Investigation into Numerical Integration

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1 Importance Sampling

The key to importance sampling is that we can think of an integrand as a probability distribution. Hence we can write

$$I = \int_{volume} P(\vec{x}) g(\vec{x}) d^N x \tag{1}$$

Assuming the distribution is normalised we can then approximate the integral to

$$I \approx \frac{1}{N} \sum_{i=1}^{N} g(\vec{x_i}) \tag{2}$$

2 Integrating $\cos^2(x)$

Using Equation 1 and setting $P(\vec{x}) = 1$, $g(\vec{x}) = \cos^2(x)$ we can perform the integral as in Equation 2.

2.1 Finding the error in the value

In order to approximate the error in this method with different values of N we can take a sample of 100 different values for each value of N. We can then calculate the standard deviation among these 100 values to see how accurate this method is for any given N. This is shown in Figure 1.

N	Mean	Std. Dev.
10	0.729913765866	0.0584584499866
100	0.728009655427	0.022552488229
1000	0.727503409834	0.00700622952894
10000	0.727190923513	0.0020022253523
100000	0.727357604272	0.000705901363029
1000000	0.727312439746	0.000244233723048
10000000	0.727318292933	0.0000662636889731

Figure 1: Summary of measured quantities and their uncertainties in samples of 100

This can be plotted and then extrapolated as shown in Figure 2

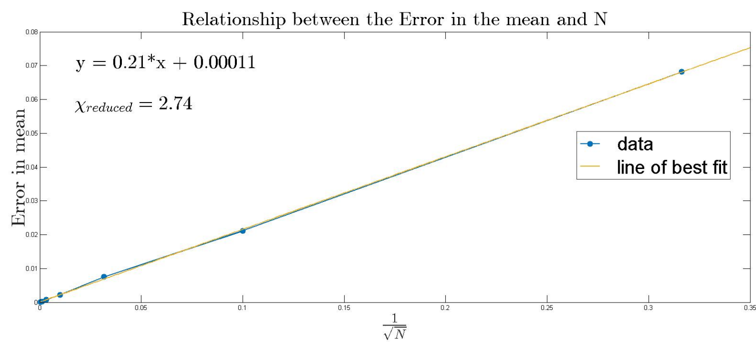


Figure 2: Relationship between error and N

For this particular example we now have the relation (where we ignore the constant)

$$\sigma_{\mu=0.21\frac{1}{\sqrt{N}}} \tag{3}$$

If we would like to calculate how large N should be for the error to be accurate to the 10th decimal place then we could do a calculation like the following :
$N = (0.21 \times 10^{10})^2$
$= 4.41 \times 10^{18}$

3 Finding volume of unit N-sphere

We can also use Monte Carlo methods to determine the volume of a unit N-sphere by accepting and rejecting points as appropriate and taking a ratio.
For example if we consider an N-dimensional vector

$$A = \begin{bmatrix} a_1 \\ a_2 \\ ... \\ a_n \end{bmatrix} \tag{4}$$

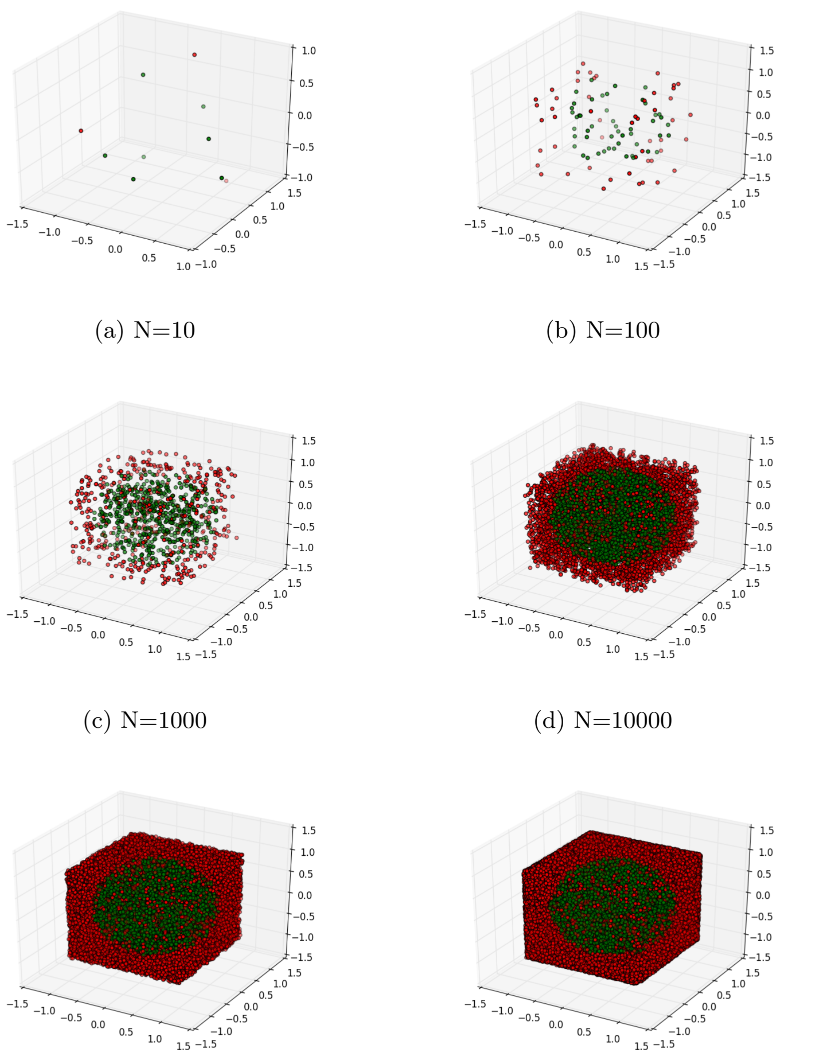
The surface of the unit N-sphere is given by

$$A \cdot A = 1 \tag{5}$$

Thus by taking the ratio

$$\text{Volume of sample space} \times \frac{\text{Accepted points}}{\text{Total points}} \tag{6}$$

we can get an estimate for the volume of an N-dimensional sphere. This can be visualised for a unit sphere in Figure 3.



(a) N=10

(b) N=100

(c) N=1000

(d) N=10000

(e) N=100000

(f) N=1000000

Figure 3: Visualisation of determining the volume of a unit sphere by Monte Carlo methods with different numbers of points

4 Metropolis Algorithm

For cases where we know the probability distribution but cannot normalise it we have to resort to other methods.

One such method is by only taking into account values generated by the Metropolis algorithm. The Metropolis algorithm explores the sample space by taking a random walk through the sample space accepting points according to some probability.

When using this method, it is important to monitor the rejection rate of the algorithm to ensure the end result is of good quality.

For example if we wanted to calculate the integral

$$\int_{-\infty}^{\infty} P_\beta(x)V(x)dx \tag{7}$$

where $P_\beta \propto e^{-\beta V(x)}$
This integral could then be approximated as

$$\frac{1}{N}\sum_{i=1}^{N} V(x_i) \tag{8}$$

where x_i is generated by the Metropolis algorithm at the given value of β
The analytic answer can be obtained by the following

$$I = \frac{\int_{-\infty}^{\infty} P_\beta(x)V(x)dx}{\int_{-\infty}^{\infty} P_\beta(x)dx} \tag{9}$$

$$\frac{\int_{-\infty}^{\infty} e^{-\beta V(x)}V(x)dx}{\int_{-\infty}^{\infty} P_\beta(x)dx} \tag{10}$$

$$\frac{-\frac{d}{d\beta}\int_{-\infty}^{\infty} e^{-\beta V(x)}dx}{\int_{-\infty}^{\infty} e^{-\beta V(x)}dx} \tag{11}$$

We are interested in the particular case $V(x) = \frac{x^2}{2}$
Making use of the Gaussian integral we obtain $\int_{-\infty}^{\infty} e^{-\beta V(x)}dx = \sqrt{\frac{2\pi}{\beta}}$
After substituting this into Equation 11 we arrive at the analytic answer of $\frac{1}{2\beta}$
A comparison between the analytic and calculated value is given in Figure 4

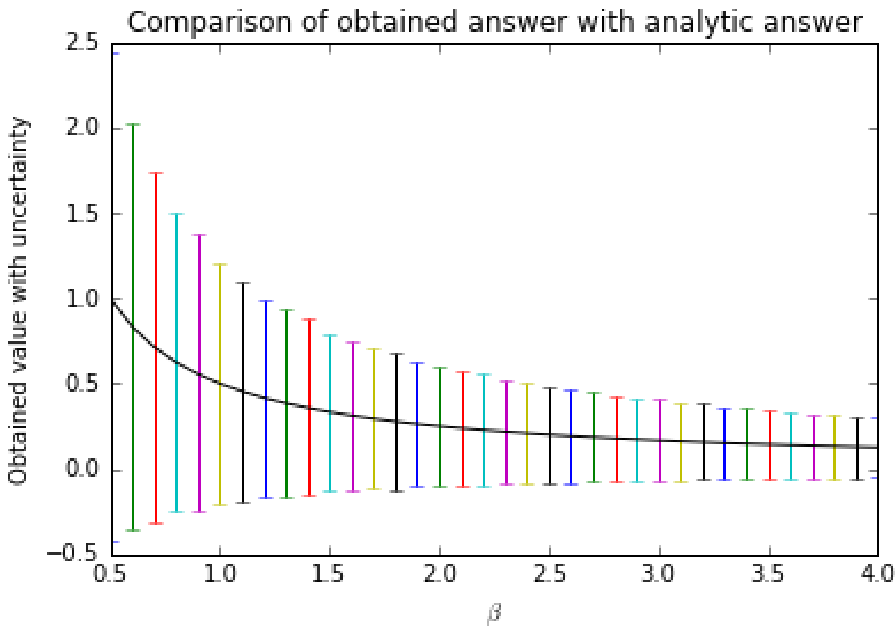
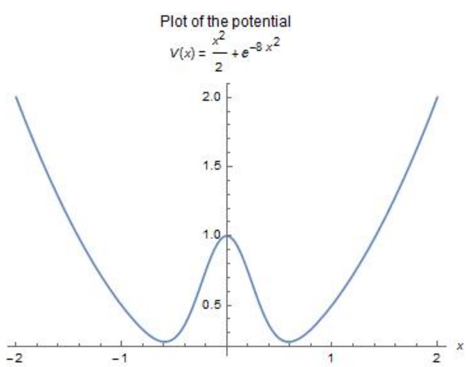
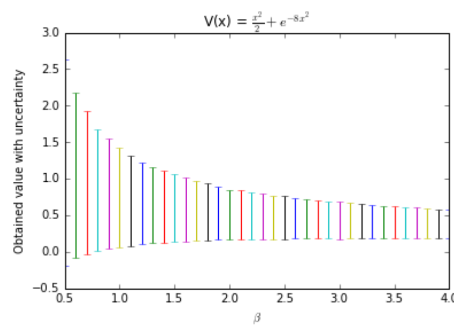


Figure 4: Comparison of analytic and calculated values

The same is done for the potential $V(x) = \frac{x^2}{2} + e^{-8x^2}$ and the results are summarised in Figure 5



(a) Potential function



(b) Calculated values using Metropolis algorithm

Figure 5: New potential function and corresponding calculated values