Resampling Algorithms for High Energy Physics Simulations

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Aim

- Let
  - $\{(\mathsf{X}_n, \mathcal{X}_n)\}_{n \in \mathbb{N}}$ be *measurable spaces*;
  - $\{Q_n\}_{n \in \mathbb{N}}$ *transition kernels*;
  - γ_0 be a *measure* on $(\mathsf{X}_0, \mathcal{X}_0)$.
- For each $n \in \mathbb{N}$, define the measure

$$\gamma_{0:n}(dx_{0:n}) := \gamma_0(dx_0) \prod_{m=0}^{n-1} Q_m(x_m, dx_{m+1})$$

  on the *path space* $\mathsf{X}_{0:n} := \mathsf{X}_0 \times \cdots \times \mathsf{X}_n$.
- We aim at forming *weighted samples* $\{(\xi_{0:n}^i, \omega_n^i)\}_{i=1}^N$, $n \in \mathbb{N}$, targeting the sequence $\{\gamma_{0:n}\}_{n \in \mathbb{N}}$ in the sense that for all n and h,

$$\frac{1}{N} \sum_{i=1}^{N} \omega_n^i h(\xi_{0:n}^i) \simeq \gamma_{0:n} h := \int h(x_{0:n}) \, \gamma_{0:n}(dx_{0:n}).$$

Sequential importance sampling (SIS)

- Introduce
  - *Markov kernels* $\{P_n\}_{n \in \mathbb{N}}$ such that $Q_n \ll P_n$;
  - an initial distribution ρ on $(\mathsf{X}_0, \mathcal{X}_0)$.
- Then

$$\gamma_{0:n}(dx_{0:n}) = \frac{d\gamma_0}{d\rho}(x_0) \prod_{m=0}^{n-1} \frac{dQ_m(x_m, \cdot)}{dP_m(x_m, \cdot)}(x_{m+1}) \, \mathbb{P}_\rho(dx_{0:n}),$$

where $\mathbb{P}_\rho(dx_{0:n}) := \rho(dx_0) \prod_{m=0}^{n-1} P_m(x_m, dx_{m+1})$.

- Thus, naively, simulate each $\xi^i_{0:n}$ from $\mathbb{P}_\rho(dx_{0:n})$ and compute

$$\omega^i_n = \frac{d\gamma_0}{d\rho}(\xi^i_0) \prod_{m=0}^{n-1} \frac{dQ_m(\xi^i_m, \cdot)}{dP_m(\xi^i_m, \cdot)}(\xi^i_{m+1}).$$

SIS (cont.)

- Recursive updates $\{(\xi^i_{0:n}, \omega^i_n)\}_{i=1}^N \rightsquigarrow \{(\xi^i_{0:n+1}, \omega^i_{n+1})\}_{i=1}^N$:

for $i \leftarrow 1$ **to** N **do**

  draw $\xi^i_{n+1} \sim P_n(\xi^i_n, dx_{n+1})$;

  set $\xi^i_{0:n+1} \leftarrow (\xi^i_{0:n}, \xi^i_{n+1})$;

  set $\omega^i_{n+1} \leftarrow \omega^i_n \frac{dQ_n(\xi^i_n, \cdot)}{dP_n(\xi^i_n, \cdot)}(\xi^i_{n+1})$;

end

Example: parton shower simulation

- Given a starting scale Q, the scale q of the next emission and some additional splitting variables z have distribution

$$S_P(dq, dz|Q) := \Delta_P(\mu|Q)\delta_{(\mu,z_\mu)}(dq, dz) \\ + P(q, z)\Delta_P(q|Q)\mathbb{1}_{(\mu,Q)}(q)\, dq\, dz,$$

where

  - P is a splitting kernel;
  - μ is the infrared cutoff;
  - z_μ is a parameter point associated with the cutoff;
  - $\Delta_P(q|Q)$ is the *Sudakov form factor*

$$\Delta_P(q|Q) := \exp\left(-\int_q^Q dp \int dz\, P(p, z)\right).$$

- Our goal is to simulate the process

$$Q \overset{S_P}{\rightsquigarrow} (\tilde{q}_1, \tilde{z}_1) \overset{S_P}{\rightsquigarrow} (\tilde{q}_2, \tilde{z}_2) \overset{S_P}{\rightsquigarrow} (\tilde{q}_3, \tilde{z}_3) \overset{S_P}{\rightsquigarrow} \cdots$$

Weighted Sudakov veto (WSV) [Bel+16]

Data: $(q', z', \varepsilon'), \omega'$
Result: $(q, z, \varepsilon), \omega$
draw $(q, z) \sim S_R(dq, dz|q')$;
if $(q, z) = (\mu, z_\mu)$ **then**
  $\varepsilon \leftarrow 0$;
  $\omega \leftarrow \omega'$;
end
else
  draw $\varepsilon \sim \mathrm{Be}(\pi(q, z|q', z'))$;
  if $\varepsilon = 1$ **then**
    set $\omega \leftarrow \omega' \frac{1}{\pi(q,z|q',z')} \frac{P(q,z)}{R(q,z)}$;
  end
  else
    set $\omega \leftarrow \omega' \frac{1}{1-\pi(q,z|q',z')} \left(1 - \frac{P(q,z)}{R(q,z)}\right)$
  end
end

WSV as SIS

- Iterating the previous algorithm yields a Markovian dynamical process $\{(q_m, z_m, \varepsilon_m, \omega_m)\}_{m\in\mathbb{N}^*}$ with $q_0 = Q$ and $\omega_0 = 1$. We denote its law by $\mathbb{P}_Q$.
- Set $n_0 = 0$ and define recursively

$$n_\ell := \min\{m > n_{\ell-1} : \varepsilon_m = 1 \text{ or } q_m = \mu\}, \quad \ell > 1.$$

- By [Bel+16, Section 2.3] and the strong Markov property, with $\tilde{q}_0 = Q$,

$$\mathbb{E}_Q\left(h_p(q_{n_1}, z_{n_1}, q_{n_2}, z_{n_2}, \ldots, q_{n_p}, z_{n_p})\,\omega_{n_p}\right) \tag{1}$$
$$= \int \cdots \int h_p(\tilde{q}_1, \tilde{z}_1, \ldots, \tilde{q}_p, \tilde{z}_p) \prod_{\ell=0}^{p-1} S_P(d\tilde{q}_{\ell+1}, d\tilde{z}_{\ell+1}|\tilde{q}_\ell),$$

- Consequently, WSV can be expressed as SIS.

WSV output for the Durham y_{45} observable

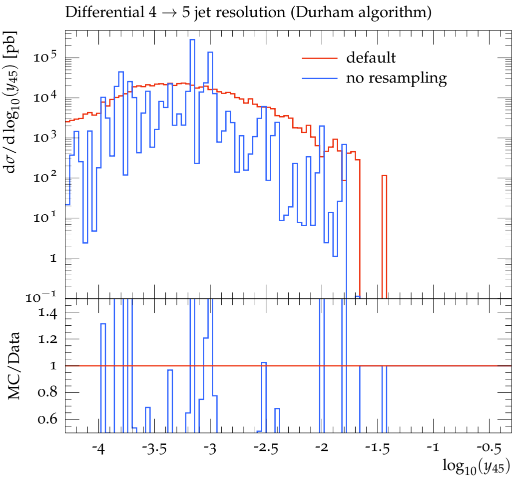


Figure: The Durham y_{45} observable as implemented in [Höc15] (default). The same observable when sampled with WSV (no resampling).

Weight degeneracy in WSV

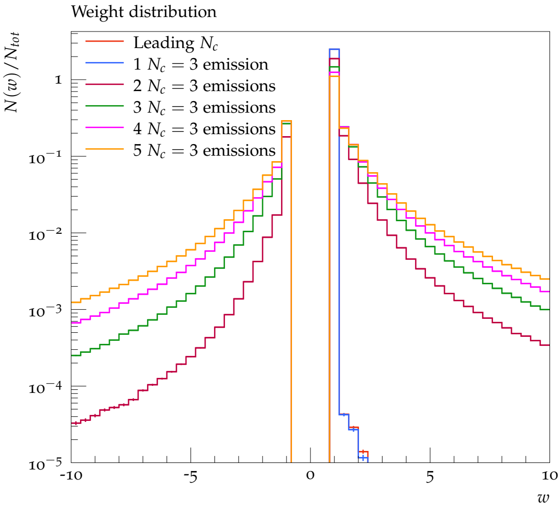
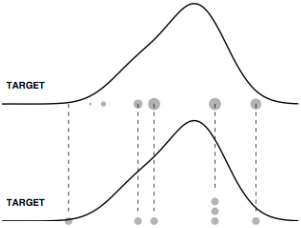


Figure: WSV weight distribution using $1, \ldots, 5$ color-corrected emissions in the `Herwig` dipole shower.

Multinomial selection [Rub87]



- Weight degeneracy is a *universal problem* of the SIS algorithm.
- Remedy: transform, at each SIS iteration, $\{(\xi^i_{0:n}, \omega^i_n)\}_{i=1}^N$ into a *uniformly weighted* sample $\{(\tilde{\xi}^i_{0:n}, \tilde{\omega}^i_n)\}_{i=1}^N$ by selecting $\{\tilde{\xi}^i_{0:n}\}_{i=1}^N$ among $\{\xi^i_{0:n}\}_{i=1}^N$ with replacement and in proportion to $\{\omega^i_n\}_{i=1}^N$ and letting

$$\tilde{\omega}^1_n = \tilde{\omega}^2_n = \cdots = \tilde{\omega}^N_n = \frac{\Omega_n}{N},$$

with $\Omega_n = \sum_{i=1}^N \omega^i_n$.

SIS with resampling (SISR) [GSS93]

Data: $\{(\xi^i_{0:n|n}, \omega^i_n)\}_{i=1}^N$
Result: $\{(\xi^i_{0:n+1|n}, \omega^i_{n+1})\}_{i=1}^N$
for $i \leftarrow 1$ **to** N **do**
  $\iota^i \sim \sum_{i=1}^N \frac{\omega^i_n}{\Omega_n} \delta_i$;
  `/* selection */`
  draw $\xi^i_{n+1|n+1} \sim P_n(\xi^{\iota^i}_{n|n}, dx_{n+1})$;
  set $\xi^i_{0:n+1|n+1} \leftarrow (\xi^{\iota^i}_{0:n|n}, \xi^i_{n+1|n+1})$;
end
for $i \leftarrow 1$ **to** N **do**
  set $\omega^i_{n+1} \leftarrow \frac{dQ_n(\xi^i_{n|n+1}, \cdot)}{dP_n(\xi^i_{n|n+1}, \cdot)}(\xi^i_{n+1|n+1}) \frac{\Omega_n}{N}$;
end

Example: WSV with resampling (WSVR)

- To cope with the weight degeneracy of WSV, furnish the same with interleaved resampling operations $\Rightarrow$ WSVR.
- Different possible resampling schedules:
  - Systematically after each WSV iteration.
  - Only at emissions (embedded chain).
  - Only when indicated by some weight skewness criterion, such as the *coefficient of variation*

$$\mathrm{CV}^2 = N \sum_{i=1}^{N} \left(\frac{\omega_n^i}{\Omega_n} - \frac{1}{N} \right)^2$$

or the *efficient sample size*

$$\mathrm{ESS} = \frac{N}{1 + \mathrm{CV}^2}.$$

WSVR output for the Durham y_{45} observable

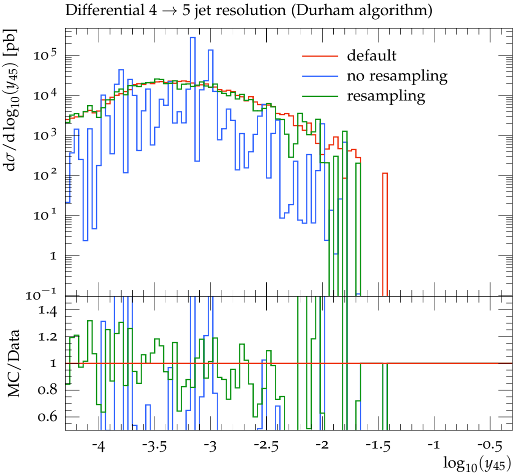


Figure: The Durham y_{45} observable as implemented in [Höc15] (default). The same observable when sampled with WSV without resampling (no resampling) and when sampled with WSVR with systematic resampling (resampling). The plot is based on 10,000 events.

Variability estimates

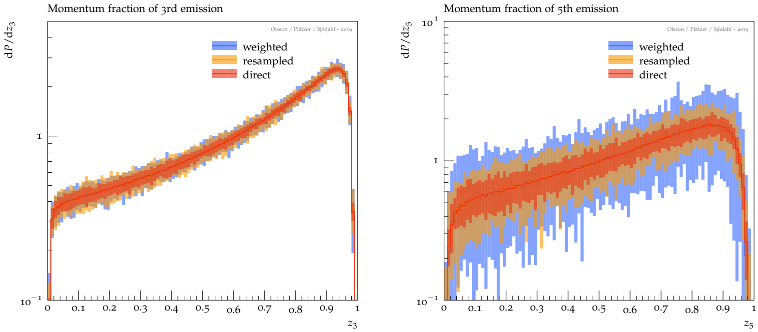


Figure: The left and right panels display momentum fractions after 2 and 5 emissions, respectively. Blue and yellow boxes correspond to WSV and WSVR, respectively.

Some theoretical properties of SISR

- The following can be established; see e.g. [Del04; DMG99].
  - For all n and h,

$$\mathbb{E}\left(\frac{1}{N}\sum_{i=1}^{N}\omega_n^i h(\xi_{0:n|n}^i)\right) = \gamma_{0:n}h.$$

  - For all n and $h \in \mathsf{L}_2(\gamma_{0:n})$ there exists $\sigma_n^2(h)$ such that, as $N \to \infty$,

$$\sqrt{N}\left(\frac{1}{N}\sum_{i=1}^{N}\omega_n^i h(\xi_{0:n|n}^i) - \gamma_{0:n}h\right) \stackrel{\mathcal{L}}{\longrightarrow} N(0, \sigma_n^2(h)).$$

- For objective functions h depending on x_n only, the sequence $\{\sigma_n^2(h)\}_{n\in\mathbb{N}}$ can, under mild ergodicity assumptions, be bounded *uniformly* in n [DMO14]. For SIS it increases exponentially.

Conclusion and future work

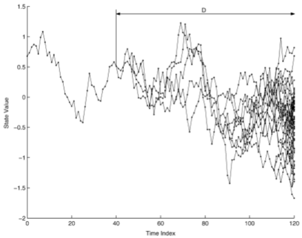


Figure: The particle path degeneracy phenomenon.

- "Change of philosophy": independent events vs. computationally efficient tool for reproducing observables.
- Particle path degeneracy phenomenon when n is large compared to N. Apply *backward-sampling* techniques [GDW04].
- Towards parallel implementations using *particle island models* [Ver+15].

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Proof of (1)

- We assume that the function π is such that for all m, $\mathbb{P}_Q$-a.s., $n_m < \infty$.
- By the functional monotone class theorem it is enough to establish (1) for $h_p(\tilde{q}_{0:p}, \tilde{z}_{0:p}) = \prod_{\ell=0}^{p} g_\ell(\tilde{q}_\ell, \tilde{z}_\ell)$.
- Proceed by induction and assume that (1) holds true for $p-1$.
- Define the weight function

$$\Psi(q, z, \varepsilon | q', z') := \mathbb{1}_{\{1\}}(\varepsilon) \frac{1}{\pi(q, z | q', z')} \frac{P(q, z)}{R(q, z)} + \mathbb{1}_{\{0\} \times \{\mu\}^{\complement}}(\varepsilon, q) \frac{1}{1 - \pi(q, z | q', z')} \left(1 - \frac{P(q, z)}{R(q, z)}\right) + \mathbb{1}_{\{\mu\}}(q).$$

Proof of (1) (cont.)

- By the tower property followed by the strong Markov property,

$$
\begin{aligned}
&\mathbb{E}_Q\left(h_p(q_{n_1}, z_{n_1}, \ldots, q_{n_p}, z_{n_p})\,\omega_{n_p}\right) \\
&= \mathbb{E}_Q\Bigg(h_{p-1}(q_{n_1}, z_{n_1}, \ldots, q_{n_{p-1}}, z_{n_{p-1}})\,\omega_{n_{p-1}} \\
&\times \mathbb{E}_Q\Bigg(g(q_{n_p}, z_{n_p}) \prod_{m=n_{p-1}+1}^{n_p} \Psi(q_m, z_m, \varepsilon_m | q_{m-1}, z_{m-1}) \mid \mathcal{F}_{n_{p-1}}\Bigg)\Bigg) \\
&= \mathbb{E}_Q\Bigg(h_{p-1}(q_{n_1}, z_{n_1}, \ldots, q_{n_{p-1}}, z_{n_{p-1}})\,\omega_{n_{p-1}} \qquad (2) \\
&\times \mathbb{E}_{q_{n_{p-1}}}\Bigg(g(q_{n_1}, z_{n_1}) \prod_{m=1}^{n_1} \Psi(q_m, z_m, \varepsilon_m | q_{m-1}, z_{m-1})\Bigg)\Bigg).
\end{aligned}
$$

Proof of (1) (cont.)

- Now, using the main result of [Bel+16, Section 2.3],

$$\mathbb{E}_{q_{n_{p-1}}}\left(g(q_{n_1}, z_{n_1}) \prod_{m=1}^{n_1} \Psi(q_m, z_m, \varepsilon_m | q_{m-1}, z_{m-1})\right) \\ = \int g(\tilde{q}_p, \tilde{z}_p)\, S_P(d\tilde{q}_p, d\tilde{z}_p | q_{n_{p-1}}).$$

- Plugging the previous identity into (2) and applying the induction hypothesis yields

$$\mathbb{E}_Q\left(h_p(q_{n_1}, z_{n_1}, \ldots, q_{n_p}, z_{n_p})\, \omega_{n_p}\right) \\ = \int \cdots \int h_p(\tilde{q}_1, \tilde{z}_1, \ldots, \tilde{q}_p, \tilde{z}_p) \prod_{\ell=0}^{p-1} S_P(d\tilde{q}_{\ell+1}, d\tilde{z}_{\ell+1} | \tilde{q}_\ell)$$

(with $\tilde{q}_0 = Q$), which was to be established.