Resampling in Sequential Monte Carlo

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Outline

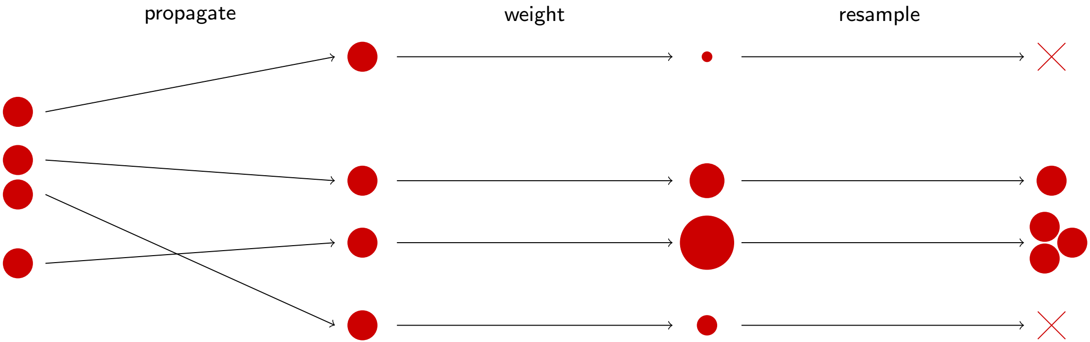
1. Introduction to sequential Monte Carlo
2. How to resample
3. Properties of resampling schemes
4. Link with genealogies

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 η_t by (random) empirical measures η_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*

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Motivation

- 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[1]

Definition

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

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

[1] Efron & Tibshirani (1994) 'An introduction to the bootstrap'

Multinomial Resampling[1]

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 $\sum v_i = N$:

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

[1]Efron & Tibshirani (1994) 'An introduction to the bootstrap'

Multinomial Resampling

Inversion Sampling

Draw uniform random variables

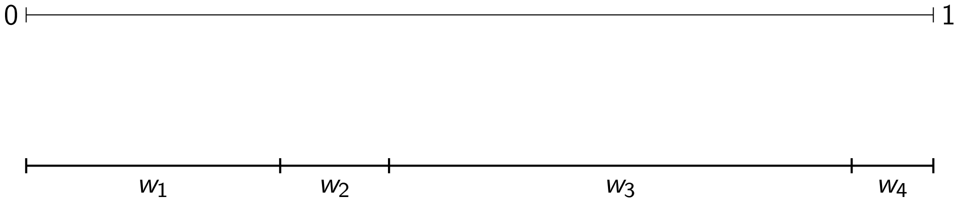
$$U_i \overset{iid}{\sim} \text{Uniform}(0,1); \qquad i = 1, \ldots, N$$

and determine the parental indices by inversion

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

Multinomial Resampling

Inversion Sampling



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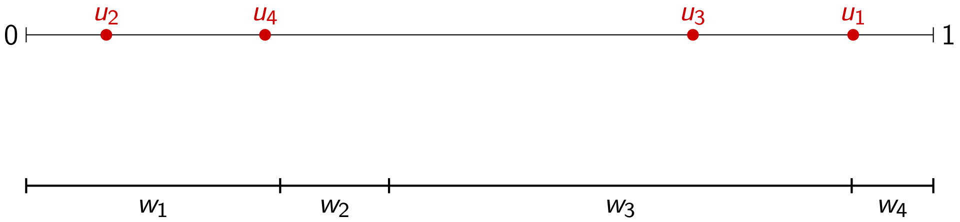

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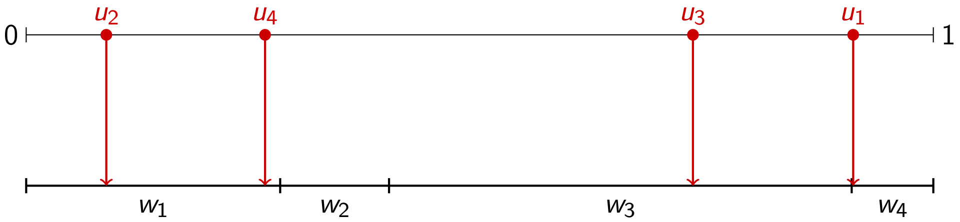


Residual Resampling[2,3]

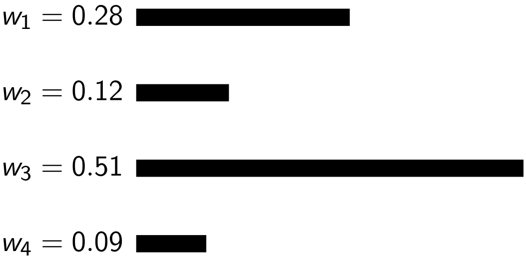
Definition

1. Deterministically assign $\lfloor Nw_i \rfloor$ offspring to particle i; i=1,. . . , 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 $r_i := \frac{1}{R}(Nw_i - \lfloor Nw_i \rfloor)$

[2] Liu & Chen (1998) 'Sequential Monte Carlo methods for dynamic systems'
[3] Whitley (1994) 'A genetic algorithm tutorial'

Residual Resampling

Illustration



Residual Resampling

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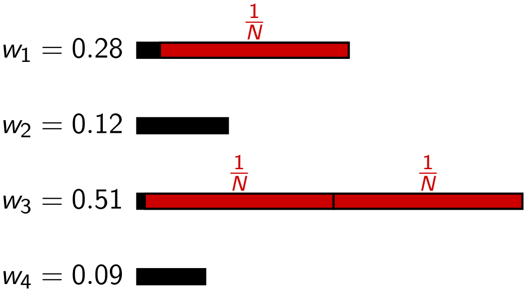

Residual Resampling

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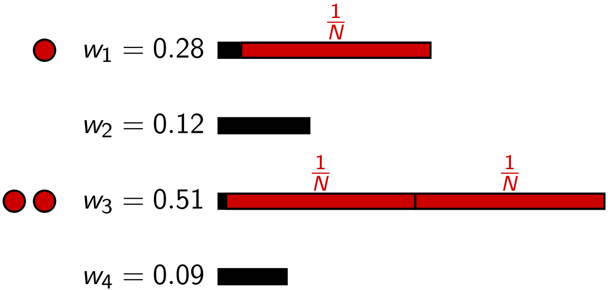


Residual Resampling

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

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

Stratified Resampling[4]

Definition

Draw uniformly from each stratified interval

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

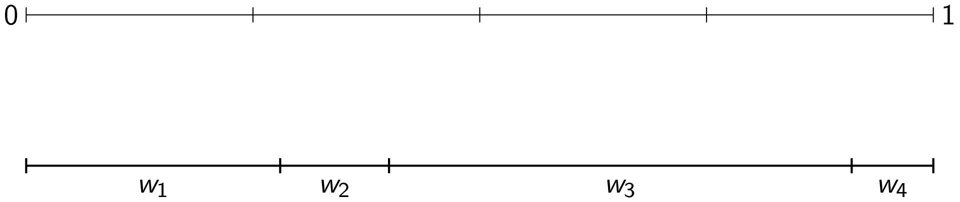
and determine the parental indices by inversion

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

[4] Kitagawa (1996) ‘Monte Carlo filter and smoother for non-Gaussian nonlinear state space models’

Stratified Resampling

Inversion Sampling



Stratified Resampling

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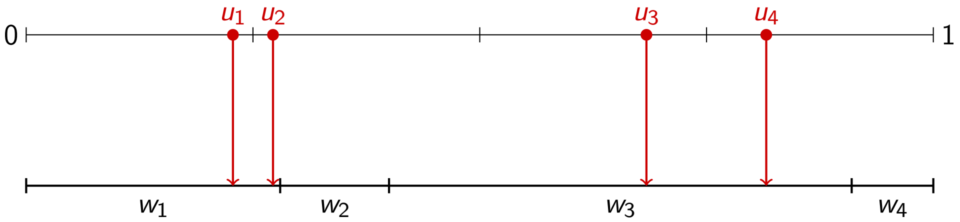


Systematic Resampling[5,6]

Definition

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

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

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

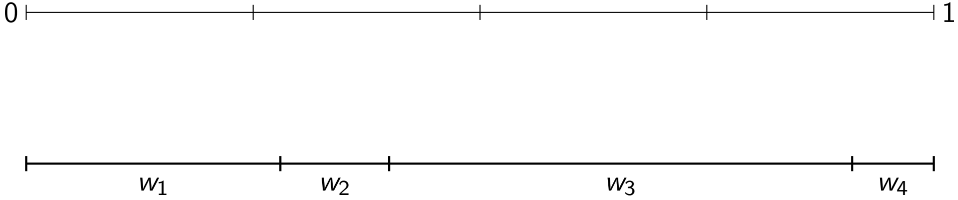
and determine the parental indices by inversion

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

[5] Carpenter, Clifford & Fearnhead (1999) 'Improved particle filter for nonlinear problems'
[6] Whitley (1994) 'A genetic algorithm tutorial'

Systematic Resampling

Inversion Sampling



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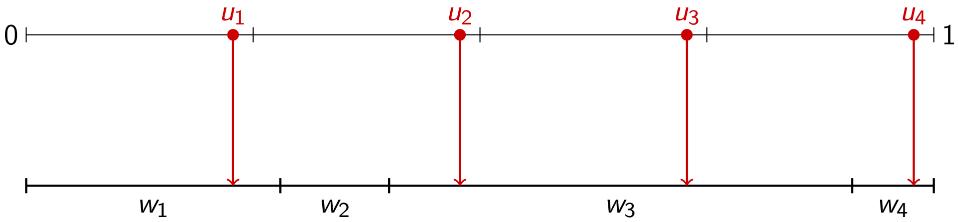

Properties of Resampling Schemes

Support of Offspring Counts

Suppose $w_i \in \left[\frac{k}{N}, \frac{k+1}{N}\right]$.
What are the possible values for v_i?

Multinomial: $v_i \in \{0, \ldots, N\}$

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

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:

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

[7]Douc, Cappé & Moulines (2005) 'Comparison of resampling schemes for particle filtering'

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In this sense we have[7]

$$\begin{aligned}\operatorname{Var}[\text{stratified}] &\leq \operatorname{Var}[\text{multinomial}]\\ \operatorname{Var}[\text{residual-stratified}] \leq \operatorname{Var}[\text{residual-multinomial}] &\leq \operatorname{Var}[\text{multinomial}]\end{aligned}$$

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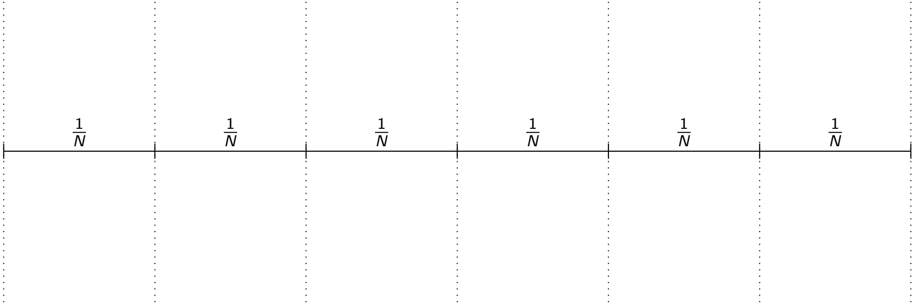
$w_{1:N} = \frac{1}{12}(3, 3, 2, 2, 1, 1)$

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

Answer: it depends on the ordering!

Properties of Resampling Schemes

Permutation Invariance



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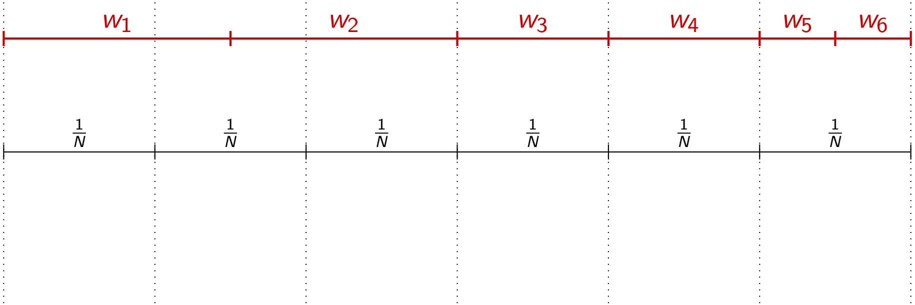

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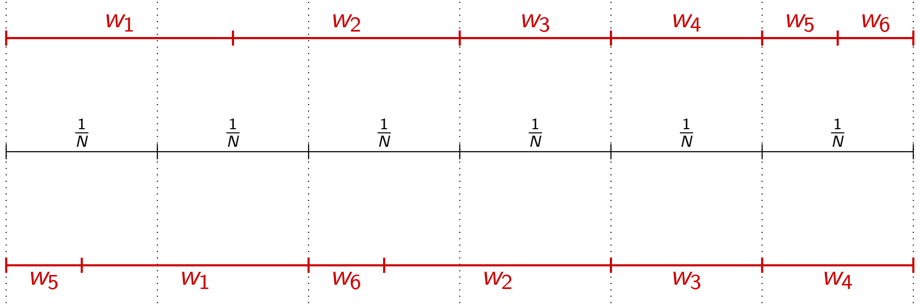

Properties of Resampling Schemes

Permutation Invariance

- Kitagawa[8] 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[9]
- Sorting by position could be a sort of proxy for sorting by weight

[8] Kitagawa (1996) 'Monte Carlo filter and smoother for non-Gaussian nonlinear state space models'

[9] 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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Degeneracy under Equal Weights

- Suppose all of the weights are multiples of $\frac{1}{N}$.
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- In particular, if $w_{1:N} = \frac{1}{N}(1, \ldots, 1)$, 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

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

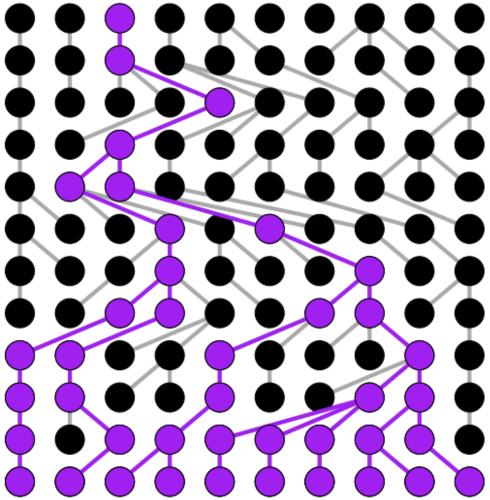
Properties of Resampling Schemes

Summary

	$\sup \lvert v_i - Nw_i \rvert$	low variance	invariant under permutations	degenerate if $w_{1:N} \propto (1, \ldots, 1)$
multinomial	N	$\times$	$\checkmark$	$\times$
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 ($N = 2$)

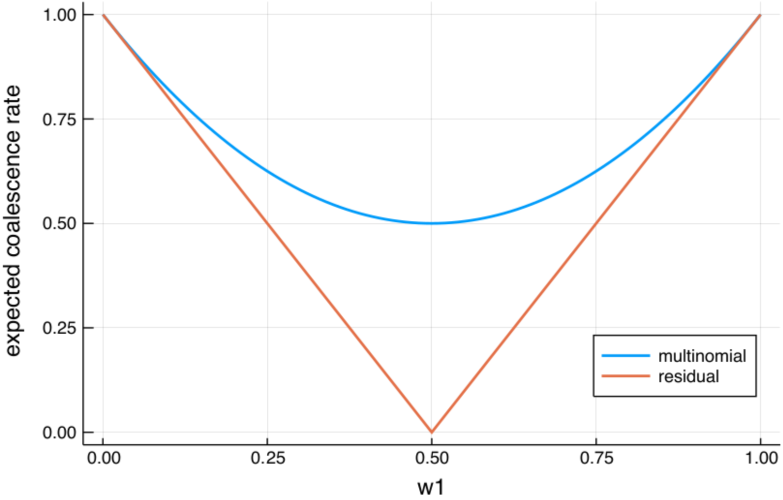
$$c_2 = \frac{1}{2}\left[v_1(v_1 - 1) + v_2(v_2 - 1)\right]$$

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



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- We also proved it in cases $N = 2$ and $N = 3$
- We conjecture that it holds for all finite N too
- It just remains to prove it for $N = 4, 5, \ldots$
- We proved that systematic resampling (and some others) dominate multinomial in expected coalescence probability, for all N.

THE END