

## Assignment 2

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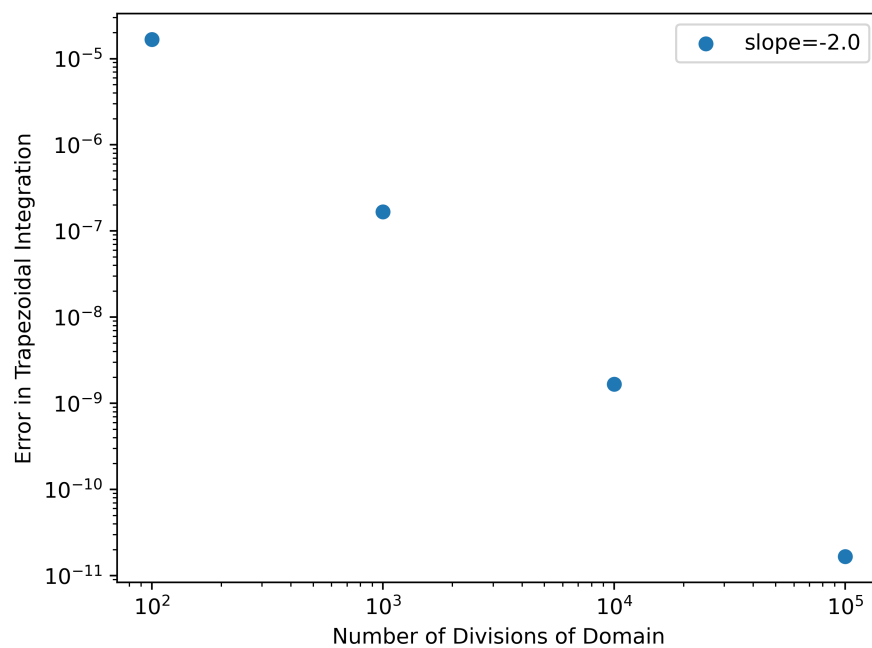
### 1. a)

Trapezoidal rule with  $N = 500$ .

$$\int_0^1 \frac{4}{1+x^2} dx = 3.1415919869231304$$

### 1. b)

$$\int_0^1 \frac{1}{1+x^2} dx$$



### 1. c)

Trapezoidal rule with  $N = 500$ .

$$\int_0^\pi \sin x dx = 1.9999934202594030$$

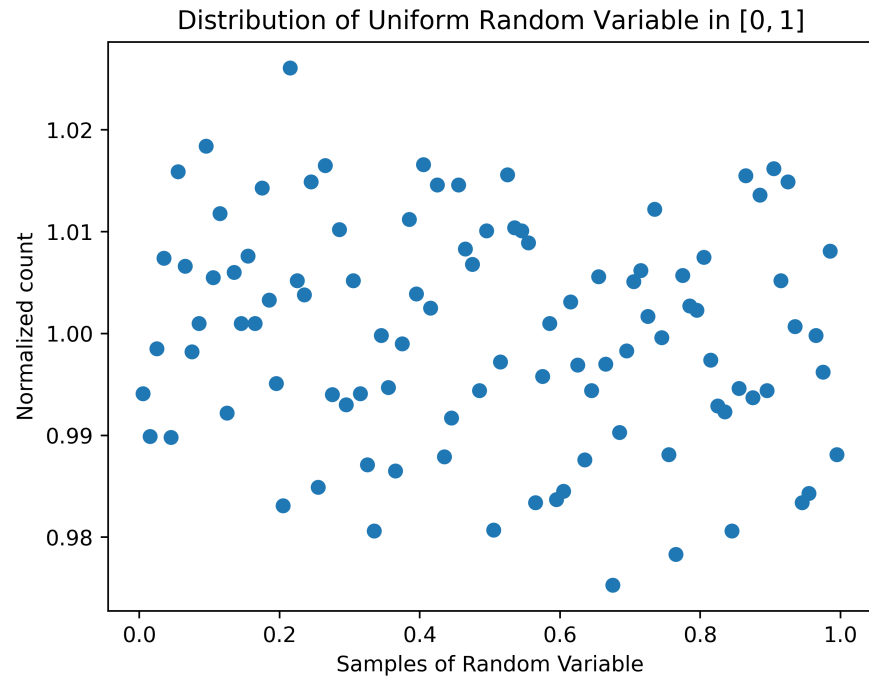
## 1. d)

Trapezoidal rule with  $N = 500$ .

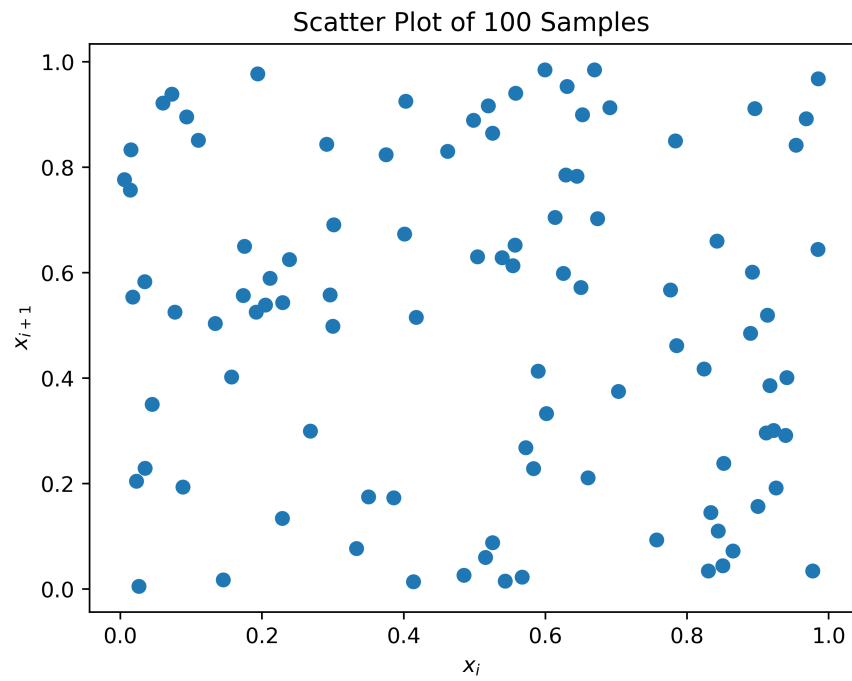
$$\int_0^\pi \frac{1}{2\pi} \exp\left(-\frac{x^2}{2}\right) dx = 0.99729988484824805$$

## 2. a)

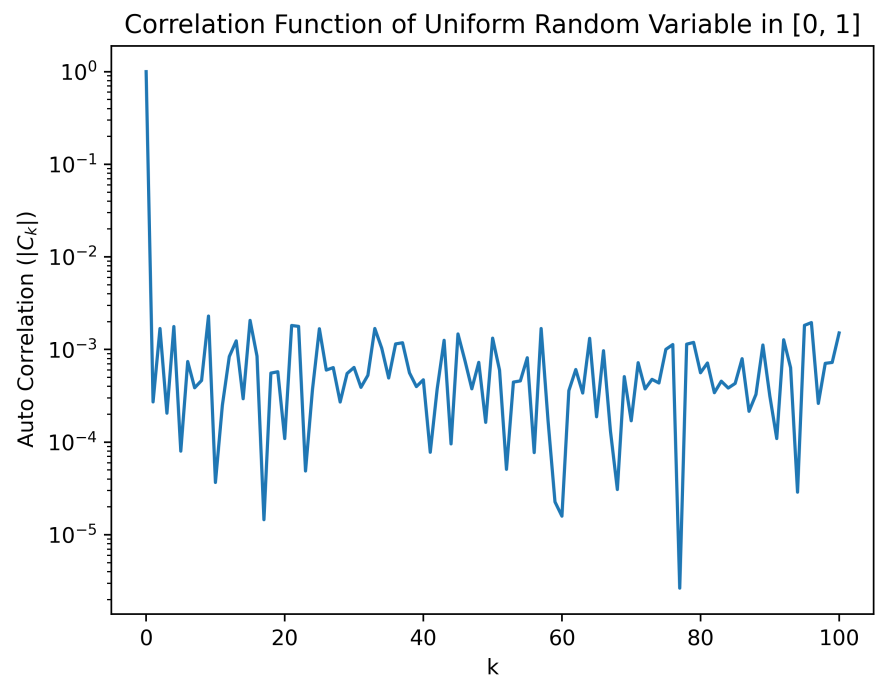
A sample size of  $10^6$  was used for the this question.



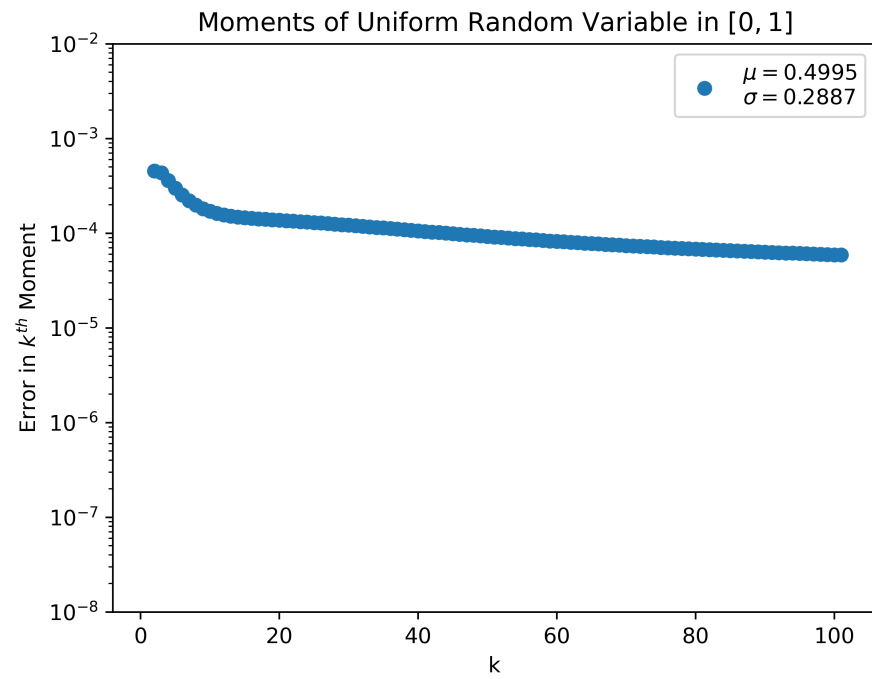
2. b)



2. c)

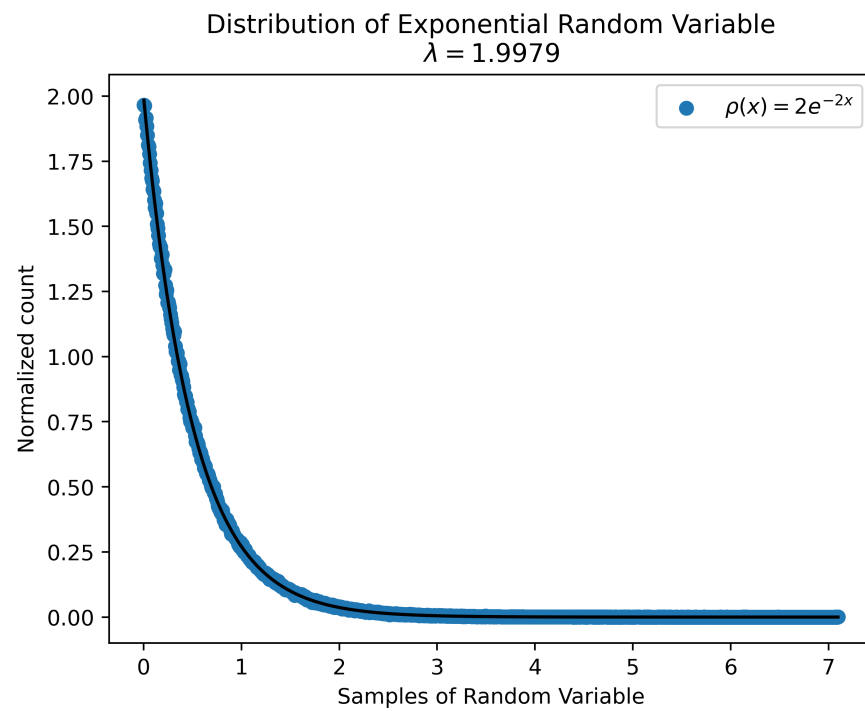


2. d)



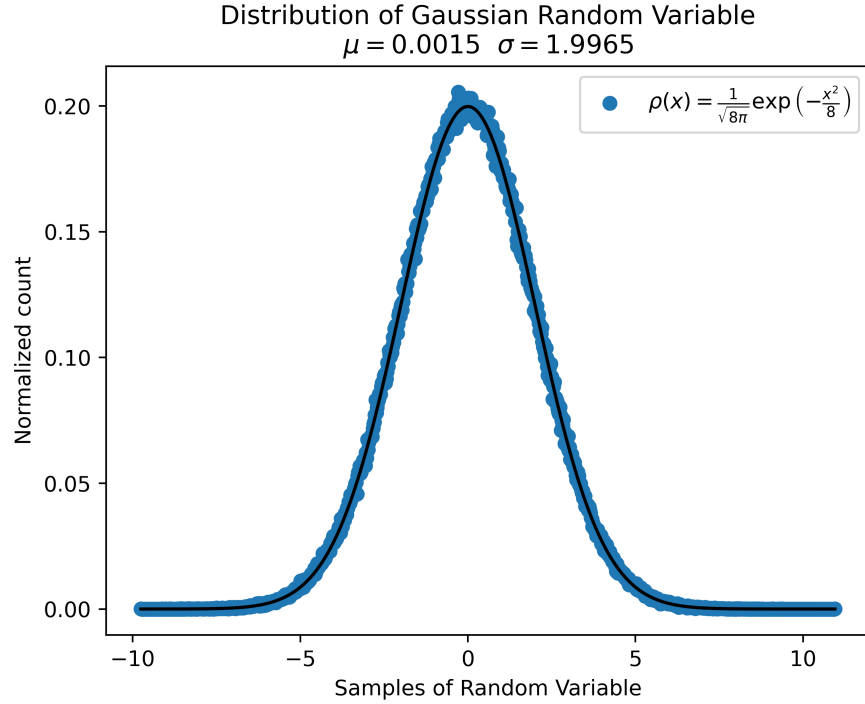
4. a)

A sample size of  $10^6$  was used for the this question.



#### 4. b)

A sample size of  $10^6$  was used for the this question.



#### 5. a)

We need to use brute force Monte Carlo in the interval  $S^6$  where  $S = [-a, a]$ , let us get an estimate of the error of neglecting the region  $\mathbb{R}^6 - S^6$ .

$$\begin{aligned}
 g(\vec{x}, \vec{y}) &\leq \exp(-\vec{x}^2 - \vec{y}^2) \\
 \Rightarrow \int_{\mathbb{R}^6 - S^6} g &\leq \int_{\mathbb{R}^6 - S^6} \exp(-\vec{x}^2 - \vec{y}^2) dx^3 dy^3 \\
 &= \int_{\mathbb{R}^6} \exp(-\vec{x}^2 - \vec{y}^2) dx^3 dy^3 - \int_{S^6} \exp(-\vec{x}^2 - \vec{y}^2) dx^3 dy^3 \\
 &= \left( \int_{\mathbb{R}} \exp(-x^2) dx \right)^6 - \left( \int_S \exp(-x^2) dx \right)^6
 \end{aligned}$$

Let  $m = \int_S \exp(-x^2) dx$ ,  $n = \int_{\mathbb{R} - S} \exp(-x^2) dx$ , then we can rewrite the above expression as

$$\begin{aligned}
 &= (m + n)^6 - m^6 \\
 &= 6m^5n + 15m^4n^2 + 20m^3n^3 + 15m^2n^4 + 6mn^5 + n^6
 \end{aligned}$$

Clearly we are only concerned with the case where  $n \ll m$ , which simplifies things to

$$\begin{aligned}
 &\leq 6m^5n + 57m^4n^2 \\
 &\leq 6(2a)^5n + 57(2a)^4n^2
 \end{aligned}$$

we can also write

$$n = \sqrt{\pi} - \int_{-a}^a e^{-x^2} dx = \sqrt{\pi} \left( 1 - \int_{-a\sqrt{2}}^{a\sqrt{2}} \mathcal{N}(x) dx \right)$$

where  $\mathcal{N}$  is the normal distribution. For  $a = 5$ ,  $5\sqrt{2}$  corresponds to atleast  $7\sigma$  deviations in the normal distribution which gives us

$$n \leq \sqrt{\pi}(1 - 0.99999999997440) \approx 4.537 \cdot 10^{-12}$$

Substituting back, we get

$$\int_{\mathbb{R}^6 - S^6} g \leq 2.222 \times 10^{-6}$$

which is a reasonable upper bound on the error.

Performing the integration with  $N = 10^6$  (we keep this constant across all Monte Carlo integration methods), we get

$$I \approx 9.8930026$$

Error estimated by Monte Carlo is 1.0814584 while actual error is 1.0693717.

## 5. b)

Now we do importance sampling with the Gaussian distribution in all 6 dimensions because the form of  $g$  is similar to a Gaussian. Performing the integration, we get

$$I \approx 10.9569892$$

Error estimated by Monte Carlo is 0.0227644 while actual error is 0.0053850.

We can also integrate using brute force in a finite region if we do the change of variables  $x_i = \tan y_i$  in each dimension, we get upon integration

$$I \approx 10.9221337$$

Error estimated by Monte Carlo is 0.0600769 while actual error is 0.0402405.

## Helium Atom Ground State

The energy of the Helium atom ground state using variational principle (using the separable solution as trial wave function) was found to be

$$E \approx -74.870595491123623 \pm 0.35615620981281765$$