

# Resampling in Sequential Monte Carlo

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# Outline

1. Introduction to sequential Monte Carlo
2. How to resample
3. Properties of resampling schemes
4. Link with genealogies

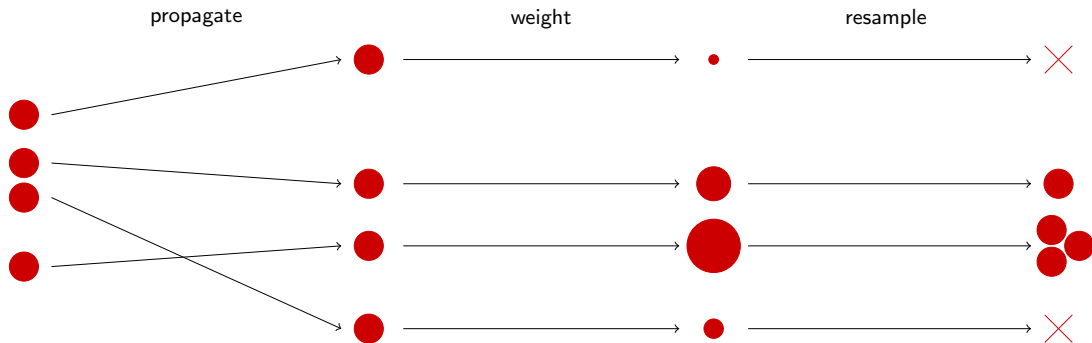
# Sequential Monte Carlo

## Motivation

- ▶ Want to approximate a sequence of target measures  $(\eta_t)_{t \in \mathbb{N}}$
- ▶ Use a system of  $N$  particles with dynamics ‘mimicking’ the target
- ▶ A ‘particle’ consists of a position and a weight:  $(x_t^{(i)}, w_t^{(i)}) = (x_i, w_i)$
- ▶ Approximate the measures  $\eta_t$  by (random) empirical measures  $\eta_t^N$  consisting of atoms at the particle positions

# Sequential Monte Carlo

## Illustration



# Resampling

## Motivation

- ▶ Resampling is necessary to prevent *weight degeneracy*
- ▶ But resampling causes *ancestral degeneracy*

# Resampling

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- ▶ Resampling is necessary to prevent *weight degeneracy*
- ▶ But resampling causes *ancestral degeneracy*
- ▶ Strategy: resample in a way that minimises 'unnecessary coalescences'

# Resampling

## Definition

We will take valid resampling schemes to be those satisfying

- ▶ The total number of particles  $N$  remains fixed
- ▶ The particles after resampling are equally weighted
- ▶ The scheme is unbiased: the expected number of offspring of particle  $i$  is equal to  $Nw_i$  for each  $i$

# Multinomial Resampling<sup>1</sup>

## Definition

Parental indices  $a_i \in \{1, \dots, N\}$ :

$$(a_i \mid w_{1:N}) \stackrel{iid}{\sim} \text{Categorical}(1 : N, w_{1:N})$$

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<sup>1</sup>Efron & Tibshirani (1994) 'An introduction to the bootstrap'



# Multinomial Resampling<sup>1</sup>

## Definition

Parental indices  $a_i \in \{1, \dots, N\}$ :

$$(a_i \mid w_{1:N}) \stackrel{iid}{\sim} \text{Categorical}(1 : N, w_{1:N})$$

Offspring numbers  $v_i \in \{0, \dots, N\}$  such that  $\sum v_i = N$ :

$$(v_{1:N} \mid w_{1:N}) \sim \text{Multinomial}(N, w_{1:N})$$

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# Multinomial Resampling

## Inversion Sampling

Draw uniform random variables

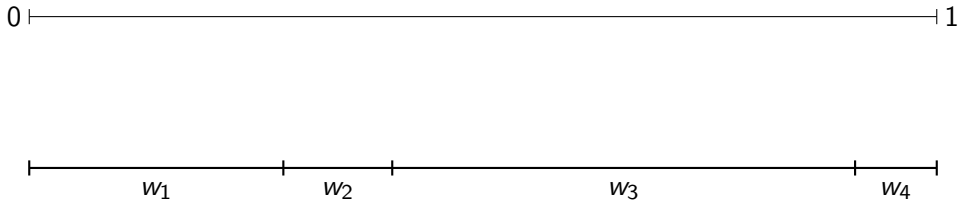
$$U_i \stackrel{iid}{\sim} \text{Uniform}(0, 1); \quad i = 1, \dots, N$$

and determine the parental indices by inversion

$$a_i = \inf \left\{ k : \sum_{j=1}^k w_j \geq U_i \right\}$$

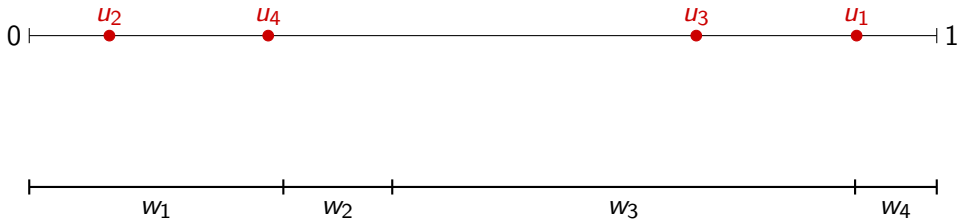
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## Inversion Sampling



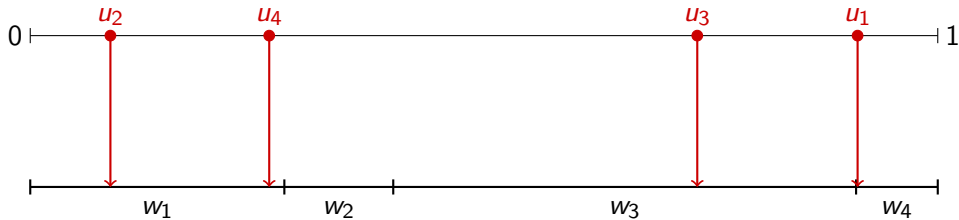
# Multinomial Resampling

## Inversion Sampling



# Multinomial Resampling

## Inversion Sampling



# Residual Resampling<sup>2,3</sup>

## Definition

1. Deterministically assign  $\lfloor Nw_i \rfloor$  offspring to particle  $i$ ;  $i=1, \dots, N$
2. There are  $R := N - \sum_{i=1}^N \lfloor Nw_i \rfloor$  offspring still to be assigned
3. Assign these randomly according to the residual weights  $r_i := \frac{1}{R}(Nw_i - \lfloor Nw_i \rfloor)$

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<sup>2</sup>Liu & Chen (1998) 'Sequential Monte Carlo methods for dynamic systems'

<sup>3</sup>Whitley (1994) 'A genetic algorithm tutorial'


# Residual Resampling

## Illustration

$w_1 = 0.28$  

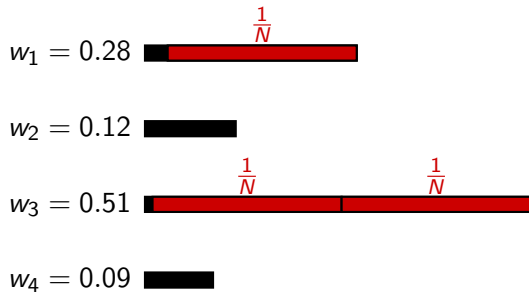
$w_2 = 0.12$  

$w_3 = 0.51$  

$w_4 = 0.09$  

# Residual Resampling

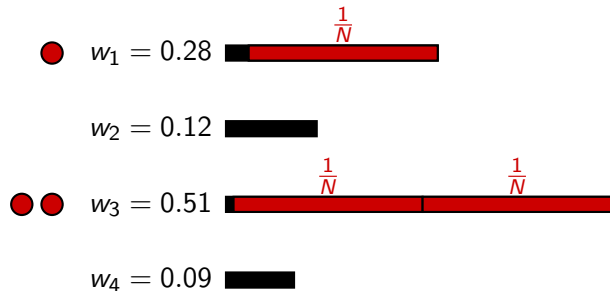
## Illustration





# Residual Resampling

## Illustration



# Residual Resampling

## Illustration

●  $r_1 \propto 0.03$  ■


$r_2 \propto 0.12$  ■■■

●●  $r_3 \propto 0.01$  ■


$r_4 \propto 0.09$  ■■■

# Residual Resampling

## Illustration

●  $r_1 = 0.12$  

$r_2 = 0.48$  

●●  $r_3 = 0.04$  

$r_4 = 0.36$  

# Residual Resampling

## Definition

If residuals are assigned using multinomial resampling, offspring counts are distributed

$$v_{1:N} \stackrel{d}{=} \lfloor Nw_{1:N} \rfloor + \text{Multinomial}(R, r_{1:N})$$

# Stratified Resampling<sup>4</sup>

## Definition

Draw uniformly from each stratified interval

$$U_i \sim \text{Uniform} \left( \frac{i-1}{N}, \frac{i}{N} \right); \quad i = 1, \dots, N$$

and determine the parental indices by inversion

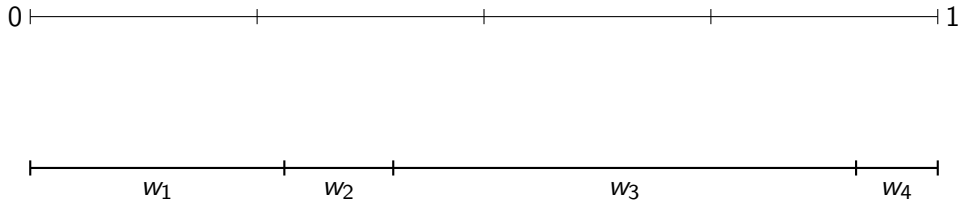
$$a_i = \inf \left\{ k : \sum_{j=1}^k w_j \geq U_i \right\}$$

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<sup>4</sup>Kitagawa (1996) 'Monte Carlo filter and smoother for non-Gaussian nonlinear state space models'

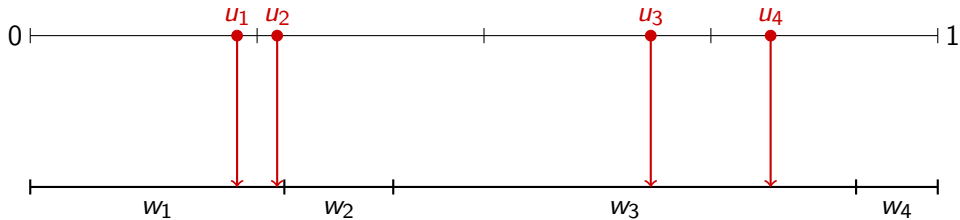
# Stratified Resampling

## Inversion Sampling



# Stratified Resampling

## Inversion Sampling



# Systematic Resampling<sup>5,6</sup>

## Definition

Draw uniformly from  $[0, \frac{1}{N}]$ , and add multiples of  $\frac{1}{N}$

$$U_1 \sim \text{Uniform} \left( 0, \frac{1}{N} \right)$$

$$U_i = U_1 + \frac{i-1}{N}; \quad i = 2, \dots, N$$

and determine the parental indices by inversion

$$a_i = \inf \left\{ k : \sum_{j=1}^k w_j \geq U_i \right\}$$

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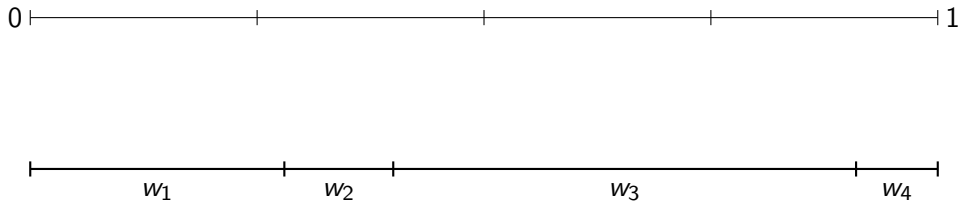
<sup>5</sup>Carpenter, Clifford & Fearnhead (1999) 'Improved particle filter for nonlinear problems'

<sup>6</sup>Whitley (1994) 'A genetic algorithm tutorial'



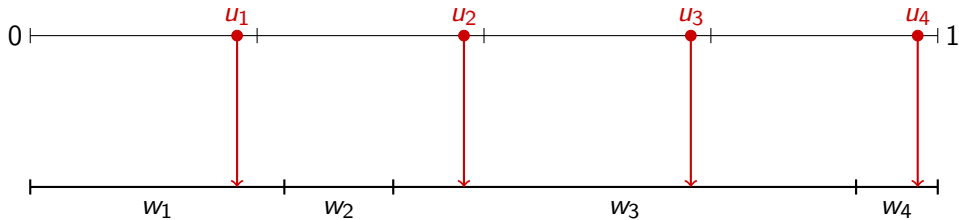
# Systematic Resampling

## Inversion Sampling



# Systematic Resampling

## Inversion Sampling



# Properties of Resampling Schemes

## Support of Offspring Counts

Suppose  $w_i \in [\frac{k}{N}, \frac{k+1}{N}]$ .

What are the possible values for  $v_i$ ?

**Multinomial:**  $v_i \in \{0, \dots, N\}$

**Residual:**  $v_i \in \{k, \dots, k + R\}$

**Stratified:**  $v_i \in \{k - 1, k, k + 1, k + 2\}$

**Systematic:**  $v_i \in \{k, k + 1\}$

# Properties of Resampling Schemes

## One-Step Variance

Consider variance of our estimator, conditional on the previous step:

$$\text{Var} \left[ \frac{1}{N} \sum_{i=1}^N \varphi(X_t^{(i)}) \mid \mathcal{G}_{t-1} \right]$$

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In this sense we have<sup>7</sup>

$$\text{Var}[\text{stratified}] \leq \text{Var}[\text{multinomial}]$$

$$\text{Var}[\text{residual-stratified}] \leq \text{Var}[\text{residual-multinomial}] \leq \text{Var}[\text{multinomial}]$$

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# Properties of Resampling Schemes

## Permutation Invariance

Stratified and systematic resampling are sensitive to the ordering of the particles.

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### Example

$$N = 6$$

$$w_{1:N} = \frac{1}{12}(3, 3, 2, 2, 1, 1)$$

Is it possible to sample offspring counts  $v_i = (1, 1, 1, 1, 1, 1)$  ?

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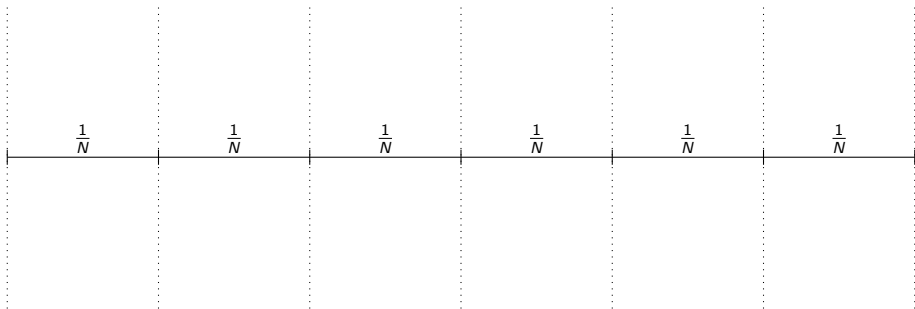
Is it possible to sample offspring counts  $v_i = (1, 1, 1, 1, 1, 1)$  ?

Answer: it depends on the ordering!



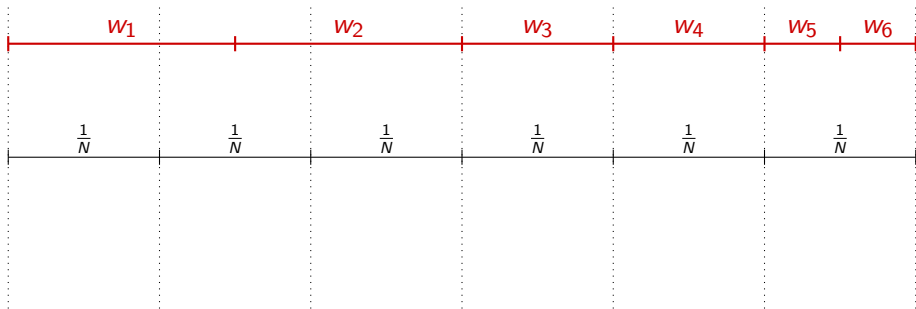
# Properties of Resampling Schemes

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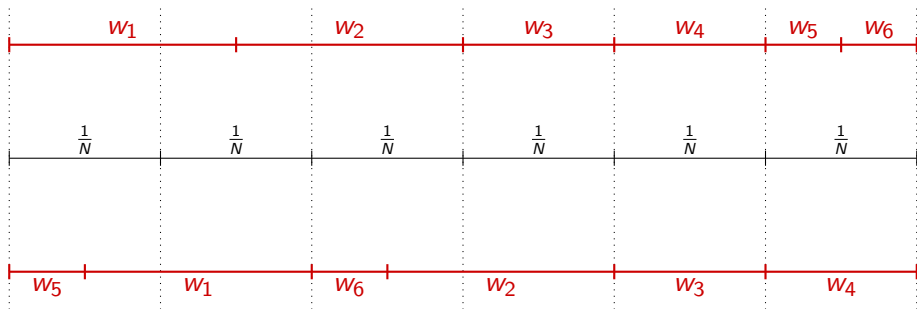
# Properties of Resampling Schemes

## Permutation Invariance



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# Properties of Resampling Schemes

## Permutation Invariance

- ▶ Kitagawa<sup>8</sup> suggested ordering the particles by their positions before resampling
- ▶ He ran an experiment suggesting that sorting reduces Monte Carlo variance
- ▶ This was later proved to be true<sup>9</sup>
- ▶ Sorting by position could be a sort of proxy for sorting by weight

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<sup>8</sup>Kitagawa (1996) 'Monte Carlo filter and smoother for non-Gaussian nonlinear state space models'

<sup>9</sup>Gerber, Chopin & Whiteley (2018) 'Negative association, ordering and convergence of resampling methods'

# Properties of Resampling Schemes

## Degeneracy under Equal Weights

- ▶ Suppose all of the weights are multiples of  $\frac{1}{N}$ .

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- ▶ In particular, if  $w_{1:N} = \frac{1}{N}(1, \dots, 1)$ , these schemes do not resample at all (assigning exactly one offspring to each particle).

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- ▶ Suppose all of the weights are multiples of  $\frac{1}{N}$ .
- ▶ Then residual, stratified and systematic resampling all yield purely deterministic assignments of offspring.
- ▶ In particular, if  $w_{1:N} = \frac{1}{N}(1, \dots, 1)$ , these schemes do not resample at all (assigning exactly one offspring to each particle).
- ▶ Under reasonable conditions, this situation has zero measure.



# Properties of Resampling Schemes

## Summary

	$\sup  v_i - Nw_i $	low variance	invariant under permutations	degenerate if $w_{1:N} \propto (1, \dots, 1)$
multinomial	$N$	×	✓	×
residual	$R$	✓	✓	✓
stratified	2	✓	×	✓
systematic	1	×	×	✓

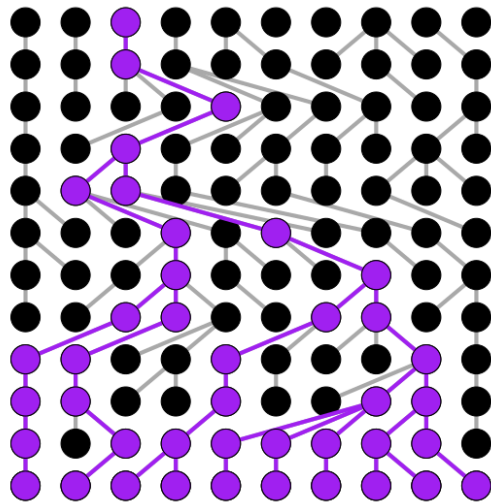
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residual	$R$	$\checkmark$	$\checkmark$	$\checkmark$
stratified	2	$\checkmark$	$\times$	$\checkmark$
systematic	1	$\times$	$\times$	$\checkmark$
residual-strat	1	$\checkmark$	$\times$	$\checkmark$

## Resampling and Genealogies

- ▶ Resampling creates a genealogy (family tree) of particles
- ▶ Properties of the genealogy affect performance of the SMC algorithm
- ▶ Different resampling schemes give different forms of genealogies
- ▶ Basic quantity for analysing genealogies is the pair coalescence probability



# Coalescence Probability

## Definition

The probability that a randomly chosen pair of particles at generation  $t$  share a common ancestor at generation  $(t - 1)$

$$c_N = \frac{1}{N(N-1)} \sum_{i=1}^N v_i(v_i - 1)$$

# Coalescence Probability

## Example

Consider the case where we have only two particles ( $N = 2$ )

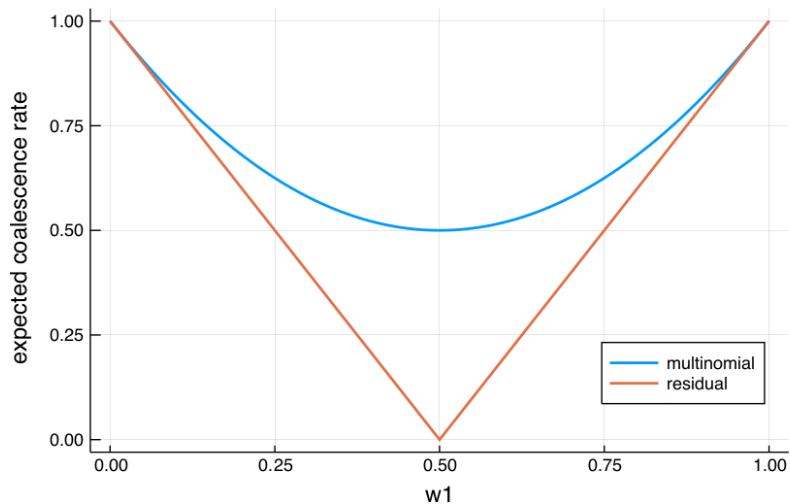
$$c_2 = \frac{1}{2} [v_1(v_1 - 1) + v_2(v_2 - 1)]$$

The expectation of  $c_2$  conditional on knowing the weights ( $w_1, w_2$ ) is

$$\begin{aligned} c_2 &= \frac{1}{2} \mathbb{E}[v_1(v_1 - 1) \mid w_{1:2}] + \frac{1}{2} \mathbb{E}[v_2(v_2 - 1) \mid w_{1:2}] \\ &= \mathbb{P}[v_1 = 2 \mid w_{1:2}] + \mathbb{P}[v_2 = 2 \mid w_{1:2}] \end{aligned}$$

# Coalescence Probability

## Example



- ▶ We proved that asymptotically (as  $N \rightarrow \infty$ ) residual resampling dominates multinomial in terms of expected coalescence probability
- ▶ We also proved it in cases  $N = 2$  and  $N = 3$

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- ▶ We conjecture that it holds for all finite  $N$  too
- ▶ It just remains to prove it for  $N = 4, 5, \dots$
- ▶ We proved that systematic resampling (and some others) dominate multinomial in expected coalescence probability, for all  $N$ .

THE END