# Sequential Monte Carlo and Rare Events 

Adam M. Johansen<br>a.m.johansen@warwick.ac.uk<br>http://go.warwick.ac.uk/amjohansen/talks/<br>ST912 Statistical Frontiers Seminar<br>February 2022



## Overview

Motivating Problem Estimating (very) Small Probabilities Monte Carlo Solutions Sequential Monte Carlo algorithms<br>Feynman-Kac Formulae A mathematical description<br>Splitting-type Algorithms SMC for Rare Events<br>Unbiased Splitting Unbiased Algorithms in Continuous Time

# Rare Event Estimation/Simulation 

A Motivating Problem

## Context

- Given a probability space $(\Omega, \mathcal{F}, \mathbb{P})$,
- and a random element $X:(\Omega, \mathcal{F}) \rightarrow(E, \mathcal{E})$,
- what is $\mathbb{P}(X \in A)=\mathbb{P} \circ X^{-1}(A)=\mathbb{P}(\{\omega \in \Omega: X(\omega) \in A\})$,
- for some $A \in \mathcal{E}$ such that $\mathbb{P}(X \in A) \ll 1$ ?



## Some Simple Examples

1. A really simple problem.

- Let

$$
f(x)=\frac{1}{\sqrt{2 \pi}} \exp \left(-\frac{x^{2}}{2}\right)
$$

- What is $\mathbb{P}(X \in A)$ if $A=[a, \infty)$ for $a \gg 1$ ?
- Simple semi-analytic solution $1-\Phi(a)$.

2. A somewhat harder problem:

- Let

$$
f(\mathbf{x})=\frac{1}{\sqrt{|2 \pi \Sigma|}} \exp \left(-\frac{1}{2} \mathbf{x}^{T} \Sigma^{-1} \mathbf{x}\right)
$$

- What is $\mathbb{P}(X \in A)$ if $A=\otimes_{i=1}^{d}\left[a_{i}, b_{i}\right]$ ?
- What can we say about $\left.\operatorname{Law}(X)\right|_{A}$

3. Getting more interesting:

- Let $d X_{t}=a\left(X_{t}\right) d t+b\left(X_{t}\right) d B_{t}$.
- What is $\mathbb{P}\left(\zeta\left(X_{[0, T]}\right) \in A\right)$ ?
- What is $\mathbb{P}\left(X_{\sigma} \in A\right)$ if $\sigma=\inf \left\{t: X_{t} \in A \cup R\right\}$ ?


## Sampling Approaches

## The Monte Carlo Method

- Given a probability density, $f$, and $\varphi: E \rightarrow \mathbb{R}$

$$
I=\int_{E} \varphi(x) f(x) d x
$$

- Simple Monte Carlo solution:
- Sample $X_{1}, \ldots, X_{N} \stackrel{\text { i.i.d. }}{\sim} f$.
- Estimate $\hat{I}=\frac{1}{N} \sum_{i=1}^{N} \varphi\left(X_{i}\right)$.

Justified by the law of large numbers... and the central limit theorem.

- Can also be viewed as approximating $\pi(d x)=f(x) d x$ with

$$
\widehat{\pi}^{N}(d x)=\frac{1}{N} \sum_{i=1}^{N} \delta_{x_{i}}(d x)
$$

Justified by Glivenko-Cantelli type results.

## The Monte Carlo Method and Rare Events

- Use $\mathbb{P}(X \in A) \equiv \mathbb{E}\left[\mathbb{I}_{A}(X)\right]=I\left(\mathbb{I}_{A}\right)$.
- Then, directly:

$$
\mathbb{P}(X \in A) \approx \hat{I}_{n}\left(\mathbb{I}_{A}\right)=\frac{\left|A \cap\left\{X_{1}, \ldots, X_{n}\right\}\right|}{n}
$$

## Simple Monte Carlo and the Toy Problem

| $a$ | $\log \left(\hat{l}_{10^{k}}\left(\mathbb{I}_{[a, \infty)}\right)\right)$ |  |  |  |  |  |  |  | $\log$ |
| :--- | ---: | ---: | ---: | ---: | ---: | ---: | ---: | ---: | ---: |
|  | k | 1 | 2 | 3 | 4 | 5 | 6 | 7 | $1-\Phi(a)$ |
| 1 | -2.30 | -1.66 | -1.80 | -1.82 | -1.83 | -1.84 | -1.84 | -1.84 |  |
| 2 |  | -3.91 | -3.73 | -3.76 | -3.78 | -3.79 | -3.79 | -3.78 |  |
| 3 |  |  |  | -6.91 | -6.81 | -6.59 | -6.60 | -6.61 | -6.61 |
| 4 |  |  |  |  | -10.12 | -10.26 | -10.42 | -10.36 |  |
| 5 |  |  |  |  |  |  |  | -14.73 | -15.06 |
| 6 |  |  |  |  |  |  |  |  | -20.74 |

Simple calculations reveal:

$$
\begin{aligned}
& >\mathbb{E}\left[\hat{l}_{n}\left(\mathbb{I}_{[a, \infty)}\right)\right]=\mathbb{P}(X \in[a, \infty)) \\
& >\operatorname{Var}\left[\hat{l}_{n}\left(\mathbb{I}_{[a, \infty)}\right)\right]=\frac{1}{n} \mathbb{P}(X \in[a, \infty))(1-\mathbb{P}(X \in[a, \infty)))
\end{aligned}
$$

- So the relative standard deviation is $\sim(n \mathbb{P}(X \in[a, \infty)))^{-1 / 2}$.


## Simple Monte Carlo and the Toy Problem

| $a$ | $\log \left(\hat{l}_{0^{\kappa}}\left(\mathbb{I}_{[a, \infty)}\right)\right)$ |  |  |  |  |  |  | $\log$ |  |
| :--- | ---: | ---: | ---: | ---: | ---: | ---: | ---: | ---: | ---: |
|  | $k$ | 1 | 2 | 3 | 4 | 5 | 6 | 7 | $1-\Phi(a)$ |
| 1 | -2.30 | -1.66 | -1.80 | -1.82 | -1.83 | -1.84 | -1.84 | -1.84 |  |
| 2 |  | -3.91 | -3.73 | -3.76 | -3.78 | -3.79 | -3.79 | -3.78 |  |
| 3 |  |  | -6.91 | -6.81 | -6.59 | -6.60 | -6.61 | -6.61 |  |
| 4 |  |  |  |  | -10.12 | -10.26 | -10.42 | -10.36 |  |
| 5 |  |  |  |  |  |  | -14.73 | -15.06 |  |
| 6 |  |  |  |  |  |  |  | -20.74 |  |

Simple calculations reveal:

- $\mathbb{E}\left[\hat{I}_{n}\left(\mathbb{I}_{[a, \infty)}\right)\right]=\mathbb{P}(X \in[a, \infty))$
- $\operatorname{Var}\left[\hat{I}_{n}\left(\mathbb{I}_{[a, \infty)}\right)\right]=\frac{1}{n} \mathbb{P}(X \in[a, \infty))(1-\mathbb{P}(X \in[a, \infty)))$
- So the relative standard deviation is $\sim(n \mathbb{P}(X \in[a, \infty)))^{-1 / 2}$.


## Variance Reduction

- Want $\hat{p}_{n}$ such that $\hat{p}_{n} \approx \mathbb{P}(X \in A)=: p$ :
- Ideally, with $\mathbb{E}\left[\hat{p}_{n}\right]=p$.
- Such that $\operatorname{Var}\left(\hat{p}_{n}\right) \ll p^{2}$.
- For modest $n$.
- Controlling variance is the key issue.
- Importance Sampling.
- Splitting.
- Interacting Particle Systems.
- Sequential Monte Carlo.


## The Importance-Sampling Identity

- Given $g$, such that
- $f(x)>0 \Rightarrow g(x)>0$
- and $f(x) / g(x)<\infty$, define $w(x)=f(x) / g(x)$ and:

$$
\int \varphi(x) f(x) d x=\int \varphi(x) f(x) g(x) / g(x) d x=\int \varphi(x) w(x) g(x) d x
$$

- This suggests the importance sampling estimator:
- Sample $X_{1}, \ldots, X_{N} \stackrel{\text { i.i.d. }}{\sim} g$.
- Estimate $\widehat{I}=\frac{1}{N} \sum_{i=1}^{N} w\left(X_{i}\right) \varphi\left(X_{i}\right)$.
- Can also be viewed as approximating $\pi(d x)=f(x) d x$ with

$$
\widehat{\pi}^{N}(d x)=\frac{1}{N} \sum_{i=1}^{N} w\left(X_{i}\right) \delta_{X_{i}}(d x) .
$$

## Importance Sampling Example



## Importance Sampling Variance

The variance of this estimator is:

$$
\begin{aligned}
& \operatorname{Var}\left[\frac{1}{n} \sum_{i=1}^{n} w\left(Y_{i}\right) \varphi\left(Y_{i}\right)\right] \\
= & \frac{1}{n} \operatorname{Var}\left[w\left(Y_{1}\right) \varphi\left(Y_{1}\right)\right] \\
= & \frac{1}{n}\left\{\mathbb{E}\left[\left(w\left(Y_{1}\right) \varphi\left(Y_{1}\right)\right)^{2}\right]-\mathbb{E}\left[w\left(Y_{1}\right) \varphi\left(Y_{1}\right)\right]^{2}\right\} \\
= & \frac{1}{n}\left\{\int(w(y) \varphi(y))^{2} g(d y)-\left(\int w(y) \varphi(y) g(d y)\right)^{2}\right\} \\
= & \frac{1}{n}\left\{\int w(y) \varphi^{2}(y) f(d x)-\mathbb{E}[\varphi(X)]^{2}\right\}
\end{aligned}
$$

## Optimal Importance Sampling

## Proposition

Let $X \sim f$, where $f(d x)=f(x) d x$, with values in $(E, \mathcal{E})$ and let $\phi: \mathbb{R} \rightarrow(0, \infty)$ a function of interest. The proposal which minimizes the variance of the importance sampling estimator of $\mathbb{E}[\varphi(X)]$ is $g(x) d x$, where:

$$
g(x)=\frac{f(x) \varphi(x)}{\int f(y) \varphi(y) d y}
$$

Note: if $E \supset A \supset \operatorname{supp} \varphi(x)$, it suffices for $\left.\left.f\right|_{A} \ll g\right|_{A}$.

## Importance Sampling and the Toy Problem

| $a$ | $k$ | $\log \left(\hat{l}_{10^{k}}\left(\mathbb{I}_{[a, \infty)}\right)\right)$ |  |  |  |  |  |  |  | $\log$ |
| :--- | ---: | ---: | ---: | ---: | ---: | ---: | ---: | :---: | :---: | :---: |
|  | 1 | 2 | 3 | 4 | 5 | 6 | 7 |  |  |  |
| $1-\Phi(a)$ |  |  |  |  |  |  |  |  |  |  |
| 1 | -1.72 | -1.84 | -1.83 | -1.84 | -1.84 | -1.84 | -1.84 |  |  |  |
| 2 | -3.63 | -3.78 | -3.79 | -3.78 | -3.78 | -3.78 | -3.78 |  |  |  |
| 3 | -6.43 | -6.59 | -6.63 | -6.60 | -6.61 | -6.61 | -6.61 |  |  |  |
| 4 | -10.16 | -10.34 | -10.40 | -10.35 | -10.36 | -10.36 | -10.36 |  |  |  |
| 5 | -14.85 | -15.04 | -15.12 | -15.06 | -15.07 | -15.06 | -15.06 |  |  |  |
| 6 | -20.51 | -20.72 | -20.81 | -20.73 | -20.73 | -20.74 | -20.74 |  |  |  |
| 7 | -27.16 | -27.37 | -27.46 | -27.38 | -27.39 | -27.38 | -27.38 |  |  |  |
| 8 | -34.79 | -35.01 | -35.10 | -35.02 | -35.01 | -35.01 | -35.01 |  |  |  |
| 9 | -43.41 | -43.64 | -43.73 | -43.63 | -43.63 | -43.63 | -43.62 |  |  |  |
| -20.74 |  |  |  |  |  |  |  |  |  |  |
|  |  |  | -27.38 |  |  |  |  |  |  |  |
| -43.63 |  |  |  |  |  |  |  |  |  |  |

Using $g(x)=\exp (-(x-a)) \mathbb{I}_{[a, \infty)}(x)$.

## Self-Normalised Importance Sampling

- Often, $f$ is known only up to a normalising constant.
- If $v(x)=c f(x) / g(x)=c w(x)$, then

$$
\frac{\mathbb{E}_{g}(v \varphi)}{\mathbb{E}_{g}(v \mathbf{1})}=\frac{\mathbb{E}_{g}(c w \varphi)}{\mathbb{E}_{g}(c w \mathbf{1})}=\frac{c \mathbb{E}_{f}(\varphi)}{c \mathbb{E}_{f}(\mathbf{1})}=\mathbb{E}_{f}(\varphi)
$$

- Estimate the numerator and denominator with the same sample:

$$
\widehat{\imath}=\frac{\sum_{i=1}^{N} v\left(X_{i}\right) \varphi\left(X_{i}\right)}{\sum_{i=1}^{N} v\left(X_{i}\right)}
$$

- Biased for finite samples, but consistent.
- Typically reduces variance.


## Discrete Time Markov Processes and Rare Events

- Often rare events are described in terms of a process.
- In discrete time, say

$$
X_{1} \sim p_{1}\left(x_{1}\right) d x_{1} \quad X_{n} \mid X_{1: n-1} \sim p_{n}\left(x_{n} \mid x_{n-1}\right) d x_{n}
$$

where each $X_{i}$ takes values in a space $E$.

- Questions might be of the form what is $\mathbb{P}\left(\xi\left(X_{1: n}\right) \in A\right)$ for $\xi: E^{n} \rightarrow \mathbb{R}$ and $A \subset \mathbb{R}$ :
- E.g. If $E=\mathbb{R}, p_{1}\left(x_{1}\right) \propto \exp \left(-x_{1}^{2} / 2\right)$ and

$$
p_{n}\left(x_{n} \mid x_{n-1}\right) \propto \exp \left(-\left(x_{n}-x_{n-1}^{2}\right) / 2\right) \text { and } A=[a, \infty) .
$$

- If $p_{1}, \ldots$ characterizes the evolution of differential group delay in a fibre optic cable $A=[a, \infty)$ and

$$
\xi\left(x_{1: n}\right)=\max \left\{\left\|\sum_{p=1}^{q} \xi^{\prime}\left(x_{q}\right)\right\|: q \leq n\right\}
$$

where $\xi^{\prime}$ is essentially a projection of the underlying state one arrives at a real engineering problem.

- We'll return to continuous time processes later.


## Importance Sampling for DTMPs

- Sample $\left\{X_{1: n}^{(i)}\right\}$ at time $n$ from $q_{n}\left(x_{1: n}\right)$, define

$$
w_{n}\left(x_{1: n}\right) \propto \frac{p_{n}\left(x_{1: n}\right)}{q_{n}\left(x_{1: n}\right)}
$$

where $\left.p_{n}\left(x_{1: n}\right)=p_{1}\left(x_{1}\right) \prod_{m=2}^{n} p_{( } m x_{m} \mid x_{m-1}\right)$.

- set $W_{n}^{(i)}=w_{n}\left(X_{1: n}^{(i)}\right) / \sum_{j} w_{n}\left(X_{1: n}^{(j)}\right)$,
- then $\left\{W_{n}^{(i)}, X_{n}^{(i)}\right\}$ is a consistently weighted sample.
- This seems inefficient.


## Sequential Importance Sampling (SIS) I

- Importance weight

$$
\begin{aligned}
w_{n}\left(x_{1: n}\right) & \propto \frac{p_{1}\left(x_{1}\right) \prod_{m=2}^{n} p_{m}\left(x_{m} \mid x_{m-1}\right)}{q_{n}\left(x_{1: n}\right)} \\
& =\frac{p_{1}\left(x_{1}\right)}{q_{n}\left(x_{1}\right)} \prod_{m=2}^{n} \frac{p_{m}\left(x_{m} \mid x_{m-1}\right)}{q_{n}\left(x_{m} \mid x_{1: m-1}\right)}
\end{aligned}
$$

- Given $\left\{W_{n-1}^{(i)}, X_{1: n-1}^{(i)}\right\}$ targetting $p_{n-1}\left(x_{1: n-1}\right)$
- Let $q_{n}\left(x_{1: n-1}\right)=q_{n-1}\left(x_{1: n-1}\right)$,
- sample $X_{n}^{(i)} \stackrel{\text { i.i.d. }}{\sim} q_{n}\left(\cdot \mid X_{1: n-1}^{(i)}\right)$ or even $q_{n}\left(\cdot \mid X_{n-1}^{(i)}\right)$.


## Sequential Importance Sampling (SIS) II

- And update the weights:

$$
\begin{aligned}
w_{n}\left(x_{1: n}\right) & =w_{n-1}\left(x_{1: n-1}\right) \frac{p\left(x_{n} \mid x_{n-1}\right)}{q_{n}\left(X_{n} \mid x_{n-1}\right)} \\
W_{n}^{(i)} & =w_{n}\left(X_{1: n}^{(i)}\right) \\
& =w_{n-1}\left(X_{1: n-1}^{(i)}\right) \frac{p\left(X_{n}^{(i)} \mid X_{n-1}^{(i)}\right)}{q_{n}\left(X_{n}^{(i)} \mid X_{n-1}^{(i)}\right)} \\
& =W_{n-1}^{(i)} \frac{p\left(X_{n}^{(i)} \mid X_{n-1}^{(i)}\right)}{q_{n}\left(X_{n}^{(i)} \mid X_{n-1}^{(i)}\right)}
\end{aligned}
$$

- If $\int p\left(x_{1: n} \mid y_{1: n}\right) d x_{n} \approx p\left(x_{1: n-1} \mid y_{1: n-1}\right)$ this makes sense.
- We only need to store $\left\{W_{n}^{(i)}, X_{n-1: n}^{(i)}\right\}$.
- Same computation every iteration.


## Importance Sampling on Huge Spaces Doesn't Work

- It's said that IS breaks the curse of dimensionality:

$$
\sqrt{N}\left[\frac{1}{N} \sum_{i=1}^{N} w\left(X_{i}\right) \varphi\left(X_{i}\right)-\int \varphi(x) f(x) d x\right] \xrightarrow{d} \mathcal{N}\left(0, \operatorname{Var}_{g}[w \varphi]\right)
$$

- This is true.
- But it's not enough.
- $\operatorname{Var}_{g}[w \varphi]$ increases (often exponentially) with dimension.
- Eventually, an SIS estimator (of $p\left(x_{1: n}\right)$ ) will fail.
- But $p\left(x_{n}\right)=\int p\left(x_{1: n}\right) d x_{1: n-1}$ is a fixed-dimensional distribution... which has implications which we will revisit.


## Multilevel Splitting

## Returning to continuous time processes

## Splitting

An insight dating back to the 1950s:


Allowing $\sigma_{B_{i}}=\inf \left\{t: X_{t} \in B_{i} \cup A\right\}$ :

$$
\mathbb{P}\left(X_{\sigma_{B}} \in B\right)=\mathbb{P}\left(X_{\sigma_{B_{1}}} \in B_{1}\right) \prod_{i=2}^{m} \mathbb{P}\left(X_{\sigma_{B_{i}}} \in B_{i} \mid X_{\sigma_{B_{i-1}}} \in B_{i-1}\right)
$$

where $B_{1} \subset B_{2} \subset \cdots \subset B_{m}=B$ and $A$ is positive recurrent for $X$.
We can estimate each term separately.

## The Discrete Skeleton of MLS

Algorithmically, this idealised algorithm reduces a continuous-time problem to a discrete-time on:

- Let $\lambda$ denote the initial distribution: $X(0) \sim \lambda$.
- Define $U_{i}=\left(\sigma_{B_{i}}, X_{B_{i}}\left(\sigma_{i}\right)\right), i=1, \ldots, m$
- Let $M_{i}:\left(\mathbb{R}_{\geq 0} \times \mathbb{R}^{d}\right) \times \mathcal{S} \rightarrow[0,1]$ denote the Markov kernels of this discrete-time process ${ }^{1}$.
- Define $G_{i}: \mathbb{R}_{\geq 0} \times \mathbb{R}^{d} \rightarrow\{0,1\}$ as:

$$
G_{i}(t, x)= \begin{cases}1, & \text { if } x \in B_{i} \\ 0, & \text { otherwise }\end{cases}
$$

${ }^{1}$ Where $\mathcal{S}$ be the Borel sigma algebra associated with $\mathbb{R}_{\geq 0} \times \mathbb{R}^{d}$

## The Algorithm

Algorithm Idealised Multilevel Splitting
Given $\lambda ; G_{1}, \ldots, G_{m} ; M_{1}, \ldots, M_{m} ; N_{0}$; and $R_{1}, \ldots, R_{m-1}$ :

1. For $j=1, \ldots, N_{0}$, draw independently:

$$
X_{1}^{j}(0) \sim \lambda \text { and } U_{1}^{j} \sim M_{1}\left(\left(0, X_{1}^{j}(0)\right), \cdot\right) .
$$

2. Let $S_{1}=\left\{U_{1}^{j}: G_{1}\left(U_{1}^{j}\right)=1\right\}$ be the survivors, and $N_{1}=\left|S_{1}\right|$.
3. For $i=2, \ldots, m$ :
3.1 If $N_{i-1}=0$, return $\hat{p}=0$.
3.2 Given $S_{i-1}=\left\{\bar{U}_{i-1}^{j}\right\}_{j=1}^{N_{i-1}}$, for all $(j, k) \in\left\{\left(j^{\prime}, k^{\prime}\right): 1 \leq j^{\prime} \leq N_{i-1}, 1 \leq k^{\prime} \leq R_{i-1}\right\}$ sample independently $U_{i}^{j, k} \sim M_{i}\left(\bar{U}_{i-1}^{j}, \cdot\right)$.
3.3 Let $S_{i}=\left\{U_{i}^{j, k}: G_{i}\left(U_{i}^{j, k}\right)=1\right\}$, and $N_{i}=\left|S_{i}\right|$.
4. Return $\hat{p}=\frac{N_{m}}{N_{0} \prod_{i=1}^{m-1} R_{i}}$.

Requires the choice of $R_{1}, \ldots, R_{m-1}$ and samples from
$M_{1}, \ldots, M_{m}$.
Statistics

## Beyond Idealised Multilevel Splitting

Fixed-effort Splitting Addresses the first issue.

- Rather than fixing $R_{i}$, fix $N_{i}$.
- Sample $N_{i}$ times with replacement from the survivors from the previous iteration.
- Or something motivated by similar considerations.
- Can be analysed directly, but it can also be viewed as a particular instance of sequential Monte Carlo.
Multilevel Splitting with Couplings Addresses the second.
- Avoid sampling from $M_{1}, \ldots, M_{m}$.
- Instead sample from a more tractable transition.
- Utilizes $\varepsilon$-strong simulation from the law of diffusion processes.
- And an additional modification to make the algorithm tractable.


## SMC: Sequential Importance Resampling

## Resampling

- We can produce unweighted samples from weighted ones.
- Given $\left\{W_{i}, X_{i}\right\}_{i=1}^{N}$ an unbiased resampling $\left\{\tilde{X}_{i}\right\}_{i=1}^{N}$ is such that

$$
\mathbb{E}\left[\left.\frac{1}{N} \sum_{i=1}^{N} \varphi\left(\tilde{X}_{i}\right) \right\rvert\,\left\{W_{i}, X_{i}\right\}_{i=1}^{N}\right]=\sum_{i=1}^{N} W_{i} \varphi\left(X_{i}\right)
$$

for any continuous bounded $\varphi$.

- Simplest option: sample from empirical distribution

$$
\tilde{X}_{1}, \ldots, \tilde{X}_{N} \stackrel{i i d}{\sim} \sum_{j=1}^{N} W_{j} \delta_{X_{j}}(\cdot)
$$

- Other approaches reduce the additional variance.


## The SIR[esampling] Algorithm

- Problem: variance of the weights in SIS builds up over time.
- Solution? Given $\left\{W_{n-1}^{(i)}, X_{1: n-1}^{(i)}\right\}$ :

1. Resample, to obtain $\left\{\frac{1}{N}, \widetilde{X}_{1: n-1}^{(i)}\right\}$.
2. Sample $X_{n}^{(i)} \sim q_{n}\left(\cdot \mid \widetilde{X}_{n-1}^{(i)}\right)$.
3. Set $X_{1: n-1}^{(i)}=\widetilde{X}_{1: n-1}^{(i)}$.
4. Set $W_{n}^{(i)} \propto p_{n}\left(X_{n}^{(i)} \mid X_{n-1}^{(i)}\right) / q_{n}\left(X_{n}^{(i)} \mid X_{n-1}^{(i)}\right)$ with $\sum_{i} W_{n}^{(i)}=1$.

- And continue as with SIS.
- Actually, we only need to be able to evaluate up to a normalizing constant: see step 4.
- There is a cost, but this really works... at least for some problems.

Iteration 2


Iteration 3


Iteration 4


Iteration 5


Iteration 6


Iteration 7


Iteration 8


Iteration 9


Iteration 10


## What Are the Target and Proposal for Splitting?

- Let

$$
\begin{aligned}
q_{1}\left(\tau_{1}, x_{1}\right) & =\int \lambda\left(d x_{0}\right) M_{1}\left(\left(0, x_{0}\right), \cdot\right) \\
q_{i} & =\int M_{i}\left(\left(\sigma_{i}, x_{i}\right), \cdot\right) \quad i=2, \ldots, m
\end{aligned}
$$

- Let $G_{i}\left(\tau_{i}, x_{i}\right)=\mathbb{I}_{B_{i}}\left(x_{i}\right)$
- Set

$$
\gamma_{i}\left(d\left(\tau_{j}, x_{j}\right)_{j=1}^{i}\right)=q_{1}\left(\tau_{1}, x_{1}\right) G_{1}\left(\tau_{1}, x_{1}\right) \prod_{j=1}^{i} q_{i}\left(\left(\tau_{i-1}, x_{i-1}\right), d\left(\tau_{i}, x_{i}\right)\right)
$$

$$
p_{i} \propto \gamma_{i}
$$

- In sampling we only need $\gamma_{i}$ and can recover estimates of its normalizing constant.


## Feynman-Kac Formulæ

## A Probabilistic Perspective

This entire section can be skipped and the rest of the presentation should remain accessible, it's here only for those who are interested in the probabilistic foundations of these algorithms.

## Feynman-Kac Formulæ

- A natural description for measure-valued stochastic processes.
- Model for:
- Particle motion in absorbing environments.
- Classes of branching particle system.
- Simple genetic algorithms.
- Particle filters and related algorithms.

Elements of this framework:

- Probabilistic Construction
- Semigroup[oid] Structure
- McKean Interpretations
- Particle Approximations
- Selected Results


# Probabilistic Construction 

Following Del Moral (2004)

## The Canonical Markov Chain

- Consider the filtered probability space:

$$
\left(\Omega, \mathcal{F},\left\{\mathcal{F}_{n}\right\}_{n \in \mathbb{N}}, \mathbb{P}_{\mu}\right)
$$

- Let $\left\{X_{n}\right\}_{n \in \mathbb{N}}$ be a Markov chain such that for any $n \in \mathbb{N}$ :

$$
\mathbb{P}_{\mu}\left(X_{1: n} \in d x_{1: n}\right)=\mu\left(d x_{1}\right) \prod_{i=2}^{n} M_{i}\left(x_{i-1}, d x_{i}\right)
$$

$$
X_{i}: \Omega \rightarrow E_{i} \quad \mu \in \mathcal{P}\left(E_{1}\right) \quad M_{i}: E_{i-1} \rightarrow \mathcal{P}\left(E_{i}\right)
$$

- $\left(E_{i}, \mathcal{E}_{i}\right)$ are measurable spaces.
- The $X_{i}$ are $\mathcal{E}_{i} / \mathcal{F}_{i}$-measurable.
- Using Kolmogorov's/Tulcea's extension theorem there exists a unique process-valued extension.


## Some Operator Notation

Given two measurable spaces, $(E, \mathcal{E})$ and $(F, \mathcal{F})$, a measure $\mu$ on $(E, \mathcal{E})$ and a Markov kernel, $K: E \rightarrow \mathcal{P}(F)$, define:

$$
\begin{aligned}
\mu\left(\varphi_{E}\right) & :=\int \mu(d x) \varphi_{E}(x) & \\
\mu K\left(\varphi_{F}\right) & :=\int \mu(d x) K(x, d y) \varphi_{F}(y) & \mu K \in \mathcal{P}(F) \\
K\left(\varphi_{F}\right)(x) & :=\int K(x, d y) \varphi_{F}(y) & K\left(\varphi_{F}\right): E \rightarrow \mathbb{R}
\end{aligned}
$$

with $\varphi_{E}, \varphi_{F}$ suitably measurable functions.
Given two functions, $g, h: E \rightarrow \mathbb{R}$, define $g \cdot h: E \rightarrow \mathbb{R}$ via $(g \cdot h)(x)=g(x) h(x)$.

Given $e: E \rightarrow \mathbb{R}$ and $f: F \rightarrow \mathbb{R}$, let $(e \otimes f)(x, y):=e(x) f(y)$.

## The Feynman-Kac Formulæ

- Given $\mathbb{P}_{\mu}$ and potential functions:

$$
\left\{G_{i}\right\}_{i \in \mathbb{N}} \quad G_{i}: E_{i} \rightarrow[0, \infty)
$$

- Define two path measures weakly:

$$
\begin{aligned}
\mathbb{Q}_{n}\left(\varphi_{1: n}\right) & =\frac{\mathbb{E}\left[\varphi_{1: n}\left(X_{1: n}\right) \prod_{i=1}^{n-1} G_{i}\left(X_{i}\right)\right]}{\mathbb{E}\left[\prod_{i=1}^{n-1} G_{i}\left(X_{i}\right)\right]} \\
\widehat{\mathbb{Q}}_{n}\left(\varphi_{1: n}\right) & =\frac{\mathbb{E}\left[\varphi_{1: n}\left(X_{1: n}\right) \prod_{i=1}^{n} G_{i}\left(X_{i}\right)\right]}{\mathbb{E}\left[\prod_{i=1}^{n} G_{i}\left(X_{i}\right)\right]}
\end{aligned}
$$

where $\varphi_{1: n}: \otimes_{i=1}^{n} E_{i} \rightarrow \mathbb{R}$.

## Example (Filtering via FK Formulæ: Prediction)

- Let $\mu\left(x_{1}\right)=f\left(x_{1}\right), M_{n}\left(x_{n-1}, d x_{n}\right)=f\left(x_{n} \mid x_{n-1}\right) d x_{n}$.
- Let $G_{n}\left(x_{n}\right)=g\left(y_{n} \mid x_{n}\right)$.
- Then:

$$
\begin{aligned}
\mathbb{Q}_{n}\left(\varphi_{1: n}\right) & =\mathbb{E}\left[\varphi_{1: n}\left(X_{1: n}\right) \prod_{i=1}^{n-1} G_{i}\left(X_{i}\right)\right] / \mathbb{E}\left[\prod_{i=1}^{n-1} G_{i}\left(X_{i}\right)\right] \\
& =\mathbb{E}\left[\varphi_{1: n}\left(X_{1: n}\right) \prod_{i=1}^{n-1} g\left(y_{i} \mid X_{i}\right)\right] / \mathbb{E}\left[\prod_{i=1}^{n-1} g\left(y_{i} \mid X_{i}\right)\right] \\
& =\frac{\int\left[f\left(x_{1}\right) \prod_{i=2}^{n} f\left(x_{i} \mid x_{i-1}\right)\right]\left[\prod_{j=1}^{n-1} g\left(y_{j} \mid x_{j}\right)\right] \varphi_{1: n}\left(x_{1: n}\right) d x_{1: n}}{\int\left[f\left(x_{1}\right) \prod_{i=2}^{n} f\left(x_{i} \mid x_{i-1}\right)\right]\left[\prod_{j=1}^{n-1} g\left(y_{j} \mid x_{j}\right)\right] d x_{1: n}} \\
& =\int p\left(x_{1: n} \mid y_{1: n-1}\right) \varphi_{1: n}\left(x_{1: n}\right) d x_{1: n}
\end{aligned}
$$

## Example (Filtering via FK Formulæ: Update/Filtering)

- Whilst:

$$
\begin{aligned}
\widehat{\mathbb{Q}}_{n}\left(\varphi_{1: n}\right) & =\mathbb{E}\left[\varphi_{1: n}\left(X_{1: n}\right) \prod_{i=1}^{n} G_{i}\left(X_{i}\right)\right] / \mathbb{E}\left[\prod_{i=1}^{n} G_{i}\left(X_{i}\right)\right] \\
& =\mathbb{E}\left[\varphi_{1: n}\left(X_{1: n}\right) \prod_{i=1}^{n} g\left(y_{i} \mid X_{i}\right)\right] / \mathbb{E}\left[\prod_{i=1}^{n} g\left(y_{i} \mid x_{i}\right)\right] \\
& =\frac{\int\left[f\left(x_{1}\right) \prod_{i=2}^{n} f\left(x_{i} \mid x_{i-1}\right)\right]\left[\prod_{j=1}^{n} g\left(y_{j} \mid x_{j}\right)\right] \varphi_{1: n}\left(x_{1: n}\right) d x_{1: n}}{\int\left[f\left(x_{1}\right) \prod_{i=2}^{n} f\left(x_{i} \mid x_{i-1}\right)\right]\left[\prod_{j=1}^{n} g\left(y_{j} \mid x_{j}\right)\right] d x_{1: n}} \\
& =\int p\left(x_{1: n} \mid y_{1: n}\right) \varphi_{1: n}\left(x_{1: n}\right) d x_{1: n}
\end{aligned}
$$

## Feynman-Kac Marginal Measures

We are typically interested in marginals:

$$
\begin{array}{rlrl}
\text { "Predicted" } & \text { "Updated" } \\
\gamma_{n}\left(\varphi_{n}\right) & =\mathbb{E}\left[\varphi_{n}\left(X_{n}\right) \prod_{i=1}^{n-1} G_{i}\left(X_{i}\right)\right] & \widehat{\gamma}_{n}\left(\varphi_{n}\right) & =\mathbb{E}\left[\varphi_{n}\left(X_{n}\right) \prod_{i=1}^{n} G_{i}\left(X_{i}\right)\right] \\
\eta_{n}\left(\varphi_{n}\right) & =\frac{\mathbb{E}\left[\varphi_{n}\left(X_{n}\right) \prod_{i=1}^{n-1} G_{i}\left(X_{i}\right)\right]}{\mathbb{E}\left[\prod_{i=1}^{n-1} G_{i}\left(X_{i}\right)\right]} & \widehat{\eta}_{n} & =\frac{\mathbb{E}\left[\varphi_{n}\left(X_{n}\right) \prod_{i=1}^{n} G_{i}\left(X_{i}\right)\right]}{\mathbb{E}\left[\prod_{i=1}^{n} G_{i}\left(X_{i}\right)\right]} \\
& =\gamma_{n}\left(\varphi_{n}\right) / \gamma_{n}(\mathbf{1}) & & =\widehat{\gamma}_{n}\left(\varphi_{n}\right) / \widehat{\gamma}_{n}(\mathbf{1})
\end{array}
$$

Key property:

$$
\begin{aligned}
& \eta_{n}\left(A_{n}\right)=\int_{E_{1} \times \ldots E_{n-1} \times A_{n}} \mathbb{Q}_{n}\left(d x_{1: n}\right) \\
& \widehat{\eta}_{n}\left(A_{n}\right)=\int_{E_{1} \times \ldots E_{n-1} \times A_{n}} \widehat{\mathbb{Q}}_{n}\left(d x_{1: n}\right)
\end{aligned}
$$

## A Glimpse of the Theory

A Dynamic Systems View:

How do the marginal distributions evolve?
Don't worry about the details in these slides.

## Some Recursive Relationships

- The unnormalized marginals obey:

$$
\widehat{\gamma}_{n}\left(\varphi_{n}\right)=\gamma_{n}\left(\varphi_{n} \cdot G_{n}\right) \quad \gamma_{n}\left(\varphi_{n}\right)=\widehat{\gamma}_{n-1} M_{n}\left(\varphi_{n}\right)
$$

- Whilst the normalized marginals satisfy:

$$
\begin{array}{rlrl}
\widehat{\eta}_{n}\left(\varphi_{n}\right) & =\frac{\widehat{\gamma}_{n}\left(\varphi_{n}\right)}{\widehat{\gamma}_{n}(\mathbf{1})} & \eta_{n}\left(\varphi_{n}\right) & =\frac{\gamma_{n}\left(\varphi_{n}\right)}{\gamma_{n}(\mathbf{1})} \\
& =\frac{\gamma_{n}\left(\varphi_{n} \cdot G_{n}\right)}{\gamma_{n}\left(G_{n}\right)} & & =\frac{\widehat{\gamma}_{n-1} M_{n}\left(\varphi_{n}\right)}{\widehat{\gamma}_{n-1} M_{n}(\mathbf{1})} \\
& =\frac{\eta_{n}\left(\varphi_{n} \cdot G_{n}\right)}{\eta_{n}\left(G_{n}\right)} & & =\frac{\widehat{\eta}_{n-1} M_{n}\left(\varphi_{n}\right)}{\widehat{\eta}_{n-1} M_{n}(\mathbf{1})} \\
& & =\widehat{\eta}_{n-1} M_{n}\left(\varphi_{n}\right)
\end{array}
$$

- So:

$$
\widehat{\eta}_{n}=\frac{\widehat{\eta}_{n-1} M_{n}\left(\varphi_{n} \cdot G_{n}\right)}{\widehat{\eta}_{n-1} M_{n}\left(G_{n}\right)}
$$

## The Boltzmann-Gibbs Operator

- Given $\nu \in \mathcal{P}(E)$ and $G: E \rightarrow \mathbb{R}$ :

$$
\begin{array}{rlrl}
\Psi_{G}: & & \mathcal{P}(E) & \rightarrow \mathcal{P}(E) \\
\Psi_{G}: & \nu & \rightarrow \Psi_{G}(\nu)
\end{array}
$$

- The Boltzmann-Gibbs Operator $\Psi_{G}$ is defined weakly by:

$$
\forall \varphi \in \mathcal{C}_{b}: \quad \Psi_{G}(\nu)(\varphi)=\frac{\nu(G \cdot \varphi)}{\nu(G)}
$$

- or equivalently, for all measurable sets $A$ :

$$
\begin{aligned}
\Psi_{G}(A) & =\frac{\nu\left(G \cdot \mathbb{I}_{A}\right)}{\nu(G)} \\
& =\frac{\int_{A} \nu(d x) G(x)}{\int_{E} \nu\left(d x^{\prime}\right) G\left(x^{\prime}\right)}
\end{aligned}
$$

## Example (Boltzmann-Gibbs Operators and Bayes' Rule)

- Let $\mu(d x)=f(x) \lambda(d x)$ be a prior measure.
- Let $G(x)=g(y \mid x)$ be the likelihood.
- Then:

$$
\begin{aligned}
\Psi_{G}(\mu)(\varphi) & =\frac{\mu(G \cdot \varphi)}{\mu(G)}=\frac{\int \mu(d x) G(x) \varphi(x)}{\int \mu\left(d x^{\prime}\right) G\left(x^{\prime}\right)} \\
& =\frac{\int f(x) g(y \mid x) \varphi(x) \lambda(d x)}{\int f\left(x^{\prime}\right) g\left(y \mid x^{\prime}\right) \lambda\left(d x^{\prime}\right)} \\
& =\int f(x \mid y) \varphi(x) \lambda(d x)
\end{aligned}
$$

with

$$
f(x \mid y):=\frac{f(x) g(y \mid x)}{\int f(x) g(y \mid x) \lambda(d x)}
$$

- So: $\Psi_{g(y \mid \cdot)}$ : Prior $\rightarrow$ Posterior.


## Markov Semigroups

- A semigroup $\mathcal{S}$ comprises:
- A set, $S$.
- An associative binary operation, $\cdot$.
- A Markov Chain with homogeneous transition $M$ has dynamic semigroup $M_{n}$ :
- $M_{0}(x, A)=\delta_{x}(A)$.
- $M_{1}(x, A)=M(x, A)$.
- $M_{n}(x, A)=\int M(x, d y) M_{n-1}(y, A)$.
- $\left(M_{n} \cdot M_{m}\right)(x, A)=\int M_{n}(x, d y) M_{m}(y, A)=M_{n+m}(x, A)$.
- A linear semigroup.
- Key property:

$$
\mathbb{P}\left(X_{n+m} \in A \mid X_{m}=x\right)=M_{n}(x, A)
$$

## Markov Semigroupoids

- A semigroupoid, $\mathcal{S}^{\prime}$ comprises:
- A set, $S$.
- A partial associative binary operation, •.
- A Markov Chain with inhomogeneous transitions $M_{n}$ has dynamic semigroupoid $M_{p: q}$ :
- $M_{p: p}(x, A)=\delta_{x}(A)$.
- $M_{p: p+1}(x, A)=M_{p+1}(x, A)$.
- $M_{p: q}(x, A)=\int M_{p+1}(x, d y) M_{p+1: q}(y, A)$.
- $\left(M_{p: q} \cdot M_{q: r}\right)(x, A)=\int M_{p: q}(x, d y) M_{q: r}(y, A)=M_{p: r}(x, A)$.
- A linear semigroupoid.
- Key property:

$$
\mathbb{P}\left(X_{n+m} \in A \mid X_{m}=x\right)=M_{m, n+m}(x, A)
$$

## An Unnormalized Feynman-Kac Semigroupoid

- We previously established:

$$
\gamma_{n}=\widehat{\gamma}_{n-1} M_{n} \quad \widehat{\gamma}_{n}\left(\varphi_{n}\right)=\gamma_{n}\left(\varphi_{n} \cdot G_{n}\right)
$$

- Defining

$$
Q_{p}\left(x_{p-1}, d x_{p}\right)=G_{p-1}\left(x_{p-1}\right) M_{p}\left(x_{p-1}, d x_{p}\right)
$$

we obtain $\gamma_{n}=\gamma_{n-1} Q_{n}$.

- We can construct the dynamic semigroupoid $Q_{p: q}$ :
- $Q_{p: p}(x, A)=\delta_{x}(A)$.
- $Q_{p: p+1}(x, A)=Q_{p+1}(x, A)$.
- $Q_{p: q}(x, A)=\int Q_{p+1}(x, d y) Q_{p+1: q}(y, A)$.
- $\left(Q_{p: q} \cdot Q_{q: r}\right)(x, A)=\int Q_{p: q}(x, d y) Q_{q: r}(y, A)=Q_{p: r}(x, A)$.
- Just a Markov semigroupoid for general measures:
$\forall p \leq q: \gamma_{q}=\gamma_{p} Q_{p: q}$.


## A Normalised Feynman-Kac Semigroupoid

- We previously established:

$$
\eta_{n}=\widehat{\eta}_{n-1} M_{n} \quad \widehat{\eta}_{n}(\varphi)=\frac{\eta_{n}\left(\varphi_{n} \cdot G_{n}\right)}{\eta_{n}\left(G_{n}\right)}
$$

- From the definition of $\Psi_{G_{n}}: \widehat{\eta}_{n}=\Psi_{G_{n}}\left(\eta_{n}\right)$.
- Defining $\Phi_{n}: \mathcal{P}\left(E_{n-1}\right) \rightarrow \mathcal{P}\left(E_{n}\right)$ as:

$$
\Phi_{n}: \eta_{n-1} \rightarrow \Psi_{G_{n-1}}\left(\eta_{n-1}\right) M_{n}
$$

we have the recursion $\eta_{n}=\Phi_{n}\left(\eta_{n-1}\right)$ and the nonlinear semigroupoid, $\Phi_{p: q}$ :

- $\Phi_{p: p}(x, A)=\delta_{x}(A)$.
- $\Phi_{p: p+1}(x, A)=\Phi_{p+1}(x, A)$.
- $\Phi_{p: q}(x, A)=\Phi_{p+1: q}\left(\Phi_{p+1}\left(\eta_{p}\right)\right)$ for $q>p+1$.
- $\left(\Phi_{p: q} \cdot \Phi_{q: r}\right)(x, A)=\int \Phi_{q: r}(y, A) \Phi_{p: q}(x, d y)=\Phi_{p: r}(x, A)$.
- Again: $\forall p \leq q: \eta_{q}=\eta_{p} \Phi_{p: q}$.


# McKean Interpretations 

Microscopic mass transport.

## McKean Interpretations of Feynman-Kac Formulæ

- Families of Markov kernels consistent with FK Marginals.
- A collection $\left\{K_{n, \eta}\right\}_{n \in \mathbb{N}, \eta \in \mathcal{P}\left(E_{n-1}\right)}$ is a McKean Interpretation if:

$$
\forall n \in \mathbb{N}: \eta_{n}=\Phi_{n}\left(\eta_{n-1}\right)=\eta_{n-1} K_{n, \eta_{n-1}}
$$

- Not unique. . . and not linear.
- Selection/Mutation approach seems natural:
- Choose $S_{n, \eta}$ such that $\eta S_{n, \eta}=\Psi_{G_{n}}(\eta)$.
- Set $K_{n+1, \eta}=S_{n, \eta} M_{n+1}$.
- Still not unique:
- $S_{n, \eta}\left(x_{n}, \cdot\right)=\Psi_{G_{n}}(\eta)$
$-S_{n, \eta}\left(x_{n}, \cdot\right)=\epsilon_{n} G_{n}\left(x_{n}\right) \delta_{x_{n}}(\cdot)+\left(1-\epsilon_{n} G_{n}\left(x_{n}\right)\right) \Psi_{G_{n}}(\eta)(\cdot)$


## Particle Interpretations

## Stochastic discretisations.

## Particle Interpretations of Feynman-Kac Formulæ I

Given a McKean interpretation, we can attach an $N$-particle model.

- Denote $\xi_{n}^{(N)}=\left(\xi_{n}^{(N, 1)}, \xi_{n}^{(N, 2)}, \ldots, \xi_{n}^{(N, N)}\right) \in E_{n}^{N}$.
- Allow

$$
\left(\Omega^{N}, \mathcal{F}^{N}=\left(\mathcal{F}_{n}^{N}\right)_{n \in \mathbb{N}}, \xi^{(N)}, \mathbb{P}_{\eta_{0}}^{N}\right)
$$

to indicate a particle-set-valued Markov chain.

- Let $\eta_{n-1}^{(N)}=\frac{1}{N} \sum_{i=1}^{N} \delta_{\xi_{n-1}^{(N, i)}}$.
- Allow the elementary transitions to be:

$$
\mathbb{P}\left(\xi_{n}^{(N)} \in d \xi_{n}^{(N)} \mid \xi_{n-1}^{(N)}\right)=\prod_{p=1}^{N} K_{n, \eta_{n-1}^{(N)}}\left(\xi_{n-1}^{(N, p)}, d \xi_{n}^{(N, p)}\right)
$$

## Particle Interpretations of Feynman-Kac Formulæ II

- Consider $K_{n, \eta}=S_{n-1, \eta} M_{n}$

$$
\mathbb{P}\left(\xi_{n}^{(N)} \in d \xi_{n}^{(N)} \mid \xi_{n-1}^{(N)}\right)=\prod_{p=1}^{N} S_{n-1, \eta_{n-1}^{(N)}} M_{n}\left(\xi_{n-1}^{(N, p)}, d \xi_{n}^{(N, p)}\right)
$$

- Defining:

$$
\begin{aligned}
\mathcal{S}_{n-1}^{(N)}\left(\xi_{n-1}^{(N)}, d \widehat{\xi}_{n}^{(N)}\right) & =\prod_{i=1}^{N} S_{n, \eta_{n-1}^{(N)}}\left(\xi_{n-1}^{(N, p)}, d \widehat{\xi}_{n-1}^{(N, p)}\right) \\
\mathcal{M}_{n}^{(N)}\left(\widehat{\xi}_{n-1}^{(N)}, d \xi_{n}^{(N)}\right) & =\prod_{i=1}^{N} M_{n}\left(\widehat{\xi}_{n-1}^{(N, p)}, \xi_{n}^{(N, p)}\right)
\end{aligned}
$$

it is clear that:

$$
\mathbb{P}\left(\xi_{n}^{(N)} \in d \xi_{n}^{(N)} \mid \xi_{n-1}^{(N)}\right)=\int_{E_{n-1}^{N}} \mathcal{S}_{n-1, \eta_{n-1}^{(N)}}\left(\xi_{n-1}^{(N)}, d \hat{\xi}_{n-1}^{(N)}\right) \mathcal{M}_{n}\left(\widehat{\xi}_{n-1}^{(N)}, d \xi_{n}^{(N)}\right)
$$

## Selection, Mutation and Structure

- A suggestive structural similarity:

$$
\begin{array}{llll}
\eta_{n-1} \in \mathcal{P}\left(E_{n-1}\right) & \xrightarrow[\longrightarrow]{S_{n-1, \eta_{n-1}}} \quad \widehat{\eta}_{n} \in \mathcal{P}\left(E_{n-1}\right) & \xrightarrow{M_{n}} \quad \eta_{n} \in \mathcal{P}\left(E_{n}\right) \\
\xi_{n-1}^{(N)} \in E_{n-1}^{N} & \stackrel{\text { Select }}{\longrightarrow} & \widehat{\xi}_{n}^{(N)} \in E_{n-1}^{N} & \xrightarrow{\text { Mutate }} \\
\xi_{n}^{(N)} \in E_{n}^{N}
\end{array}
$$

- Selection:

$$
\begin{aligned}
& S_{n-1, \eta_{n-1}^{(N)}}=\Psi_{G_{n-1}}\left(\eta_{n-1}^{(N)}\right)=\sum_{i=1}^{N} \frac{G_{n-1}\left(\xi_{n-1}^{(N, i)}\right)}{\sum_{j=1}^{N} G_{n-1}\left(\xi_{n-1}^{(N, j)}\right)} \delta_{\xi_{n-1}^{(N, i)}} \\
& \quad \widehat{\xi}_{n-1}^{(N, i)} \stackrel{\text { i.i.d. }}{\sim} \Psi_{G_{n-1}}\left(\eta_{n-1}^{(N)}\right)
\end{aligned}
$$

- Mutation (conditionally independent):

$$
\xi_{n}^{(N, i)} \sim M_{n}\left(\widehat{\xi}_{n-1}^{(N, i)}, d \xi_{n}^{(N, i)}\right)
$$

- Semigroupoid

$$
\mathbb{P}^{N}\left(\xi_{n}^{(N)} \in d x_{n}^{(N)} \mid \xi_{n-1}^{(N)}\right)=\prod_{i=1}^{N} \Phi_{n}\left(\eta_{n-1}^{(N)}\right)\left(d x_{n}^{(N, i)}\right)
$$

## Selected Results

## Local Error Decomposition

$$
\begin{aligned}
& \eta_{1} \quad \rightarrow \quad \eta_{2}=\Phi_{2}\left(\eta_{1}\right) \quad \rightarrow \quad \eta_{3}=\Phi_{1: 3}\left(\eta_{1}\right) \quad \rightarrow \quad \cdots \quad \rightarrow \Phi_{1: n}\left(\eta_{1}\right) \\
& \left.\begin{array}{ccccccc}
\Downarrow & & & & \\
\eta_{1}^{N} & \rightarrow & \Phi_{2}\left(\eta_{1}^{N}\right) & \rightarrow & \Phi_{1: 3}\left(\eta_{1}^{N}\right) & \rightarrow & \ldots
\end{array}\right) \rightarrow \Phi_{1: n}\left(\eta_{1}^{N}\right) \\
& \eta_{n-1}^{N} \rightarrow \Phi_{n}\left(\eta_{n-1}^{N}\right) \\
& \Downarrow \\
& \eta_{n}^{N}
\end{aligned}
$$

Formally: $\eta_{n}^{N}-\eta_{n}=\sum_{p=1}^{n} \Phi_{p, n}\left(\eta_{p}^{N}\right)-\Phi_{p, n}\left(\Phi_{p}\left(\eta_{p-1}^{N}\right)\right)$

## Some Unbiasesness

Theorem (Del Moral 2004: Theorem 7.4.2)
Under mild regularity conditions, for any $n \in \mathbb{N}$ and some bounded, measurable $\varphi_{n}$ :

$$
\mathbb{E}\left[\eta^{N}\left(\varphi_{n}\right)\right]=\gamma_{n}\left(\varphi_{n}\right) .
$$

N.B. Typically the corresponding result does not hold for normalised measures:

$$
\mathbb{E}\left[\eta_{n}^{N}\left(\varphi_{n}\right)\right] \neq \eta_{n}\left(\varphi_{n}\right) .
$$

although it does asymptotically with bias $\mathcal{O}\left(N^{-1}\right)$.

## Law of Large Numbers and Weak Convergence

Theorem (Del Moral 2004: Theorem 7.4.4)
Under regularity conditions, for any $n \geq 1, p \geq 1, \varphi_{n} \in \mathcal{C}_{b}\left(E_{n}\right)$ :

$$
\sqrt{N} \mathbb{E}\left[\left|\eta_{n}^{N}\left(\varphi_{n}\right)-\eta_{n}\left(\varphi_{n}\right)\right|^{p}\right]^{1 / p} \leq c_{p, n}\left\|\varphi_{n}\right\|_{\infty}
$$

By a Borel-Cantelli argument:

$$
\lim _{N \rightarrow \infty} \eta_{n}^{N}\left(\varphi_{n}\right) \xrightarrow{\text { a.s. }} \eta_{n}\left(\varphi_{n}\right) .
$$

## Central Limit Theorem

## Proposition (Del Moral 2004: Proposition 9.4.2)

Under regularity conditions, for any $n \geq 1$ :

$$
\sqrt{N}\left(\eta_{n}^{N}\left(\varphi_{n}\right)-\eta_{n}\left(\varphi_{n}\right)\right) \xrightarrow{d} \mathcal{N}\left(0, \sigma_{n}^{2}\left(\varphi_{n}\right)\right)
$$

where

$$
\sigma_{n}^{2}\left(\varphi_{n}\right)=\sum_{q=1}^{n} \eta_{q}\left[\left(\bar{Q}_{q, n}\left(\varphi_{n}-\eta_{n}\left(\varphi_{n}\right)\right)\right)^{2}\right]
$$

where

$$
\bar{Q}_{q, n}\left(\varphi_{n}\right)\left(x_{q}\right)=Q_{q, n}\left(\varphi_{n}\right)\left(x_{q}\right) / \eta_{q} Q_{q, n}(\mathbf{1}) .
$$

# Exact Estimation of <br> Rare Events in Continuous Time 

## Recent work with James Hodgson and Murray Pollock

## So What's The Difficulty?

A fundamental problem remains. We cannot typically sample from the discrete time kernel associated with a stochastic process.

- We can exactly sample a broad class of scalar volatility SDEs at finite numbers of time points using exact simulation methods.
- We can constrain such paths to arbitrary finite tolerances using $\varepsilon$-strong methods.
- We cannot identify the stopping times $\sigma_{i}$ even with these methods.
- We can identify whether $X_{\sigma_{i}} \in B_{i}$ and the value of $X_{T_{i}}$ for some types of random $T_{i} \geq \sigma_{i}$.
- And that's the basis of the following method.


## $\varepsilon$-strong Methods

An $\varepsilon$-strong algorithm jointly constructs of $X$ together with a family of processes $\tilde{X}^{\varepsilon}$ indexed by $\varepsilon>0$ over $[s, t]$ such that:

1. $\sup _{r \in[s, t]}\left\|X(r)-\tilde{X}^{\varepsilon}(r)\right\| \stackrel{\text { a.s. }}{\leq} \varepsilon$ for an appropriate norm $\|\cdot\|$;
2. $\tilde{X}^{\varepsilon}$ is piece-wise constant and left-continuous on $[s, t]$ with a.s. finitely many jump;
3. $\tilde{X}^{\varepsilon}$ can be simulated exactly; and
4. Given $\varepsilon_{1}>\varepsilon_{2}>\cdots>\varepsilon_{m}>0$, for $1 \leq \ell_{1}<\ell_{2} \leq m$ it holds a.s. $\forall r \in[s, t]$ that

$$
\left\{x:\left\|\tilde{X}^{\varepsilon_{\ell_{2}}}(r)-x\right\| \leq \varepsilon_{\ell_{2}}\right\} \subset\left\{x:\left\|\tilde{X}^{\varepsilon_{\ell_{1}}}(r)-x\right\| \leq \varepsilon_{\ell_{1}}\right\}
$$

and moreover it is possible to sample explicitly $\tilde{X}^{\varepsilon_{\ell_{2}}}$ conditional on $\tilde{X}^{\varepsilon_{\ell_{1}}}$.


Figure: An schematic illustration of $\varepsilon$-strong simulation. The top row shows shows the $\varepsilon$-strong process $\tilde{X}$ developing as conditional samples are made first with tolerance $\varepsilon_{1}$, followed with $\varepsilon_{2}<\varepsilon_{1}$. The bottom row shows the fixed target path $X$, and how the $\varepsilon$-strong constraints relate to it. Pale circles indicate superseded constraints from the previous step.


Figure: Determining crossings with $\varepsilon$-strong algorithms.
The first row shows: a realisation of $X$ over a finite time horizon, an initial $\varepsilon$-strong simulation and a refinement which is sufficient to show the process crossing into $B$.
The second row shows an alternative sample path consistent with the same initial $\varepsilon$-strong simulation, an inconclusive refinement and a further refinement sufficient to conclude that the process has crossed into $A$.

## Halfway There. . .

- To implement MLS we need to be able to sample from:

$$
M_{i}\left(\left(\sigma_{i-1}, x_{i-1}\right), \cdot\right)
$$

and evaluate

$$
G_{i}\left(\sigma_{i}, x_{i}\right)=\mathbb{I}_{B_{i}}\left(x_{i}\right) .
$$

- We can now sample and evaluate $G_{i}\left(\sigma_{i}, x_{i}\right)$ without knowing $\sigma_{i}$ or $x_{i}$ explicitly.
- We cannot sample from $M_{i}$.
- We can determine if crossings occur, but not when or where.
- The next insight is that we do not need to.


## An Idea

- Splitting relies on sampling at step $i$ several times from the law of the process given the point at which it hit $B_{i-1}$.
- Traditionally, it does this independently.
- It doesn't have to do it independently.
- Any coupling of the sample paths with the correct marginals would be valid.
- We could use a coupling which makes the simulation problem tractable.


## The Underlying Picture



Figure: An illustration of Idealised Splitting with Couplings for a single particle system. The particle begins at the node labelled $x_{0}$. Level crossings are indicated by empty nodes, whereas splittings occur at the filled nodes. Between any empty node and the following filled node, the particle trajectories are coupled identically.

## The Gory Details I

- Define the bounding random time:

$$
\tilde{\sigma}_{i}=T \cdot \min \left\{m \in \mathbb{N}: m T \geq \sigma_{i}\right\}
$$

- Similarly, let $\tilde{\tau}_{i}$ be the corresponding upper bound on the first hitting time of $B_{i}$.
- Rather than split these paths into independent copies at times $\tau_{i}$, from time $\tau_{i}$ until time $\tilde{\tau}_{i}$, the "split" paths are set to be identically equal, and after this time they evolve conditionally independently given $X_{\tilde{\tau}_{i}}$.
- For $i=1, \ldots, m$, let $\tilde{M}_{i}$ denote the transition kernels for the discrete time quadruple process $V_{i}=\left(\sigma_{i}, \tilde{\sigma}_{i}, X\left(\sigma_{i}\right), \tilde{X}\left(\tilde{\sigma}_{i}\right)\right)$.
- Define also $\tilde{G}_{i}\left(V_{i}\right)=\mathbb{I}_{B_{i}}\left(X\left(\sigma_{i}\right)\right)$.
- Call the estimator for $p$ resulting from this algorithm $\tilde{p}$.


## Algorithm Idealised Splitting with Coupling

Given $\lambda$ together with $\tilde{G}_{i}, \tilde{M}_{i}$ for $i=1, \ldots, m$, an initial number of particles $N_{0}$, and splitting ratios $R_{1}, \ldots, R_{m-1}$ :

1. For $j=1, \ldots, N_{0}$ :
1.1 Draw $X_{1}^{j}(0) \sim \lambda, V_{1}^{j} \sim \tilde{M}_{1}\left(\left(0,0, X_{1}^{j}(0), X_{1}^{j}(0)\right), \cdot\right)$.
2. Let $S_{1}=\left\{V_{1}^{j}: \tilde{G}_{1}\left(V_{1}^{j}\right)=1\right\}$ be a list of the the surviving paths, and $N_{1}=\left|S_{1}\right|$.
3. For $i=2, \ldots, m$ :
3.1 If $N_{i-1}=0$, return $\tilde{p}=0$.
3.2 Otherwise given $S_{i-1}=\left\{V_{i-1}^{j}\right\}_{j=1}^{N_{i-1}}$, for each

$$
(j, k) \in\left\{\left(j^{\prime}, k^{\prime}\right): 1 \leq j^{\prime} \leq N_{i-1}, 1 \leq k^{\prime} \leq R_{i-1}\right\}:
$$

3.2.1 Sample $V_{i}^{(j, k)} \sim \tilde{M}_{i}\left(V_{i-1}^{j}, \cdot\right)$
3.3 Let $S_{i}=\left\{V_{i}^{j, k}: \tilde{G}_{i}\left(V_{i}^{j, k}\right)=1\right\}$, and set $N_{i}=\left|S_{i}\right|$.
4. Estimate

$$
\tilde{p}=\frac{N_{m}}{N_{0} \prod_{i=1}^{m-1} R_{i}}
$$

## Remark

It is not possible to implement this Algorithm as written: we cannot simulate full paths of $X$, nor make splits at times $\tau_{i}$. But the construction of MLS with couplings means that an algorithm which simply splits paths at the tractable time $\tilde{\tau}_{i}$ instead produces identical estimators for $p_{i}$.

Proposition (Hodgson, J. \& Pollock (in press))
$\tilde{p}$ is an unbiased estimator for $p: \mathbb{E}[\tilde{p}]=p$.
Proof.
Mirrors the proof for standard MLS, using the fact that the marginal law of particles between barriers is indentical to that under the simpler scheme.

## A Toy Example: Univariate Brownian Motion

- A setting in which the exact solution is known.
- We choose $A=(-\infty, 0], B=\left[3^{18}, \infty\right), B_{i}=\left[3^{i}, \infty\right)$ for $i=1, \ldots, 17$, with initial point $x_{0}=1$.
- As is well-known that for real $0<a<b$, the probability that a Brownian path started at a reaches $b$ before 0 is $a / b$ : $p=3^{-18} \approx 2.58 \times 10^{-9}$.



## Slightly More Challenging: Bivariate Brownian Motion

- The random process is again taken to be Brownian motion initialised at $W_{0}=\left(\frac{1}{2}, \frac{1}{2}\right)$.
- The reaction co-ordinate is chosen to be $\xi(x, y)=\min (x, y)$, and the levels are chosen to be $A=\xi^{-1}((-\infty, 0)), B=$ $\left.\xi^{-1}\left(\left(2^{\frac{21}{2}}, \infty\right)\right), B_{i}=\xi^{-1}\left(2^{\frac{1}{2}(i+1)}, \infty\right)\right)$ for $i=1, \ldots, 18$.
- We are not aware of any simple means by which the rare event probability can be analytically obtained in this case.



## Summary

- SMC provides a mechanism for approximating (sequences of) probability distributions via importance sampling and resampling.
- There is still scope to further develop (and understand) SMC methodology.
- There are still unsolved problems in rare event simulation and estimation.
- My own current interests include:
- Divide-and-conquer approaches to efficient distributed implementation.
- The interaction with Generalized Bayesian Inference.
- Automatic optimization of SMC algorithms.


## Some References I

- Some approachable SMC References
- Doucet, A. and Johansen, A.M.: A tutorial on particle filtering and smoothing: Fiteen years later. In D. Crisan and B. Rozovsky, editors, The Oxford Handbook of Nonlinear Filtering, pages 656-704. 2011. See Preprint.
- Chopin, N. and Papaspiliopoulos, O.: An introduction to Sequential Monte Carlo. Springer. 2020. See: SpringerLink.
- A More Technical Treatment of Feynman-Kac Formulæ
- Del Moral, P.: Feynman Kac Formulæ: Genealogical and Interacting Particle Systems. Springer, 2004. See: SpringerLink.
- Multilevel Splitting
- Origins: Kahn, H., Harris, T.E.: Estimation of particle transmission by random sampling. National Bureau of Standards Applied Mathematics Series 12, 27-30 (1951). See: https: //dornsifecms.usc.edu/assets/sites/520/docs/kahnharris.pdf.
- Unbiasedness: Amrein, M., Künsch, H.: A Variant of Importance Splitting for Rare Event Estimation: Fixed Number of Successes. ACM Transactions on Modelling and Computer Simulation 21(2), Article 13, 20pp. (2011). See: doi:10.1145/1899396.1899401.


## Some References II

- $\varepsilon$-strong Simulation for SDEs:
- M. Pollock, A. M. Johansen and G. O. Roberts, On Exact and $\varepsilon$-strong Simulation of (Jump) Diffusions. Bernoulli, 22(2):794-856, 2016. See: 10.3150/14-BEJ676.
- Exact Rare Event Estimation in Continuous Time:
- Hodgson, J., Johansen, A.M. and Pollock, M.: Unbiased simulation of rare events in continuous time. Methodology and Computing in Applied Probability, 2021. In press. See: doi:10.1007/s11009-021-09886-2.
- Some Other Uses of SMC in Rare Event Problems:
- Cérou, F., Del Moral, P., Le Gland, F., Lezaud, P.: Genetic genealogical models in rare event analysis. ALEA: Latin American Journal of Probability and Mathematical Statistics 1, 181-203 (2006). See doi:10.1007/s11222-011-9231-6.
- Del Moral, P., Garnier, J.: Genealogical particle analysis of rare events. Annals of Applied Probability 15(4), 2496-2534 (2005). See doi:10.1214/105051605000000566.
- Johansen, A., Del Moral, P., Doucet, A.: Sequential Monte Carlo samplers for rare events. In: Proceedings of the 6th International Workshop on Rare Event Simulation, pp. 256-267. Bamberg, Germany (2006). See Preprint.

