Correction to "Improved Diffusion Monte Carlo"

James F. Dama, Martin Hairer, Jonathan Weare

In the course of re-implementing the LJ7 rare event sampling example in the paper above, we discovered three textual errors and an implementation bug that does not change the conclusions of the paper but should change the reference output values in Table 1.

First, in the definition of $V(x)$, kT should be γ.

Second, in the definition of the region B, $V(x)$ should be replaced by $\gamma V(x)/\lambda$, i.e., the region was defined by distance independent of temperature and the TDMC parameters.

Third, the simulations were run with $\epsilon = 10^{-3}$ rather than $\epsilon = 10^{-4}$.

Finally, the implementation used to generate the paper's results mistakenly used

$$V(x) = \frac{\lambda}{\gamma} \min_{i \geq 2} \left\{ \sqrt{\left(x_{i,1} - \frac{1}{7} \sum_j x_{j,1} \right)^2 + \left(x_{i,2} - \frac{1}{7} \sum_j x_{j,\color{red}{1}} \right)^2} \right\} \tag{1}$$

where the second index on the x_i runs over the scalar components of the x_i vectors and the error is highlighted in red. With the example properly implemented, Table 1 of the paper should be replaced by Table 1 below. The transition probability for $\gamma = .075$ becomes lower than 10^{-13}, lower than the lowest transition probability in the original table, and therefore in this correction we replace $\gamma = 0.05$ and $\gamma = 0.025$ by two new values of γ. The algorithm continues to offer similar performance improvement at similar transition probabilities.

γ	λ	estimate	workload	$\frac{1}{2}\begin{pmatrix}\text{variance}\\ \times\text{workload}\end{pmatrix}$	brute force variance
0.4	1.6	8.26×10^{-3}	9.7	1.73×10^{-3}	8.19×10^{-3}
0.2	1.6	1.86×10^{-4}	8.6	4.84×10^{-6}	1.86×10^{-4}
0.15	1.9	3.26×10^{-6}	32	2.78×10^{-8}	3.26×10^{-6}
0.1	2.4	5.0×10^{-10}	83	2.9×10^{-14}	5.0×10^{-10}
0.08	2.6	5×10^{-13}	620	2×10^{-18}	5×10^{-13}

Table 1: Corrected version of the LJ7 example results in Table 1 of "Improved Diffusion Monte Carlo." Values were calculated using 5×10^5 replicates of each $\gamma > 0.08$ case and 1.5×10^5 replicates of the $\gamma = 0.08$ case.

While these numbers appear converged to the reported precisions, it is always possible that with more replicates the estimated values would change.