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1  """
2  CH E 210B, HW3, Problem 5
3
4  Python script to compute a volume integral of
5   $f(x, y, z) = (x^2 + y^2 + z^2)\sin(xyz)$  over the
6  volume  $x = [0, 4]$ ,  $y = [-1, 2]$ ,  $z = [0, 1]$  using a Monte Carlo Method.
7
8  We then compute the "exact" result using Mathematica's `NIntegrate` function
9  and show how the error scales with the number of points used in the MC method
10 """
11 import numpy as np
12 import matplotlib.pyplot as plt
13
14 # Global variables
15 # Box size:
16 XMIN = 0
17 XMAX = 4
18 YMIN = -1
19 YMAX = 2
20 ZMIN = 0
21 ZMAX = 1
22 # Volume of box
23 VOL = (XMAX - XMIN) * (YMAX - YMIN) * (ZMAX - ZMIN)
24
25 # Mathematica "exact" result, calculated using the command:
26 # NIntegrate[(x^2 + y^2 + z^2)*Sin[x*y*z], {x, 0, 4}, {y, -1, 2}, {z, 0, 1}]
27 EXACT_RES = 10.66249863235283
28
29 # Define function whose integral we evaluate
30 def f(x, y, z):
31     """
32     Function to numerically integrate.
33     Parameters:
34     -----
35     x, y, z : numpy.array
36         arrays of random points
37     Returns:
38     -----
39     np.array
40         array of function values evaluated at each random point
41     """
42     return (x**2 + y**2 + z**2)*np.sin(x*y*z)
43
44
45 def mc_integral(NPTS):
46     """
47     Approximates the volume integral of the function described above using a
48     Monte Carlo method.
49     Parameters:
50     -----
51     NPTS : int
52         number of MC random points
53     Returns:
54     -----
55     float
56         MC approximation of the integral
57     """
58     # Construct arrays of random points draw from uniform distribution
59     x = np.random.uniform(low=XMIN, high=XMAX, size=NPTS)

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60     y = np.random.uniform(low=YMIN, high=YMAX, size=NPTS)
61     z = np.random.uniform(low=ZMIN, high=ZMAX, size=NPTS)
62
63     # Evaluate function at each random point
64     f_vals = f(x, y, z)
65     f_avg = np.sum(f_vals) / NPTS
66
67     # Return MC approximation = (Box Volume) * (Avg f)
68     return f_avg * VOL
69
70 # Evaluate integral for N = 10000 points
71 mc_10000 = mc_integral(10000)
72 print("MC Approximation, N = 10000:", mc_10000)
73
74 # Evaluate integral for increasing NPTS, plot error vs N
75 NMIN = 1
76 NMAX = 100000
77 N = np.arange(NMIN, NMAX + 1, 5)
78 err = np.zeros(len(N))
79 for i in range(len(N)):
80     err[i] = np.abs(EXACT_RES - mc_integral(N[i]))
81
82 f, ax = plt.subplots(figsize=(6, 6))
83 act_err, = ax.plot(N, err, '.')
84 pred_err, = ax.plot(N, 1/np.sqrt(N))
85 ax.set_xlabel(r"Number of Points, $N$")
86 ax.set_ylabel("Error")
87 ax.set_title(r"MC Approximation of $\int_0^4 dx \int_{-1}^2 dy \int_0^1 dz(x^2+y^2+z^2)\sin(xyz)$")
88 ax.annotate("Expected Result: {:.3f}".format(EXACT_RES), xy=(60000, 10))
89 ax.annotate("N = 10000 Result: {:.3f}".format(mc_10000), xy=(60000, 5))
90 ax.legend([act_err, pred_err], ["Actual Error", r"Expected Error ~ $N^{-1/2}$"])
91 f.savefig("mc_integral.png")
92 plt.show()

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