PREDICTING WE VARIANCE FROM MSM

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Following Lemma 3.1 from [1], suppose we are attempting to estimate $\mathbb{E}[f]$ using WE, where f may in fact be the occupancy of the target set B for a flux calculation. Single realization estimates of f after t iterations of WE with N particles are as follows. The point, in time, estimates are:

$$\eta_t^N(f) = \sum_{i=1}^{N} w_t^i f(\xi_t^i) \tag{1}$$

where w_t^i is the weight at time t for particle i and particle i sits at position ξ_t^i. Typically, we time average this, having computed up till time t:

$$\frac{1}{t}\sum_{s=0}^{t-1}\sum_{i=1}^{N} w_s^i f(\xi_s^i). \tag{2}$$

The ensemble average of this quantity (averaged over an ensemble of WE runs),

$$\lim_{t\to\infty} t \times N \times \mathrm{Var}\left(\frac{1}{t}\sum_{s=0}^{t-1}\sum_{i=1}^{N} w_s^i f(\xi_s^i)\right) = \text{Variance Constant} \tag{3}$$

and the above constant, which we now focus on, is

$$\text{Variance Constant} = \sum_{u} \frac{\pi(u)^2}{\alpha(u)} \left\{\mathrm{Var}_{\pi(\bullet\mid u)}(Kh) + \mathrm{Var}_{\pi(\bullet\mid u)}(v) + \pi(v \mid u)^2\right\}. \tag{4}$$

In the above expression, u, is the index of the "macro" WE bins, as opposed to any "micro" bins which may have been used to construct them. $\alpha(u)$ is the fraction of walkers allocated to bin u. Quantities are computed as follows. Let K denote the transition matrix (for the recycling process) on the fine bin space. Then π is the stationary measure on the micro bins, and

$$\pi(u) = \sum_{i\in u} \pi(i) \tag{5}$$

where we are indexing the microbins over i. Next, h is computed as the solution to the Poisson equation

$$(I - K)h = f - \pi(f) \tag{6}$$

This corresponds to the h_0 from the review article, and v solves

$$v^2 = K(h^2) - (Kh)^2 \tag{7}$$

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Again, h and v are microbin functions. Then,

$$\pi(v \mid u) = \sum_{i\in u} \pi(i)v(i)/\pi(u) \tag{8}$$

$$\mathrm{Var}_{\pi(\bullet|u)}(v) = \sum_{i\in u} \pi(i)v_i^2/\pi(u) - \left(\sum_{i\in u} \pi(i)v_i/\pi(u)\right)^2 \tag{9}$$

$$\mathrm{Var}_{\pi(\bullet|u)}(Kh) = \sum_{i\in u} \pi(i)(Kh)_i^2/\pi(u) - \left(\sum_{i\in u} \pi(i)(Kh)_i/\pi(u)\right)^2 \tag{10}$$

where Kh is obtained from matrix-vector multiplication.

In the ideal setting, the dominant term in (4) is the last,

$$\pi(v)^2, \tag{11}$$

but the other two terms may play a nontrivial role.

In my experience, with sufficient microbin resolution, these are relatively (within an order of magnitude) estimates of the limiting variance.

References

[1] R. J. Webber, D. Aristoff, and G. Simpson. A splitting method to reduce MCMC variance, Dec. 2020. arXiv:2011.13899 [cs, math].