P346 Semester Project

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In the project I decided to work upon Monte Carlo Importance Sampling. Monte Carlo method, named after a casino in Los Alamos, was essentially designed by Enrico Fermi, John Von Neumann and Stanislaw Ulam in the 1930s when they were working in the Manhattan project. It uses randomness to estimated the area of a curve.

In the normal crude MCM(Monte Carlo Method), we take random x values from the initial to the final limit of the integration and then calculate the integral accordingly. But this means that if certain values of the function contribute more to the integral, like those that are higher, then these values will be counted more than they should be because of the uniform randomness of x. To counter that we use a sampling function p(x).

$$\int_a^b f(x)dx = \int_a^b \frac{f(x)}{p(x)} p(x)dx \tag{1}$$

$$\implies \int_a^b f(x)dx = \frac{1}{N}\sum_i^N \frac{f(x_i)}{p(x_i)} \tag{2}$$

where x_i are sampled according to $p(x)$.

This sampling function should mimic f(x), be normalized, integrable and it should be possible to sample points from it effectively.

To enhance the sampling even further, we introduce a function G(x) and perform a change of variables to r.

$$\begin{aligned} G(x) &= \int_0^x g(x)dx \\ r &= G(x) \end{aligned} \tag{3}$$

So,

$$I = \int_a^b \frac{f(x)}{g(x)} dG(x) = \int_0^1 \frac{f(G^{-1}(r))}{g(G^{-1}(r))} dr \approx \frac{1}{N}\sum_i^N \frac{f(G^{-1}(r_i))}{g(G^{-1}(r_i))} \tag{4}$$

Because g is normalized hence $0 \leq G(x) = r \leq 1$. Here then r_i are sampled from 0 to 1. Hence using this G function we can get an even better estimate of the integral because G contains the information of entire sampling of g. G is essentially introduced for a change of variable for the integration.

Few things to keep in mind are that the sampling function will always have a parameter which has to be calculated such that the variance of the integral is minimised. This can be done by running a loop for difference values of variance and choosing the one which gives the lowest variance.

References:

1. Variational Monte Carlo Technique, Ground State Energies of Quantum Mechanical Systems by Sukanta Deb