PHY407 Lab 10

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The workload was distributed as followings:

- **Sang Bum Yi did question 1**
- **Jianbang Lin did question 2 and 3**

Question 1

Part a)

The Brownian motion was computationally simulated by having a single particle move randomly in any of four directions (up, down, left, and right). The random move, or "random walk", was implemented with *random.randrange(int)*, which is Python's built-in function that generates a random integer between 0 and (int – 1). Since there were four available moves, the int parameter inside *randrange* function was set to 4.

The particle was confined to a square grid of 101 x 101 dimensions. For example, the particle could only move down, left, or right when it hits the top boundary. The full trajectory of the particle's random walk was recorded and can be seen in *Q1_partA_Brownian.mp4*.

Part b)

The diffusion-limited aggregation, or "DLA", was computationally simulated with 100 particles, which were confined to the 101 x 101 square grid. In DLA, the first particle started the random-walk in the centre and moved until it hit the boundary. Unlike the random-walk simulated in part 'a', particles in DLA get 'anchored' and become immovable when they hit the boundary. After the first particle got anchored, the second particle was introduced in the centre of the grid. Then it started the random-walk and moved until it hit either the boundary or any anchored particle, after which it also got anchored. The same process repeated until all 100 particles were anchored.

Since taking a record of the full trajectory of 100 particles in the DLA would have taken so long, a simulation of DLA with 15 particles in 11 x 11 square grid was instead recorded in order to show the full trajectory of particles until getting anchored, which can be seen in *Q1_partB_15particles.mp4*.

Finally, the final DLA distribution of 100 particles was recorded without the full trajectories and can be seen in *Q1_partB_100particles.mp4*.

Part c)

Building on part 'b', the square grid was expanded to 151 x 151 dimensions. Then the DLA was simulated until there is an anchored particle in the centre of the grid. The final DLA distribution can be found in Figure 1.1 below.

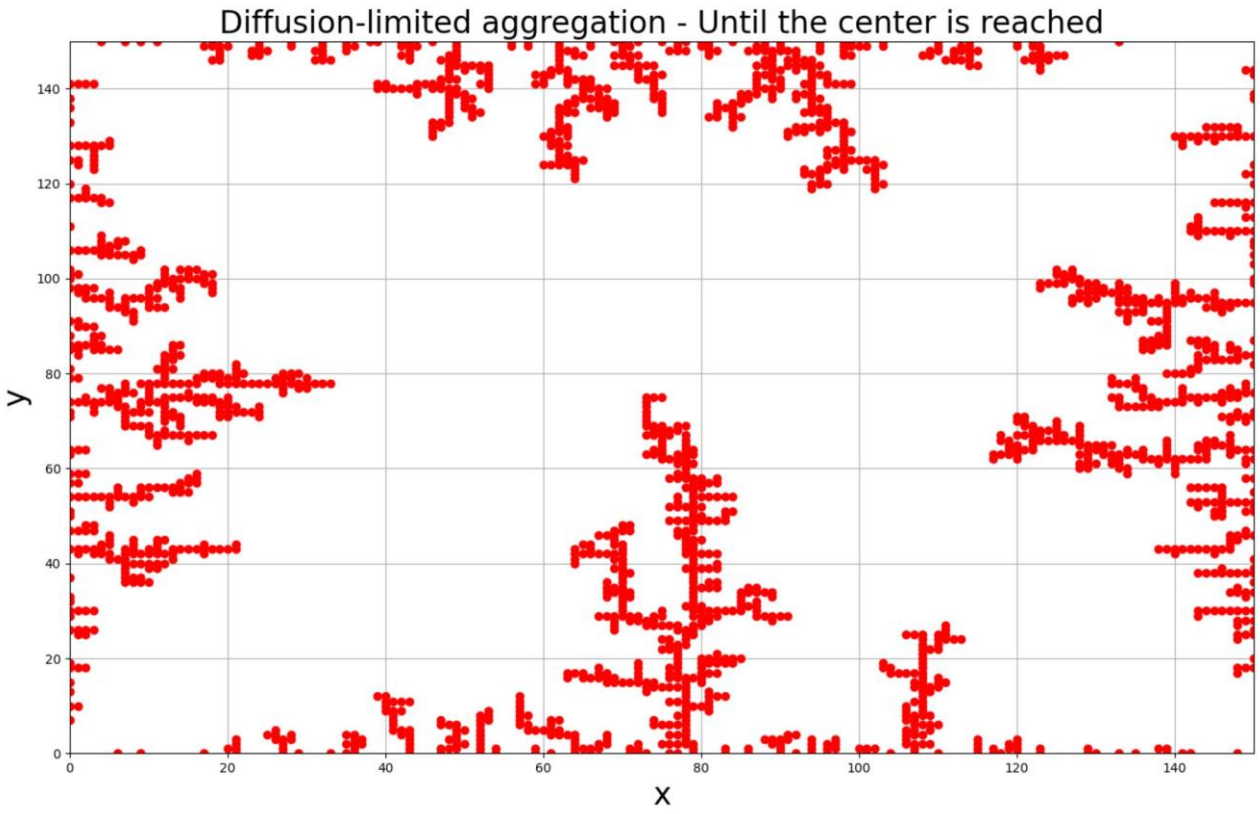

Figure 1.1: The final DLA distribution when a particle was anchored at the centre of 151 x 151 square grid. Each red dot represents an anchored particle.

In order to demonstrate the full trajectory of particles getting anchored until the centre of the grid would be occupied, the simulation of 31 x 31 square grid was recorded and can be seen in *Q1_partC_31_31.mp4*. The reduction of dimensions of the square grid was required because taking a record of the full trajectory of the DLA in 151 x 151 square grid would take so long.

Question 2:

The volume of n-dimensional hypersphere of radius R can be calculated using equation:

$$V_n(R) = \frac{R^n n^{1/2}}{\Gamma\left(\frac{n}{2}+1\right)} \qquad \text{[eq 2.1]}$$

Where Γ is the gamma function. It can also be calculated using the Monte Carlo method, which picks multiple points, values ranging from -1 to 1, these points will represent the location at n-dimensional. Then check if these points fall inside the hypersphere. Once we have number of points generated and number of points fall inside the hypersphere, we can use the following equation:

$$I = \frac{k}{N} A \qquad \text{[eq 2.2]}$$

Where I is the volume of hypersphere, k is the number of points fall inside the hypersphere, N is the total number of points used, A is the volume of hypercube, and its volume is give as 2^n, where n is the number dimension. Equation 2.2 can also be expressed as:

$$I = \int_{\nu} f(\tau)\, d\tau \qquad \text{[eq 2.3]}$$

Where f(τ) = 1 if it τ is inside the hypersphere, and f(τ) = 0 otherwise. Use this equation, the error of Monte Carlo method can be calculated:

$$\sigma = 2^n \sqrt{\frac{\frac{\sum_i \left(f(\tau_i)^2\right)}{N} - \left(\frac{\sum_i f(\tau_i)}{N}\right)^2}{N}} \qquad \text{[eq 2.4]}$$

The volume calculated using 1,000,000 points is 2.551808 +/- 0.051054, where the actual volume calculated using equation 2.1 is around 2.55, which falls into the value calculated using Monte Carlo method.

Question 3

Part a)

Given equation:

$$I = \int_0^1 \frac{x^{-1/2}}{1+e^x}\,dx \qquad \text{[eq 3.1]}$$

Two methods are used to evaluate this integral; mean value method and importance sampling. However, importance sampling gives inaccurate results if the number of sampling points is too small. To see this, 10,000 points are used to calculate integral 3.1, and this calculation is ran 100 times, and the values of integration for these two methods are shown as following:

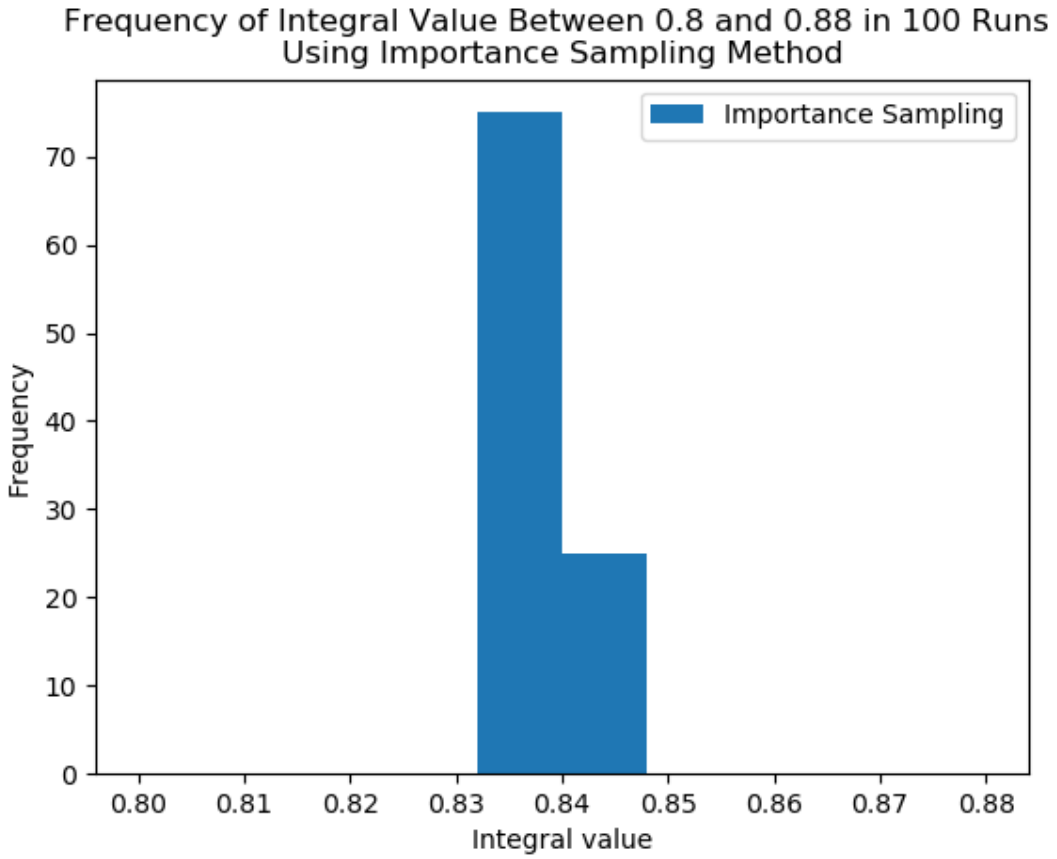

Figure 3.1: The frequency of integral values of equation 3.1 approximated using importance sampling method

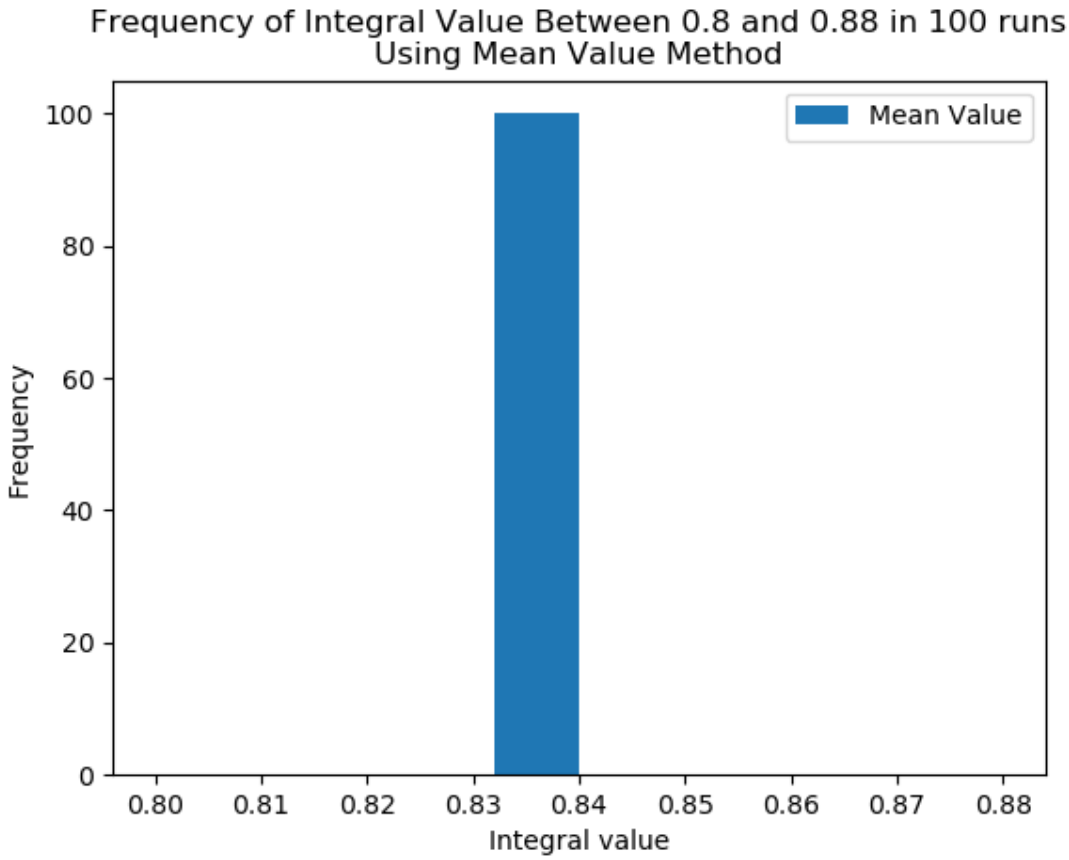

Figure 3.2: The frequency of integral values of equation 3.1 approximated using mean value method

Figure 3.1 and 3,2 show that the integral value using the mean value method is consistent, the value is 0.835908451712108. However, the values calculated using the importance sampling vary between 0.83 and 0.85, and the average of these 100 calculations is 0.8388400877961055. The actual value of this integral is 0.839, and these two methods give very accurate approximations. Importance sampling gets more accurate with more sampling points.

Part b)

To calculate the integral:

$$I = \int_0^{10} e^{-2|x-5|} \mathrm{d}x \qquad \text{[eq 3.2]}$$

By using the same method as in part a, 10,000 points are used, and repeat the calculation 100 times, the results of mean value method and importance sampling are shown as following:

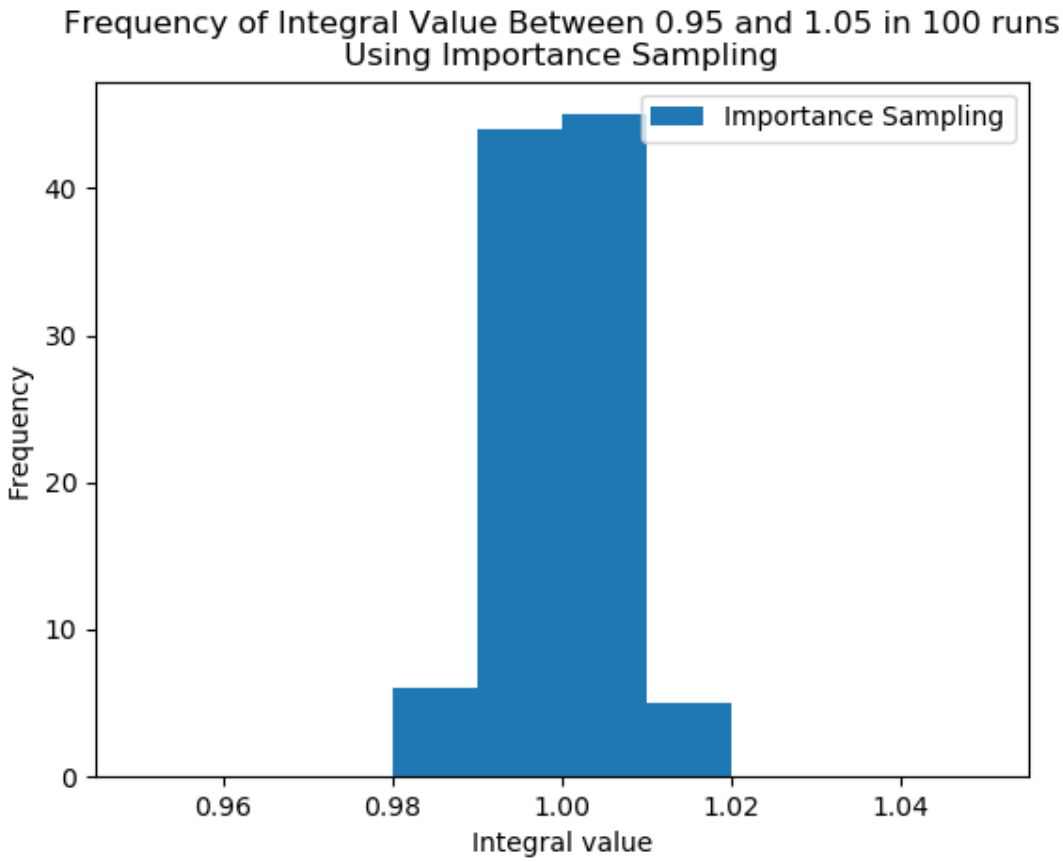

Figure 3.3: The frequency of integral values of equation 3.2 approximated using importance sampling method

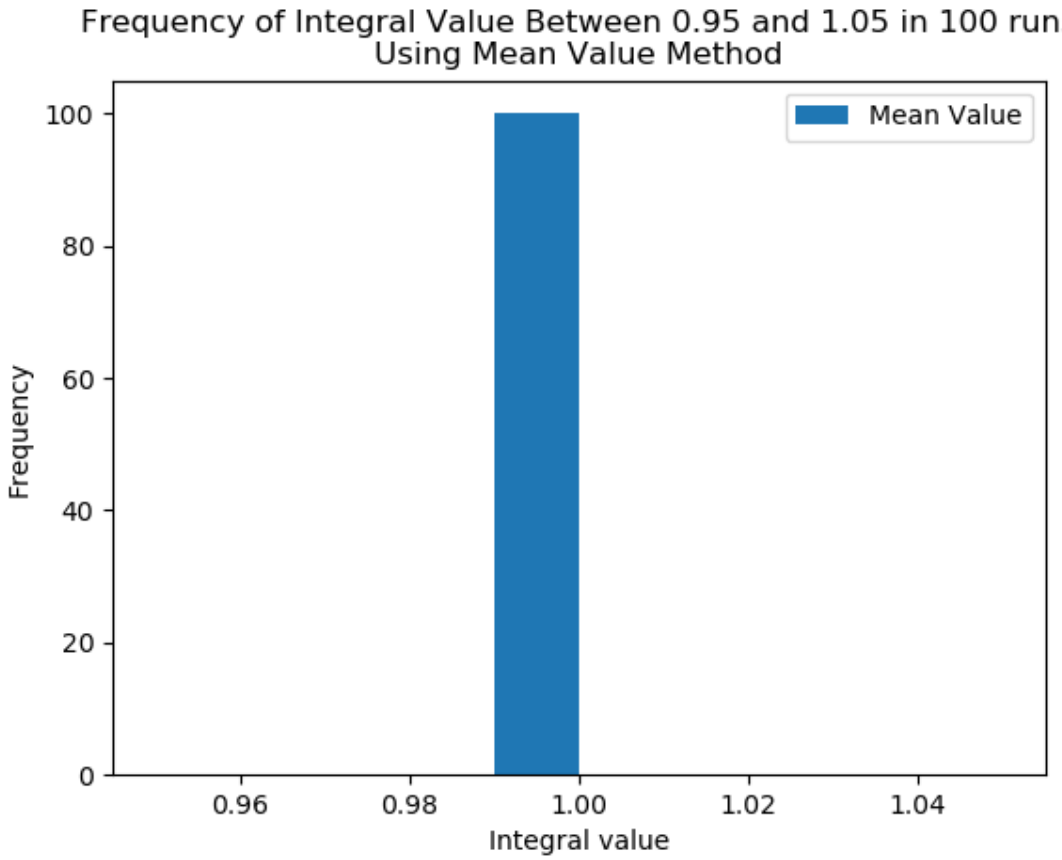

Figure 3.4: The frequency of integral values of equation 3.2 approximated using mean value method

The result is similar to result in part a, the mean value method gives a consistent approximation of value 0.9999544334111573. On the other hand, the importance sampling method gives values between 0.98 and 1.02, and by average of these 100 calculations is 1.0012123182351227. The actual value of integral 3.2 is 1, and the approximation made by these two methods are very close to the actual value.