Assignment 2

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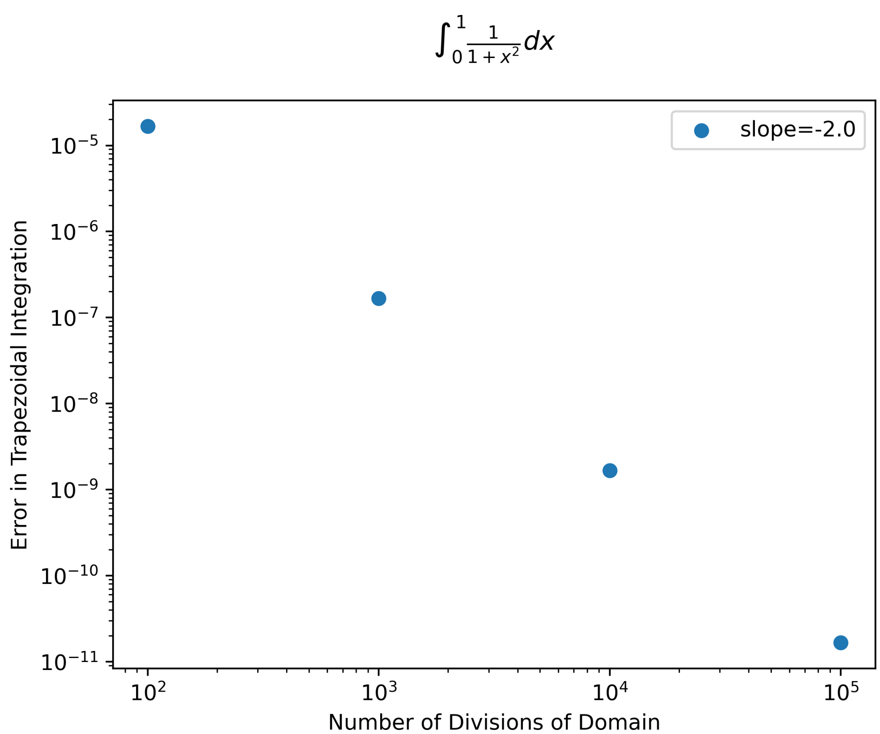
1. a)

Trapezoidal rule with $N = 500$.

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

1. b)



1. c)

Trapezoidal rule with $N = 500$.

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

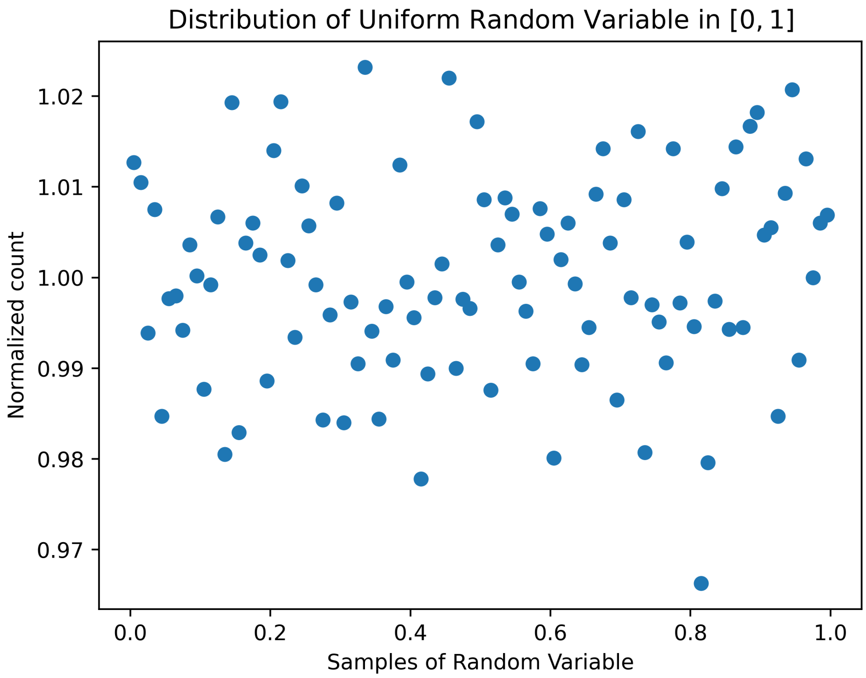
1. d)

Trapezoidal rule with $N = 500$.

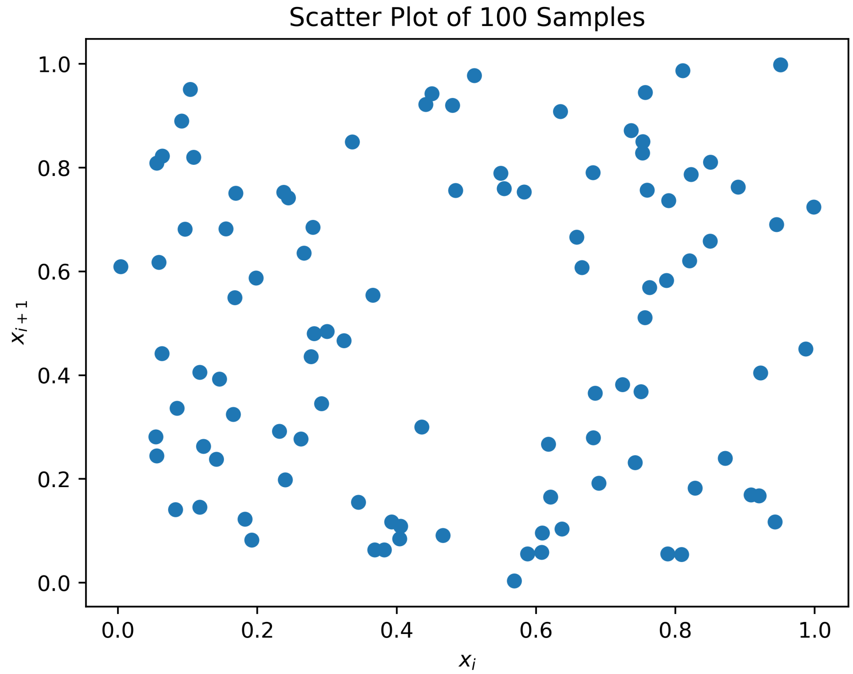
$$\int_{-3}^{3} \frac{1}{2\pi} \exp\left(-\frac{x^2}{2}\right) dx = 0.997299884848224805$$

2. a)

A sample size of 10^6 was used for this question. 100 bins were used to plot the distribution.

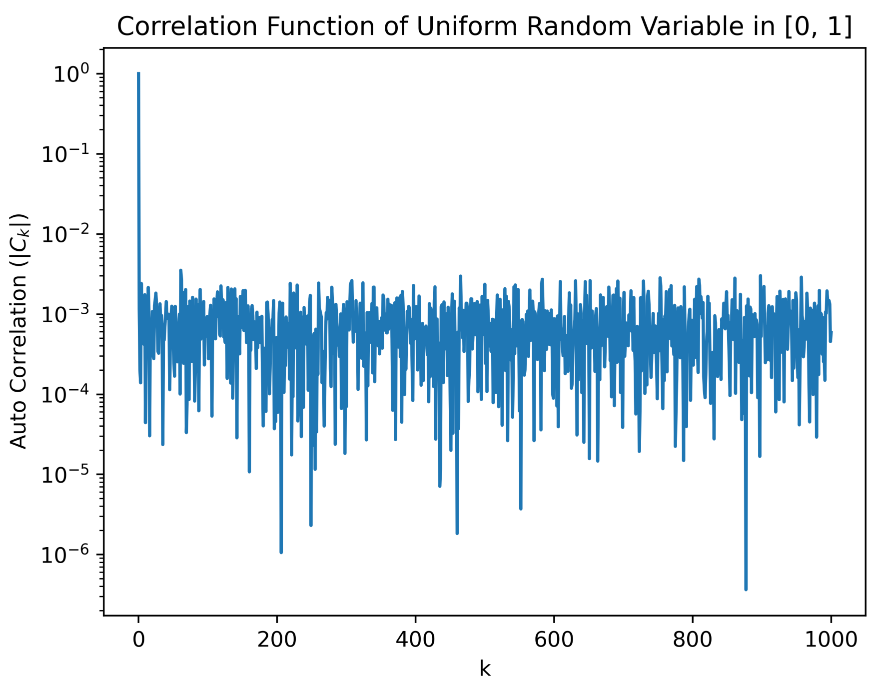


2. b)



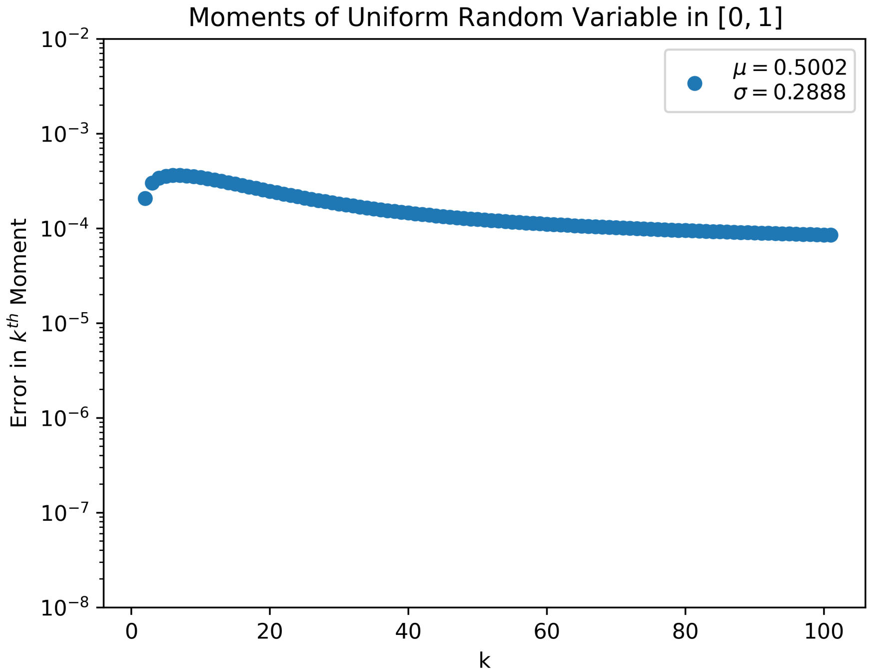
Scatter Plot of 100 Samples
1.0
0.8
0.6
0.4
0.2
0.0
0.0
0.2
0.4
0.6
0.8
1.0
x_{i+1}
x_i

2. c)



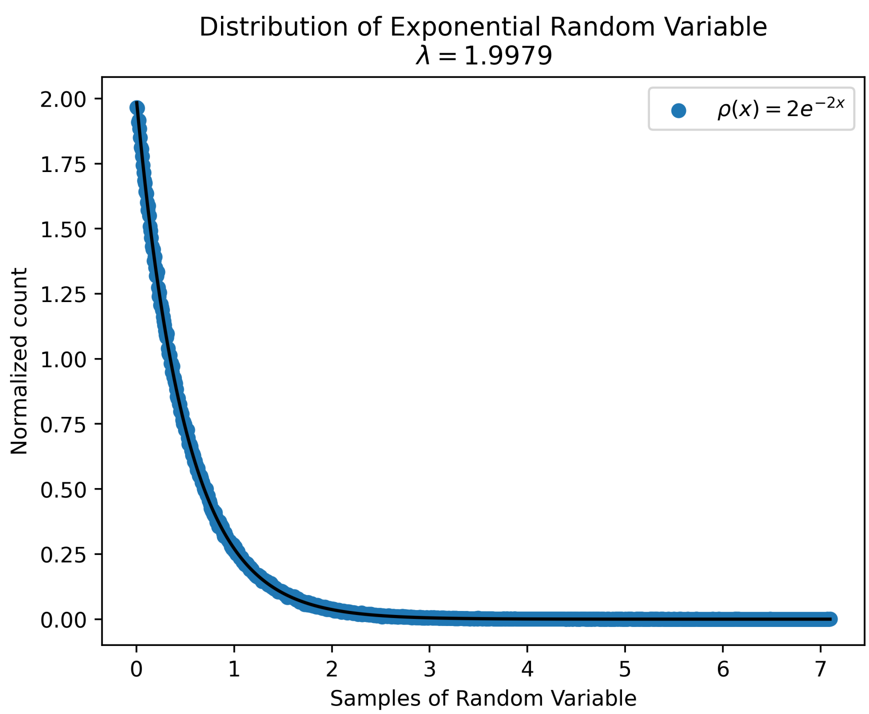
Correlation Function of Uniform Random Variable in [0, 1]
10^0
10^{-1}
10^{-2}
10^{-3}
10^{-4}
10^{-5}
10^{-6}
Auto Correlation ($|C_k|$)
0
200
400
600
800
1000
k

2. d)



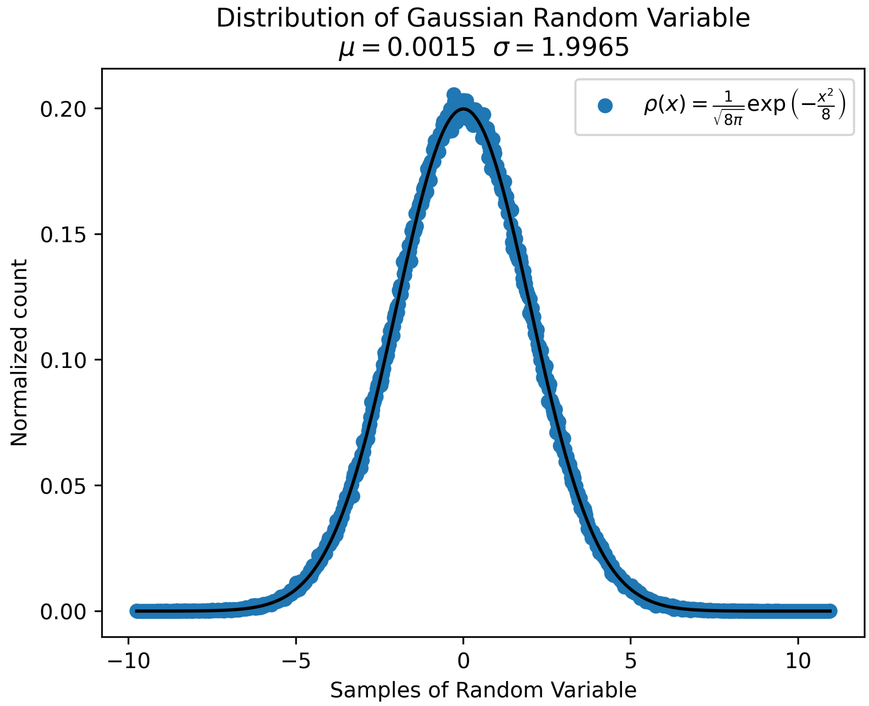
4. a)

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



4. b)

A sample size of 10^6 was used for 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 $\mathbb{R}^6 - S^6$.

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

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 7σ deviations in the normal distribution which gives us

$$n \leq \sqrt{\pi}(1 - 0.999999999997440) \approx 4.537 \cdot 10^{-12}$$

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

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