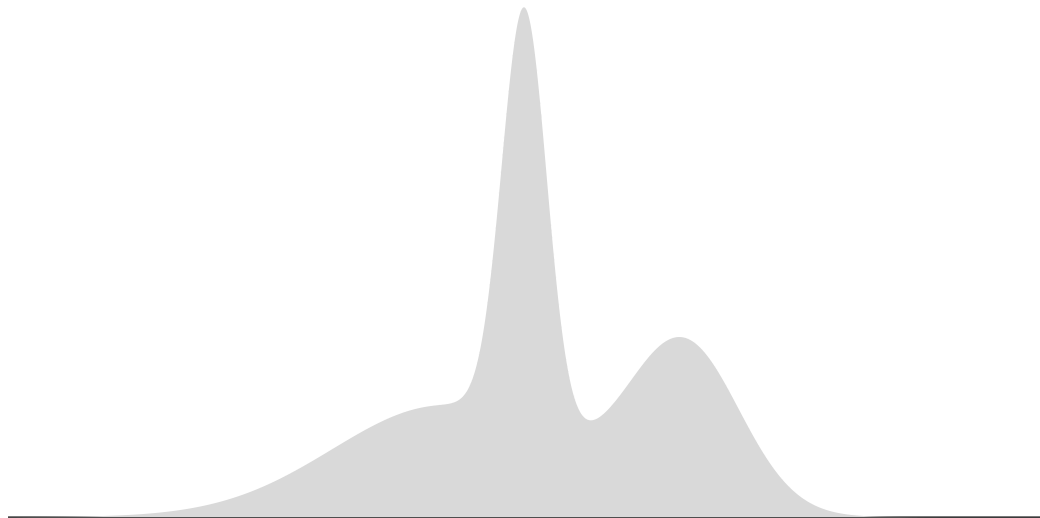
Inference problems ($s < t$):

$p(x_t \mid y_{1:s})$ “prediction”

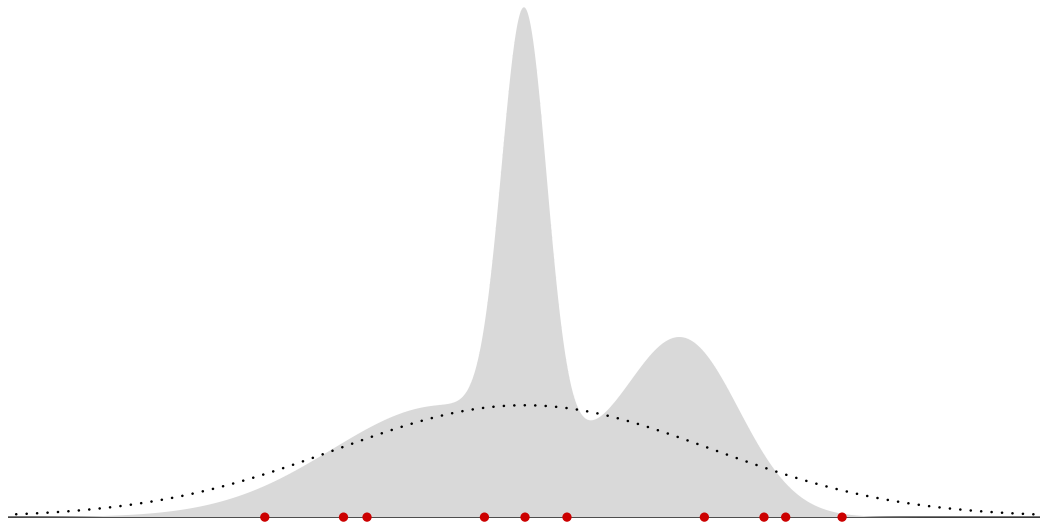
$p(x_t \mid y_{1:t})$ “filtering”

$p(x_s \mid y_{1:t})$ “smoothing”

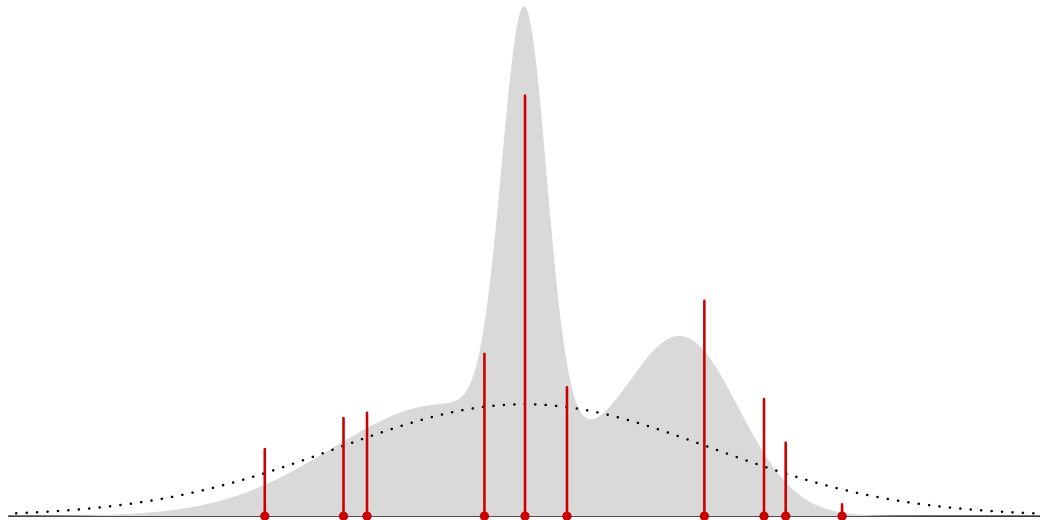
Importance sampling



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Sequential importance sampling

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- ▶ Multiplying weights over time causes *weight degeneracy*
- ▶ Can avoid this problem by resampling

Sequential Monte Carlo

Approximate a sequence of distributions by simulating a population of particles evolving in time

Sequential Monte Carlo

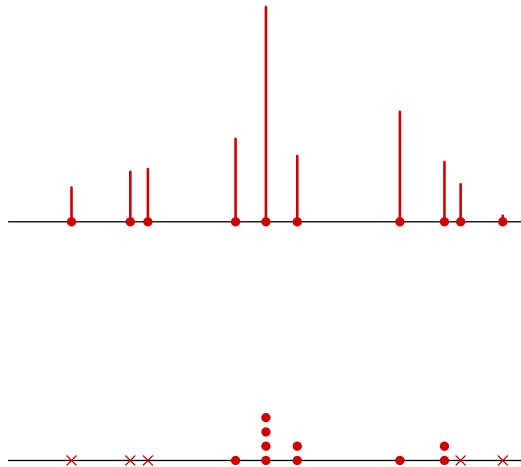
Approximate a sequence of distributions by simulating a population of particles evolving in time

Iterate these steps:

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

Resampling

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

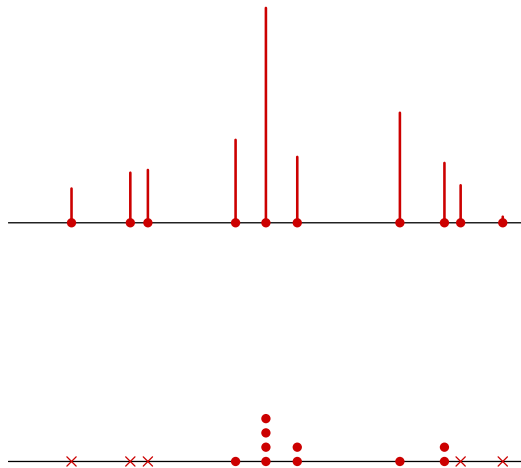


Resampling

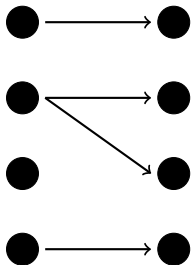
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Properties:

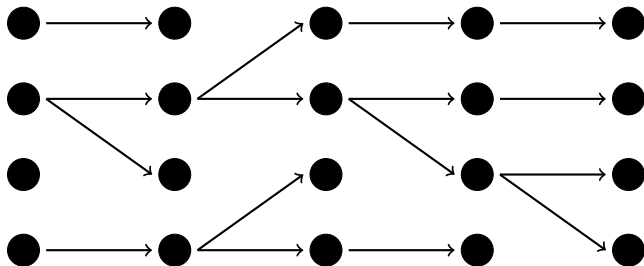
- ▶ Number of particles constant
 $\sum_{i=1}^N \nu_t^{(i)} = N$
- ▶ Equal weights after resampling
 $w_{t+}^{(i)} = 1/N$
- ▶ Unbiased
 $\mathbb{E}[\nu_t^{(i)} | w_t^{(1:N)}] = N w_t^{(i)}$



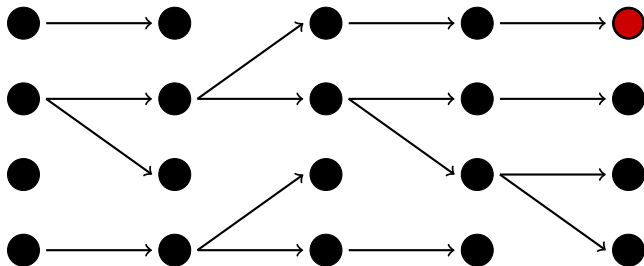
Resampling induces a genealogy



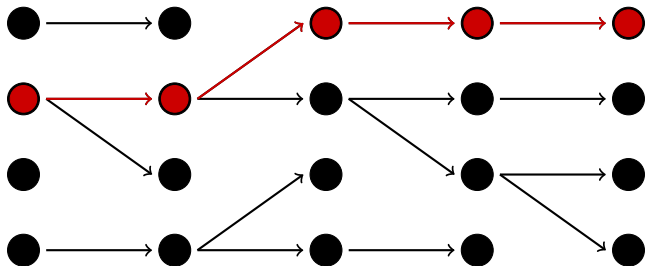
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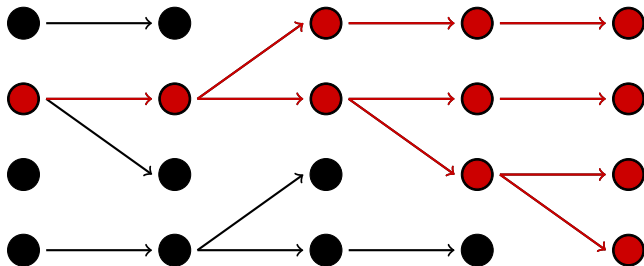
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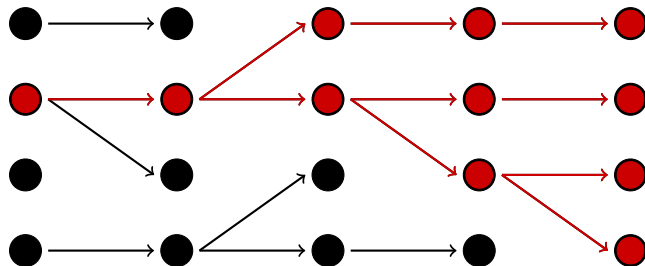
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Ancestral degeneracy: for $t \ll T$, few distinct samples are available

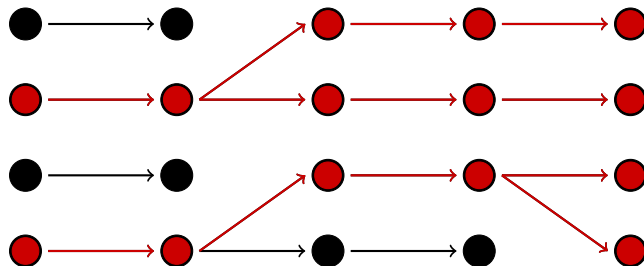
Mitigating ancestral degeneracy

Resample less often?

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



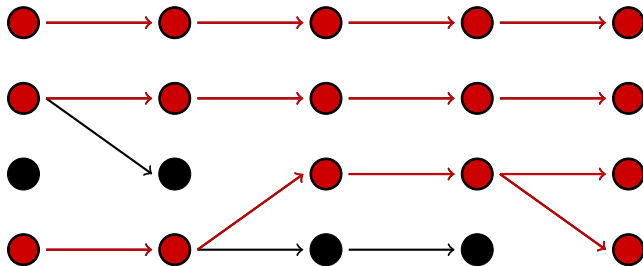
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Low-variance resampling: resample in a way that reduces the extra randomness added by the resampling step.



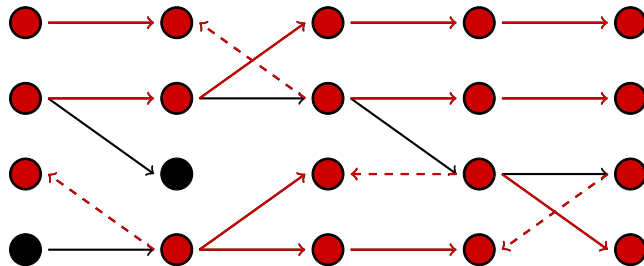
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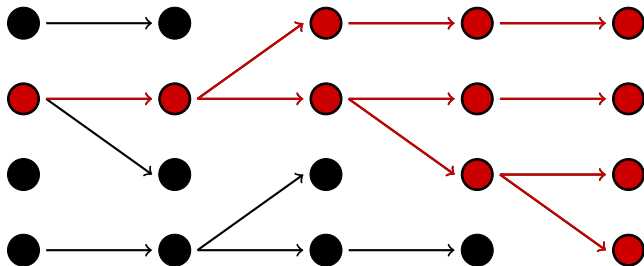
Backward simulation: use a backward pass to sample new ancestors for the terminal particles.



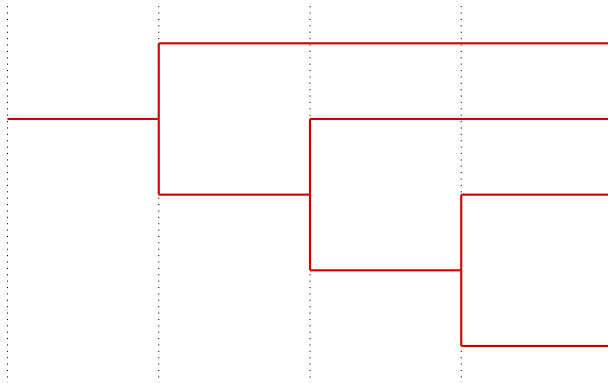
Analysing genealogies

- ▶ 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



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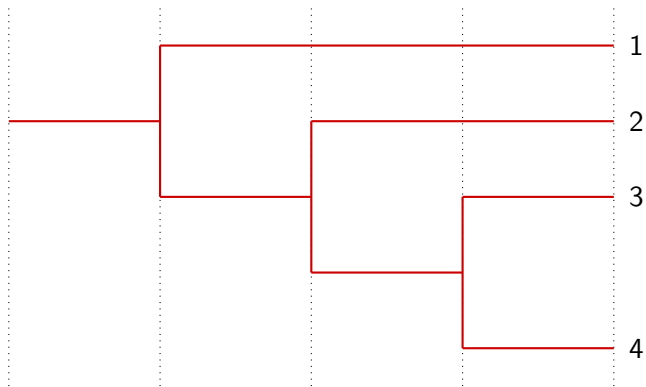
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- ▶ Label time in reverse
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- ▶ Sample $n \leq N$ terminal particles at random
- ▶ Describe genealogy by stochastic process $(G_t^{(n,N)})_{t \in \mathbb{N}_0}$ on space of partitions of $\{1, \dots, n\}$
- ▶ 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

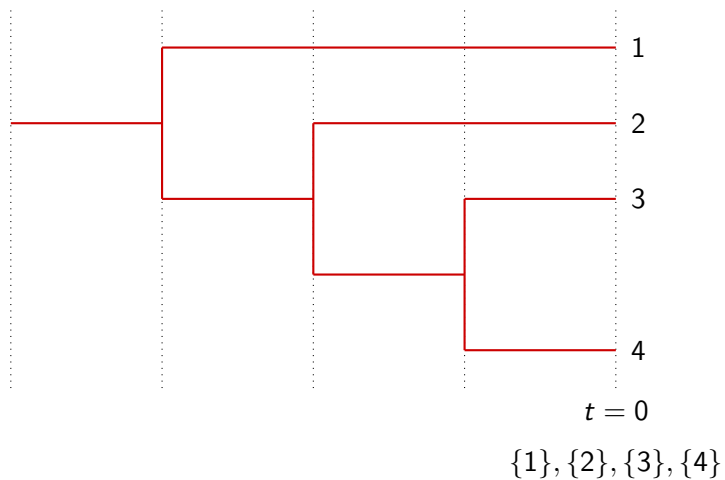
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- ▶ Elements i, j are in the same block of the partition $G_t^{(n,N)}$ iff particles i and j share a common ancestor at time t
- ▶ Initially $G_0^{(n,N)} = \{\{1\}, \dots, \{n\}\}$
- ▶ The only possible non-identity transitions are those that merge blocks
- ▶ The trivial partition $\{\{1, \dots, n\}\}$ is an absorbing state

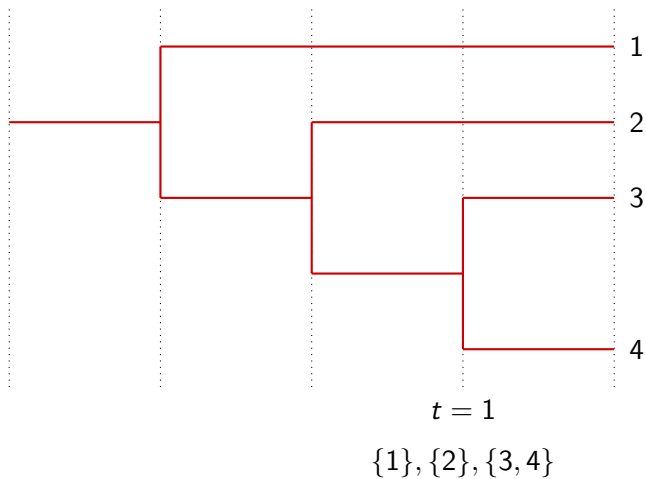
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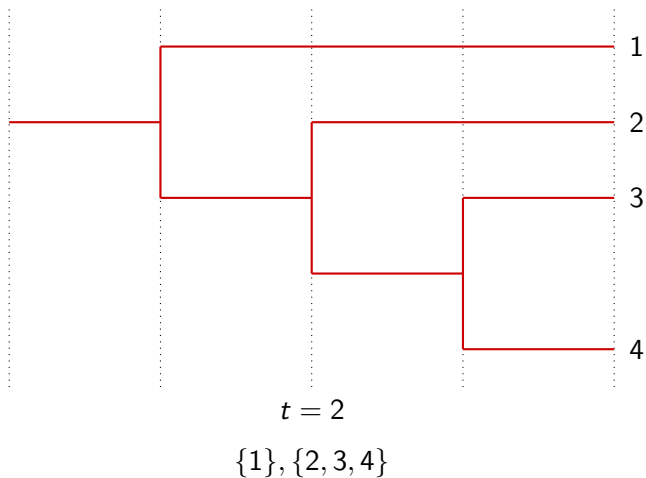
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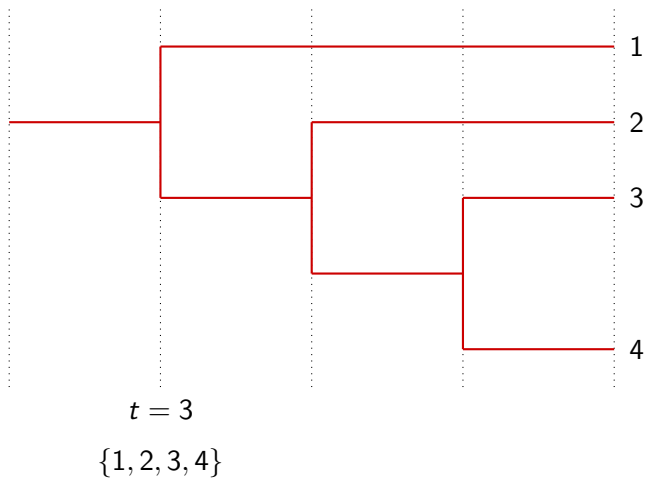
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Kingman's n -coalescent¹

- ▶ 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)

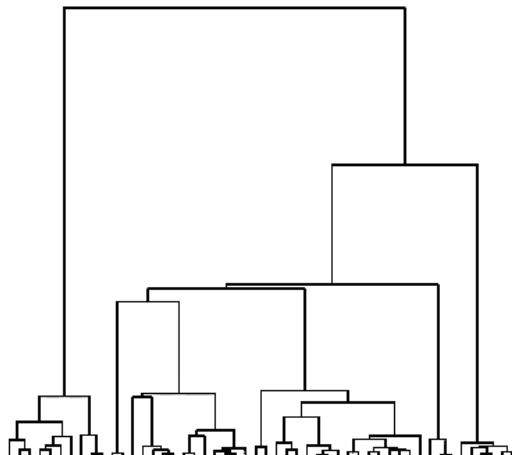


image: Wikimedia Commons

¹J F C Kingman, *Stochastic Processes & their Applications*, 1982.

Time scale

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

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

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Rescale time by inverse:

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

Main theorem

Conditions:

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- ▶ There exists a sequence (b_N) such that $\lim_{N \rightarrow \infty} b_N = 0$ and

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

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

Examples

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

Multinomial resampling

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

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

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Suppose the potentials g_t and transition densities q_t satisfy

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

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

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Stochastic rounding

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

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

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- ▶ Require further constraint $Y_1 + \dots + Y_N = N$
- ▶ **Examples:** systematic, residual-stratified, branching system³, SSP⁴ resampling

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Then the rescaled genealogies converge to the n -coalescent.

Conditional SMC

A particle Gibbs⁵ scenario...

- ▶ Want to target $p(\theta, x_{0:T} \mid y_{0:T})$

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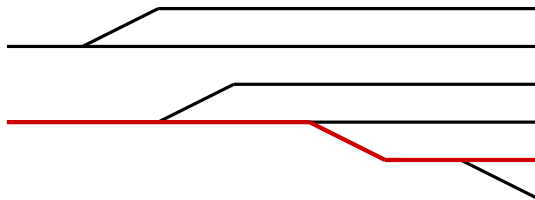
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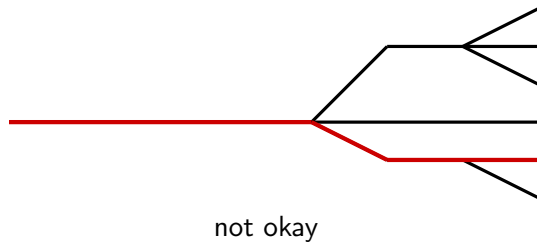
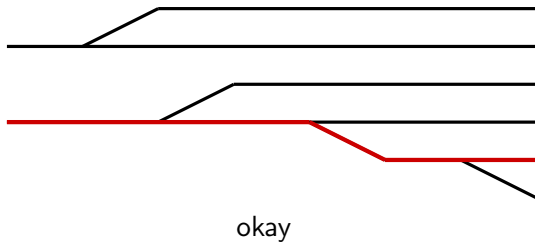
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- ▶ Standard SMC updates don't target the correct distribution
- ▶ Use SMC updates that are *conditioned* on the previous $X_{0:T}$ trajectory (states and ancestors)
- ▶ Resampling must deterministically propagate this “immortal lineage”

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Consider a conditional SMC algorithm with multinomial resampling.

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Quantities of interest

- Time to MRCA: first time when there is only one distinct lineage

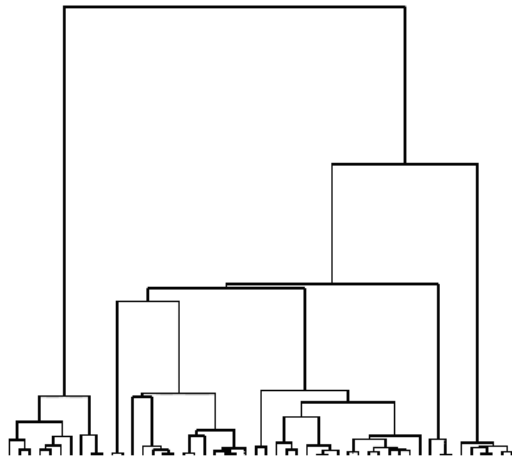


image: Wikimedia Commons

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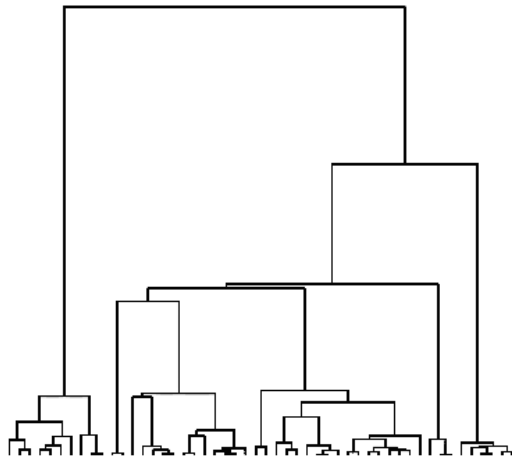


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- ▶ Total branch length: storage cost

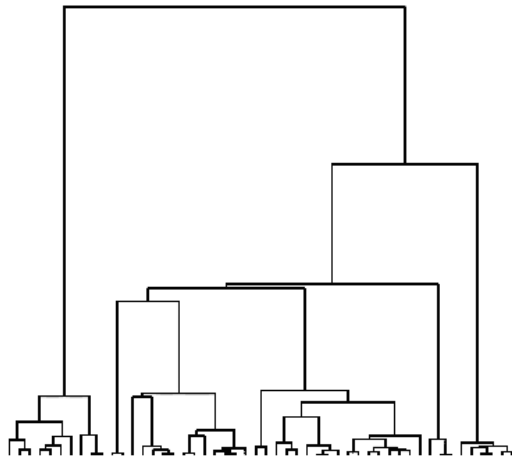


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- ▶ **Low-variance resampling**: stochastic rounding schemes have minimal variance
- ▶ **Backward simulation**: the backward-in-time process is not a pure coalescent, and is not induced by resampling

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

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

Thank you!

pre-print at [arXiv:2007.00096](https://arxiv.org/abs/2007.00096)