Computational Methods Assignment 6 - Monte Carlo Integration

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1 Question 1 - Discussion of the Method

In this program, the *Mcint* class takes a specific, potentially multivalued function of N variables to integrate between upper and lower limits, each individually specified by N-dimensional vectors. To integrate the function between the limits using importance sampling the user must supply the function to be integrated, the probability distribution to weight the samples, and an extra function supplied to either (a) generate the distribution of random numbers from a uniform deviate or (b) a function which produces numbers distributed according to the user's desired probability distribution. In this method, the function $f(\vec{x})$ (or $f(\vec{x})/p(\vec{x})$ if importance sampling) is sampled over volume V at M_{init} values, to calculate the average $V\langle f\rangle$ (or $\langle f/p\rangle$ for importance sampling). At each step, additional amount of samples are taken equal to the number currently included in the average, M. The old evaluation of the integral is multiplied by M and then the further M samples are added to it, to then divide by $2M$. As a measure of error, the standard error is used as a metric to determine the point to stop iterating the method. At each step, as well as calculating $\langle f\rangle$ (or $\langle f/p\rangle$), the value of $\langle f^2\rangle$ (or $\langle f^2/p^2\rangle$) is also calculated to obtain the standard error according to:

$$\sigma = \sqrt{\frac{\langle f^2\rangle - \langle f\rangle^2}{M}}$$

This means that the error, as expected, should decrease as $M^{-1/2}$ as the number of samples M is increased. This means that by doubling the samples it is expected that the error should decrease by a factor of $\sqrt{2}$ each time.

2 Question 2 - Uniform vs Importance sampling

The error function was supplied as the integrand and firstly the evaluation of erf(2) was performed using the uniform sampling of points in an integral, later to be calculated using a distribution $\text{pdf}_1(y) = 0.98 - 0.48y$ with a correspond cummulative distribution of:

$$\text{cdf}_1(y) = -0.24^y + 0.98y = x \implies y = \text{cdf}^{-1}(x) = \frac{0.98 - \sqrt{0.98^2 - 0.96x}}{0.48}$$

Alos to test the effect of different probability distributions on the convergence of the method, a second probability distribution function was used which bared a similar functional form to the integrand.

$$\text{pdf}_2(y) = \frac{3e^{-1/5y}}{2(1-e^{-3}} \implies y(x) = \text{cdf}_2^{-1}(x) = -\frac{2(1-e^{-1.5y}}{3(1-e^{-3})}$$

This was additionally fed into the method to assess convergence.
This was passed to the generalised integrator class along with the probability distribution function. A step constitutes the doubling of the number of samples and calculation of the average and the average square of the integrand. After 22 steps, it became too computationally cumbersome to iterate the method. After 22 steps, the value of erf(2), the standard error, and the predicted iterations required to obtain an accuracy of $\epsilon = 10^{-6}$ are shown in Table 1. This shows that implementing importance sampling results in a higher convergence of the integral, with a smaller standard error that the value obtained by uniform sampling after 22 steps. It was found that as the number of steps increased, the error associated with each step reduced by factor which became closer to $\sqrt{2}$ each time. This meant that, assuming that the error decreases by a factor

	Uniform Sampling	Importance Sampling (pdf_1)	Importance Sampling (pdf_2)
$\mathrm{erf}(x=2)$	0.995311	0.99532	0.995325
Std. Error	1.7×10^{-5}	5.9×10^{-6}	4.9×10^{-6}
Predicted Iterations for $\epsilon = 10^{-6}$	31	28	27
Corresponding required samples	1.074×10^{12}	1.342×10^{11}	6.71×10^{11}

Table 1: Results from calculation of erf(2) using both uniform sampling and importance sampling.

of $\sqrt{2}$ each step, that the number of steps required to reach the convergence criterion of $\epsilon = 10^{-6}$ could be predicted. This was found by taking the currentstandard error value at 22 steps, finding how many divisions by $\sqrt{2}$ were needed to obtain $\sigma < \epsilon$, and adding that to the number of steps already carried out (22). The number of samples this corresponds to is $M_{\text{start}} \times 2^{n_r}$ where $M_{\text{start}} = 500$ is the initial number of iterations carried out in the first step, and n_r is the number of required iterations for convergence.

This means that the number of samples required for the same accuracy is 8 times higher for the uniform sampling than the importance sampling.