

Asymptotic genealogies of sequential Monte Carlo algorithms

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Outline

1. Sequential Monte Carlo
2. Resampling and degeneracy
3. SMC genealogies
4. Examples

Sequential Monte Carlo

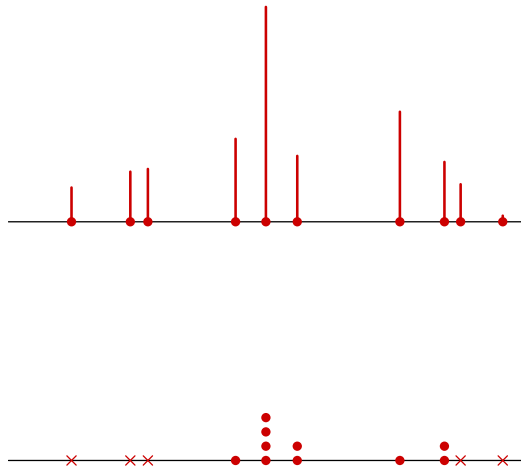
Target a sequence of distributions by simulating a population of particles evolving in time

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

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

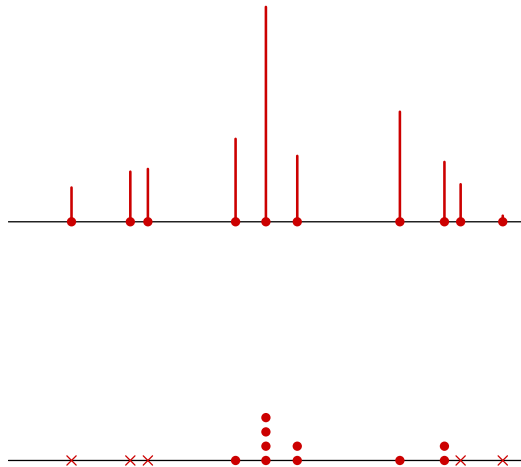
$$\sum_{i=1}^N \nu_t^{(i)} = N$$

- ▶ Equal weights after resampling

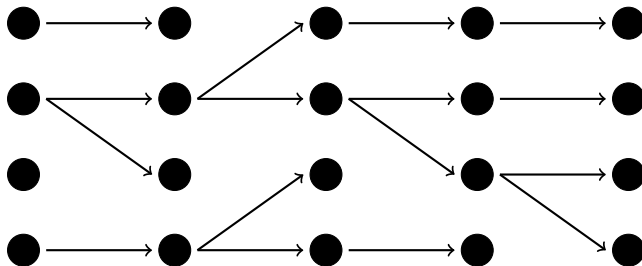
$$w_{t+}^{(i)} = 1/N$$

- ▶ Unbiased

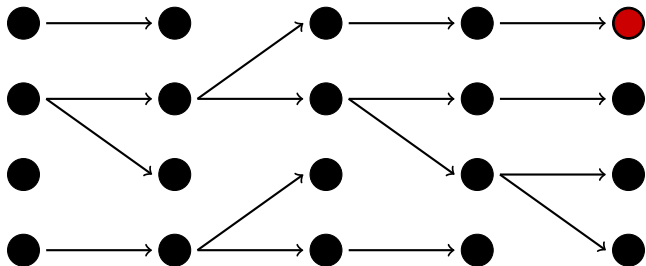
$$\mathbb{E}[\nu_t^{(i)} | w_t^{(i)}] = N w_t^{(i)}$$



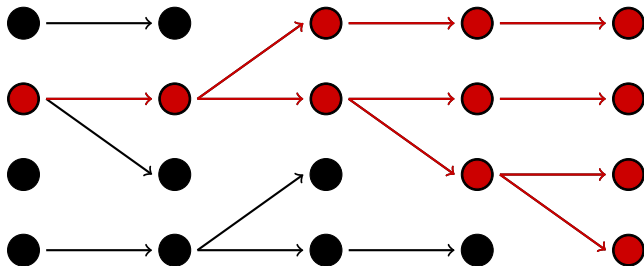
Resampling induces a genealogy



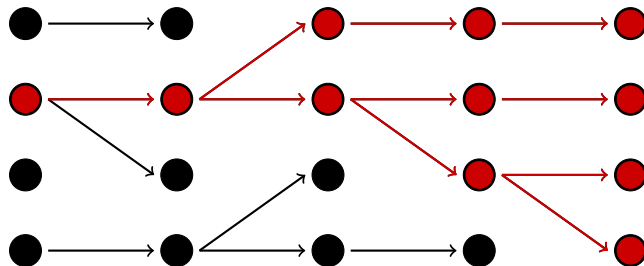
Resampling induces a genealogy



Resampling induces a genealogy



Resampling induces a genealogy

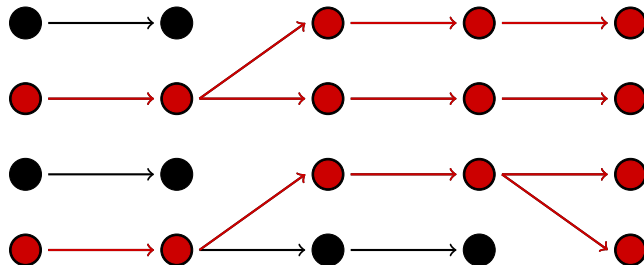


Ancestral degeneracy: for $t \ll T$, few distinct samples are available

Mitigating ancestral degeneracy

Resample less often?

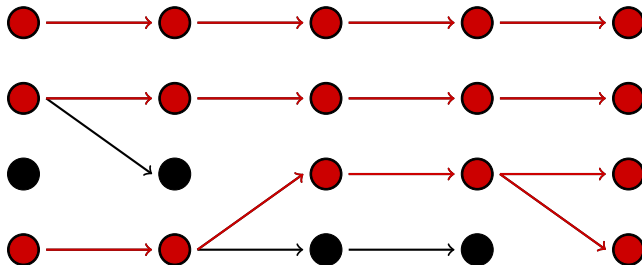
Adaptive resampling: only resample when effective sample size falls below some threshold.



Mitigating ancestral degeneracy

Resample more cleverly?

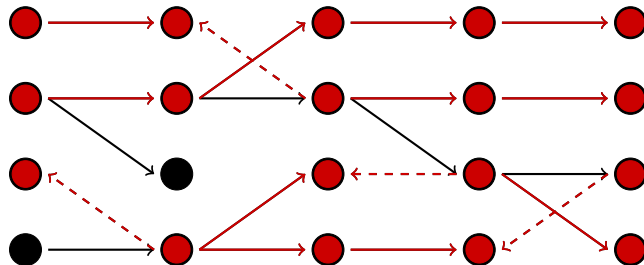
Low-variance resampling: resample in a way that reduces the extra randomness added by the resampling step.



Mitigating ancestral degeneracy

Make use of killed samples?

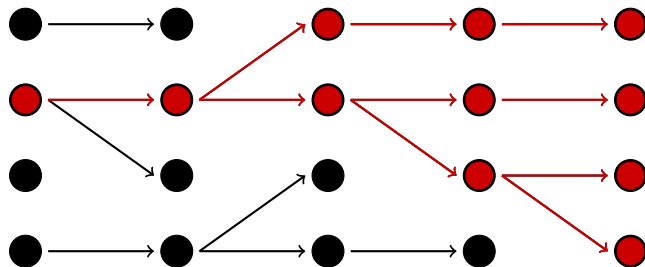
Backward simulation: use a backward pass to sample new ancestors for the terminal particles.



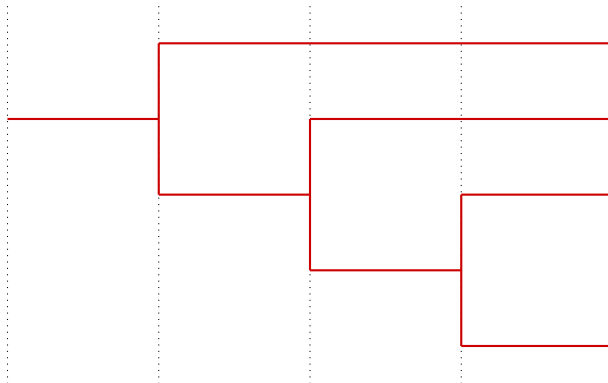
Analysing genealogies

- ▶ 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?

Encoding genealogies



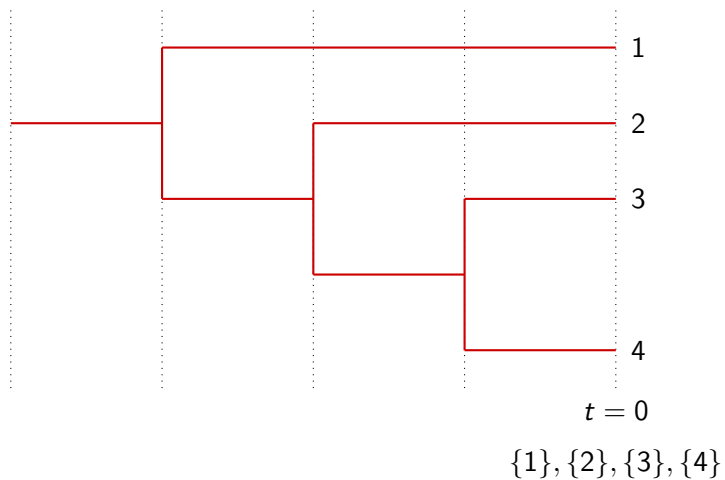
Encoding genealogies



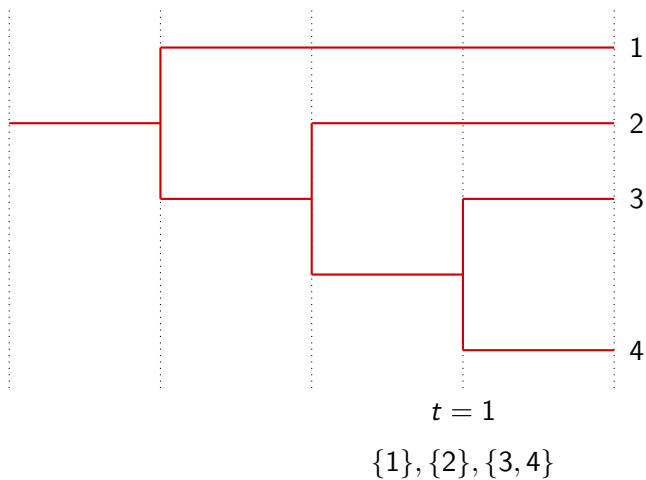
Encoding genealogies

- ▶ Label time in reverse
- ▶ Population of N particles
- ▶ Sample $n \leq N$ terminal particles
- ▶ 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

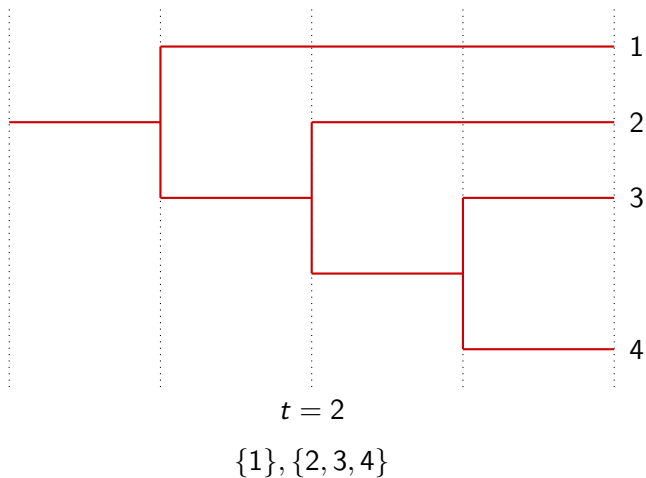
Encoding genealogies



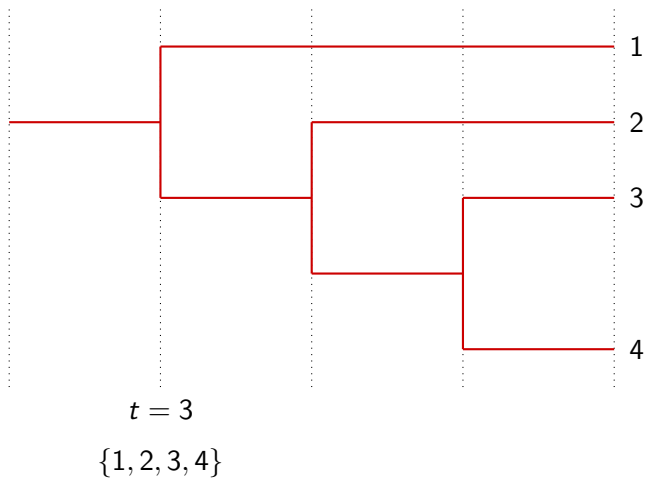
Encoding genealogies



Encoding genealogies



Encoding genealogies



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)

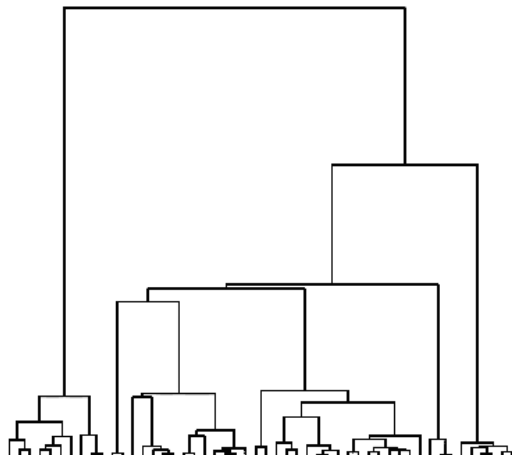


image: Wikimedia Commons

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

Time scale

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

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

Rescale time by inverse:

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

Main theorem

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 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:

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

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 $h(\cdot)$.

Then the rescaled genealogies converge to the n -coalescent.²

²J 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, residual-stratified, branching system³, SSP⁴ resampling

³D Crisan, T Lyons. *Probability Theory & Related Fields*, 1997.

⁴M Gerber, N Whiteley, N Chopin. *Annals of Statistics*, 2019.

Stochastic rounding

Resample using any stochastic rounding procedure.

Suppose the potentials g_t and transition densities q_t satisfy

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

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

Then the rescaled genealogies converge to the n -coalescent.

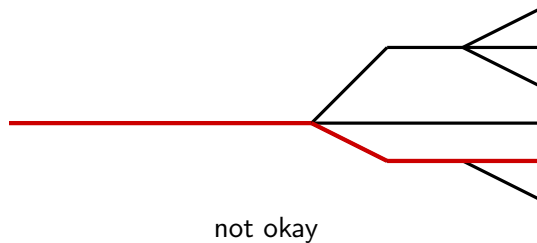
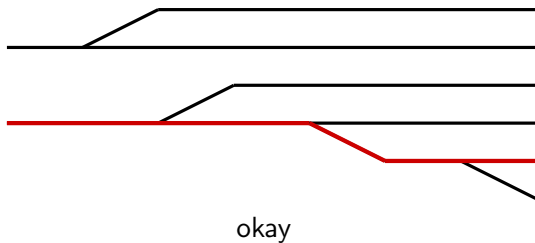
Conditional SMC

A particle Gibbs⁵ 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”

⁵C 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

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

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 : Time interval where there are exactly k distinct lineages
- ▶ Total branch length: storage cost

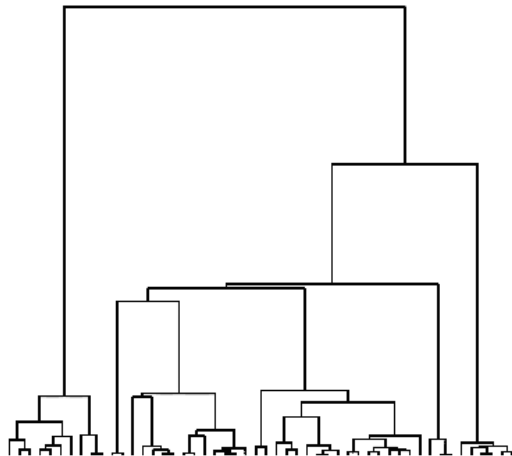


image: Wikimedia Commons

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

- ▶ 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)