Monte Carlo Errors

Our aim is to evaluate the integral

$$I = \int_V \mathrm{d}^n x\, f(\mathbf{x}). \tag{1}$$

We start by mapping the integration volume to a unit hypercube. In the simple case that each dimension of this mapping is linear, this brings out a factor of the integration volume,

$$I = \int_1 \mathrm{d}^n \rho\, V f(\boldsymbol{\rho}) \equiv \int_1 \mathrm{d}^n \rho\, w(\boldsymbol{\rho}). \tag{2}$$

In the more general case, it brings out a factor of the determinant of the Jacobian of the mapping,

$$I = \int_1 \mathrm{d}^n \rho\, J(\boldsymbol{\rho}) f(\boldsymbol{\rho}) \equiv \int_1 \mathrm{d}^n \rho\, w(\boldsymbol{\rho}). \tag{3}$$

And in the most general case, we may use more than one uniform number to generate each integration variable,

$$I = \int_1 \mathrm{d}^m \rho\, J(\boldsymbol{\rho}) f(\boldsymbol{\rho}) \equiv \int_1 \mathrm{d}^m \rho\, w(\boldsymbol{\rho}) \quad m \geq n. \tag{4}$$

In all cases, we have to integrate a suitably-defined weight function over a unit hypercube.

Our strategy is to approximate this integral by the average value of the weight function at N randomly chosen points in the hypercube:

$$I \approx I_N = \frac{1}{N} \sum_i w_i, \tag{5}$$

where $w_i = w(\boldsymbol{\rho}_i)$ and $\{\boldsymbol{\rho}_i\}$ are chosen randomly and uniformly across the hypercube, i.e. w_i has probability distribution

$$\frac{\mathrm{d}P}{\mathrm{d}w_i} = \int_1 \mathrm{d}^m \rho\, \delta\Big(w_i - w(\boldsymbol{\rho})\Big). \tag{6}$$

We can check that the expectation value of I_N is I:

$$\Big\langle I_N \Big\rangle = \frac{1}{N} \sum_i \Big\langle w_i \Big\rangle. \tag{7}$$

Since the points for different i are uncorrelated, each of the expectation values are equal:

$$\Big\langle I_N \Big\rangle = \frac{1}{N} \sum_i \Big\langle w \Big\rangle = \Big\langle w \Big\rangle, \tag{8}$$

where

$$\Big\langle I_N \Big\rangle = \Big\langle w \Big\rangle = \int \mathrm{d}w\, w\, \frac{\mathrm{d}P}{\mathrm{d}w} = \int_1 \mathrm{d}^m \rho\, w(\boldsymbol{\rho}) = I. \tag{9}$$

To work out how good an approximation to I I_N is, we work out its variance:

$$V_{I_N} \equiv \Big\langle I_N^2 \Big\rangle - \Big\langle I_N \Big\rangle^2 \tag{10}$$

$$= \Big\langle \Big(\frac{1}{N} \sum_i w_i\Big)\Big(\frac{1}{N} \sum_j w_j\Big) \Big\rangle - \Big\langle w \Big\rangle^2. \tag{11}$$

We can reorganise the sums over i and j into $j = i$ and $j \neq i$:

$$V_{I_N} = \frac{1}{N^2} \Big\langle \sum_i w_i^2 + \sum_{i \neq j} w_i w_j \Big\rangle - \Big\langle w \Big\rangle^2. \tag{12}$$

In the first sum, each term is independent, $\sum_i \left\langle w_i^2 \right\rangle = N\left\langle w^2 \right\rangle$. In the second sum, for each of the N values of i, the $N-1$ values of j are all independent, and we obtain $\sum_{i\neq j} \left\langle w_i w_j \right\rangle = N(N-1)\left\langle w \right\rangle^2$ and hence

$$V_{I_N} \;=\; \frac{1}{N}\left\langle w^2 \right\rangle - \frac{1}{N}\left\langle w \right\rangle^2. \tag{13}$$

i.e. the standard deviation of our integral estimate I_N is $\frac{1}{\sqrt{N}}$ times the standard deviation of the weight distribution, a well-known result.

In the case of a linear mapping, we can also work this out in terms of the original function:

$$\begin{aligned} V_{I_N} \;=\; \frac{1}{N}\left(\int_1 \mathrm{d}^n\rho\, w^2 - \left(\int_1 \mathrm{d}^n\rho\, w\right)^2\right) \;&=\; \frac{1}{N}\left(V\int_V \mathrm{d}^n x\, f^2 - \left(\int_V \mathrm{d}^n x\, f\right)^2\right) && (14)\\ &=\; \frac{V^2}{N}\left(\frac{1}{V}\int_V \mathrm{d}^n x\, f^2 - \left(\frac{1}{V}\int_V \mathrm{d}^n x\, f\right)^2\right) && (15)\\ &=\; \frac{V^2}{N}\left(\left\langle f^2 \right\rangle - \left\langle f \right\rangle^2\right). && (16) \end{aligned}$$

Finally, we can obtain a Monte Carlo estimate of the variance of the weight distribution from the variance of the sample. We define

$$V_N \;=\; \frac{1}{N}\sum_i w_i^2 - \Big(\frac{1}{N}\sum_i w_i\Big)^2. \tag{17}$$

Using the result for the square of I_N above, we obtain

$$\begin{aligned} \left\langle V_N \right\rangle \;&=\; \left\langle w^2 \right\rangle - \frac{1}{N^2}\left(N\left\langle w^2 \right\rangle + N(N-1)\left\langle w \right\rangle^2\right) && (18)\\ &=\; \frac{N-1}{N}\left(\left\langle w^2 \right\rangle - \left\langle w \right\rangle^2\right). && (19) \end{aligned}$$

i.e.

$$V_{I_N} \;=\; \frac{1}{N-1}\left\langle V_N \right\rangle. \tag{20}$$

i.e. the variance in the Monte Carlo estimate of the integral is the (expectation value of) the variance of the Monte Carlo sample of weights divided by $N-1$. In many applications, N is assumed large enough that this can be replaced by N.