Physics 77/88 - Fall 2024 - Homework 7

Monte-Carlo Simulation and Numerical Integration

Submit this notebook to bCourses to receive a credit for this assignment.
due: **Nov 10th 2024**
Please upload both, the .ipynb file and the corresponding .pdf

Total: 25P

In the lecture, we showed how a **M**onte-**C**arlo **S**imulation (**MCS**) can be used for estimating π. A MSC can also be used for estimating an integral numerically, even if the object of which the integral has to be calculated is high dimensional.

Consider the volume V of a N dimensional *hypersphere* or *N-ball* of radius R:

$$V_N(R) = \frac{\pi^{N/2}}{\Gamma(\frac{N}{2}+1)}\,R^N$$

Here, $\Gamma(x)$ is Euler's gamma function. Note, that for solving the problem, **no knowledge about the gamma function is needed**. In Python, we can import the gamma function via:

In [1]:
```
import math
N = 3
Result = math.gamma(N/2 + 1)
```

As an estimate, the values for the volumes of the following N are:

$N = 2$: $V = \pi\,R^2 \approx 3.142\,R^2$
$N = 3$: $V = \frac{4}{3}\pi\,R^3 \approx 4.189\,R^3$
$N = 4$: $V \approx 4.935\,R^4$
$N = 5$: $V \approx 5.264\,R^5$

and so on.

See also https://en.wikipedia.org/wiki/Volume_of_an_n-ball

The goal of the homework assignment is to learn how to apply a concept that has been introduced during the lecture for a more general case. Also, hyperspheres play an important role in Statistical Physics.

Problem 1 (20P)

Write the function **MC_ND_Sphere** using *def* that takes the number M of sampling points, the number of dimensions N and R, the radius as input arguments and approximates the volume of a N-dimensional hypersphere via a MCS.
The function should return the approximated **mean value** after 100 runs and the **standard deviation** as well as the **exact value from equation 1)**. You can use the MCS code from the lecture as backbone for your code.

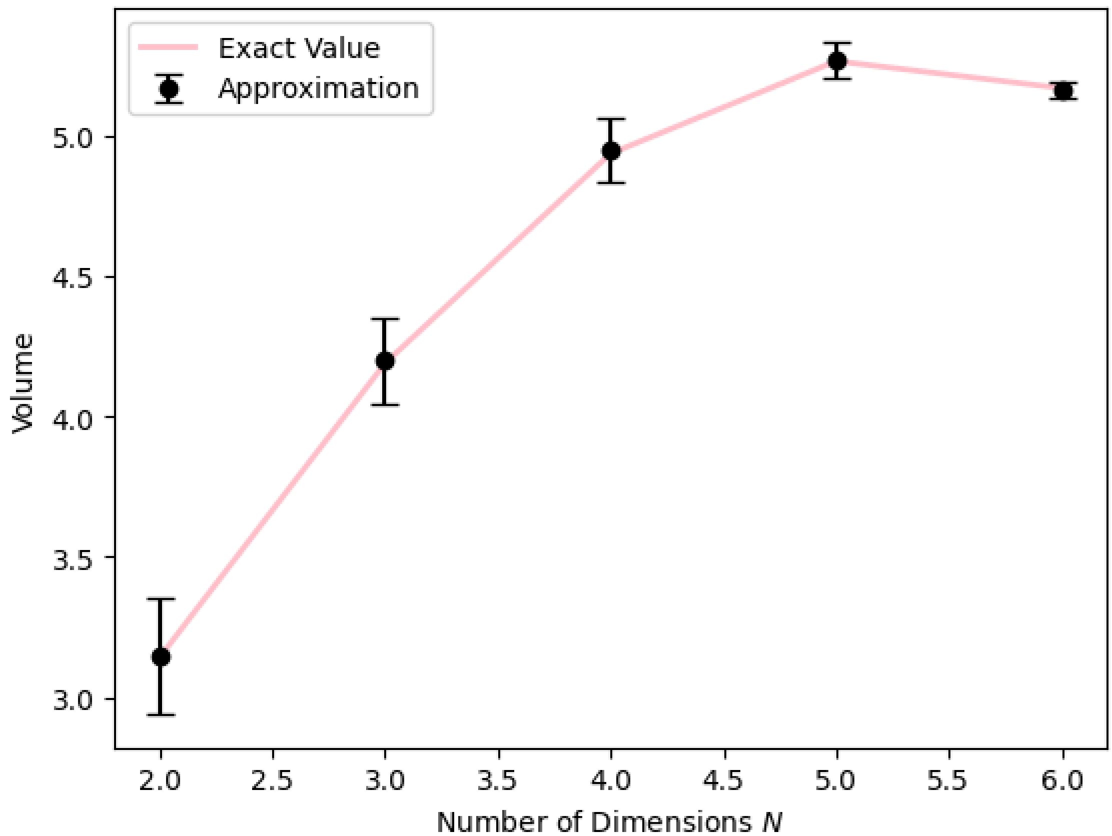
In [4]:
```
import numpy as np
import math

def MC_ND_Sphere(M, N, R):
    mreps = 100
    volumes = np.empty((mreps))
    exact_volume = (np.pi**(N/2) * R**N) / math.gamma(N/2 + 1)

    for i in range(mreps):
        points = np.random.uniform(-R, R, (M, N))
        distances = np.linalg.norm(points, axis = 1)
        inside_sphere = np.sum(distances < R)
        volumes[i] = (2 * R)**N * (inside_sphere / M)

    mean = np.mean(volumes)
    std = np.std(volumes)

    return mean, std, exact_volume
```

Problem 2 (5P)

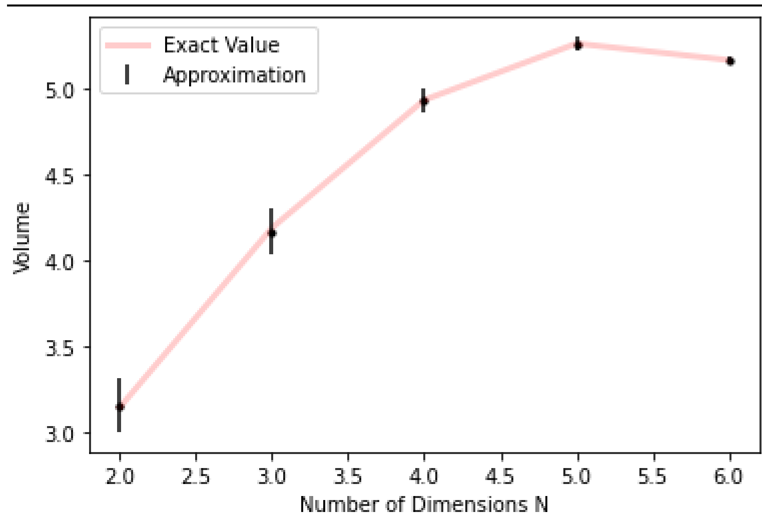
Call the function for five or six different values of N using *map*. How do you need to change the number of sampling points in order to maintain **roughly** the same accuracy for the different N? Generate a plot of your result. The plot should look similar to

In [16]:
```
import matplotlib.pyplot as plt

R = 1
dimensions = [2, 3, 4, 5, 6]
M = 10000 * [8 ** d for d in dimensions]

results = list(map(lambda M, N: MC_ND_Sphere(M, N, R), M, dimensions))

mean_volumes, std_volumes, exact_volumes = zip(*results)

plt.plot(dimensions, exact_volumes, label = "Exact Value", color = "pink", l
plt.errorbar(dimensions, mean_volumes, label = "Approximation", color = "bla
plt.xlabel("Number of Dimensions $N$")
```

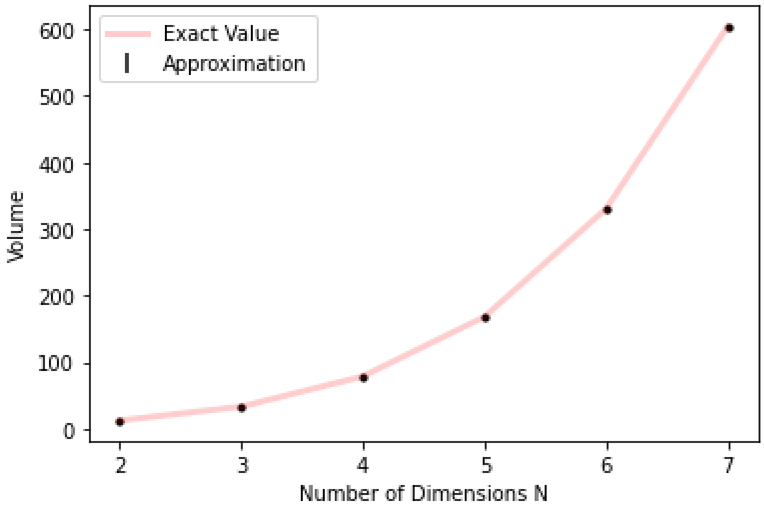
```
plt.ylabel("Volume")
plt.legend()
plt.show()
```



The number of sampling points must increase exponentially with the number of dimensions as $M = 8^N$ in order to maintain roughly the same accuracy



for $R = 1$ and similar to



Exact Value
Approximation
600
500
400
300
200
100
0
Volume
2
3
4
5
6
7
Number of Dimensions N

for $R = 2$.