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1  # -*- coding: utf-8 -*-
2  """
3  Created on Sat Nov 16 12:19:00 2019
4
5  @author: Alexm
6  """
7
8  from __future__ import division
9  import numpy as np
10 from numpy.random import rand
11 import matplotlib.pyplot as plt
12
13
14 #Part 3: Code showing the configuration of the matrix at certain intervals of the iterations
15 print('Alexandra Mulholland 17336557')
16 print('Part 3: Snapshots of the configurations of the matrix and a plot of the convergence magnetisation against i
iterations of the Metropolis algorithm')
17 #Now creating a class which consists of the Metropolis algorithm
18
19 magf=0
20 J=-1
21 #Using 'self.' which is the instance of a class (In this case the class is Ising)
22 #self.moncar therefore contains the attributes of the algorithm, which in this case
23 #is the snapshots of the configurations
24 class Ising():
25     def moncar(self, config, N, beta, magf):
26         for i in range(N):
27             for j in range(N):
28                 a = np.random.randint(0, N)
29                 b = np.random.randint(0, N)
30                 s = config[a, b]
31                 spinmag=s*magf
32                 naybor = config[(a+1)%N,b] + config[a,(b+1)%N] + config[(a-1)%N,b] + config[a,(b-1)%N]
33                 EC = 2*J*s*naybor+2*spinmag
34                 if EC < 0:
35                     s *= -1
36                 elif rand() < np.exp(-EC*beta):
37                     s *= -1
38                 config[a, b] = s
39             return config
40 #Initialising a NxN matrix consisting of random spins of 1 and -1
41     def simulate(self):
42 #simulating the Ising model
43         N =20
44         temp= 1.0
45         iterations=[] #creating an empty list
46         TS=[] #total spin of configuration
47         config = 2*np.random.randint(2, size=(N,N))-1 #again, ensuring each spin is +1 or -1 within the matrix. Ra
ndom allocation
48         f = plt.figure(figsize=(10, 10)); #dictating what size the figures showing the configuration will be
49         self.configPlot(f, config, 0, N, 1); #This is the first configuration snapshot shown in a 3 by 3 grid of c
onfiguration snapshots
50 #The zero here indicates the very first configuration i.e. the initial, random matrix
51         msrmnt = 2001 #dictates up to which point the configuration snapshot will be shown-- will be msrmnt-1
52         def TOTAL(config):
53             spin = np.sum(config)
54             return spin
55         for i in range(msrmnt): #iteration number
56             self.moncar(config, N, 1.0/temp, magf) #beta, again, is 1/Temp
57             if i == 1:self.configPlot(f, config, i, N, 2); #2nd configuration snapshot, shown at 'time' 1 i.e at t
he first loop of the monte carlo
58             if i == 10:self.configPlot(f, config, i, N, 3); #3rd configuration snapshot
59             if i == 100:self.configPlot(f, config, i, N, 4); #4th
60             if i == 1000:self.configPlot(f, config, i, N, 5); #5th
61             if i == 2000:self.configPlot(f, config, i, N, 6); #6th
62             #if i == 500:self.configPlot(f, config, i, N, 7); #7th
63             #if i == 1000:self.configPlot(f, config, i, N, 8); #8th
64             #if i == 2000:self.configPlot(f, config, i, N, 9); #9th
65             iterations.append(i+1)
66             ts1=0 #initial value-- appropriatefor random lattice
67             TOT=TOTAL(config)
68             ts1=ts1+TOT #summing the total spin value as the iterations continue

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69         TS.append(ts1)
70     plt.figure()
71     plt.plot(iterations,TS, 'd', color='blue',
72             markersize=6,
73             markerfacecolor='c',markeredgecolor='blue',
74             markeredgewidth=1)
75     plt.xlabel('Iteration number');
76     plt.ylabel('Total spin value');
77     plt.title('Plot illustating the convergence of the magnetisation');
78     #The convergence will go to |N^2|
79
80     def configPlot(self, f, config, i, N, n): #n states which configuration is which subplot ie at i=1000, n=6
81     #This method plots the grid of spins, and the simulate method calls it at various times
82         X, Y = np.meshgrid(range(N), range(N))
83         sp = f.add_subplot(3, 3, n) #The first two terms in the brackets dictate the ratio of the sides x and y
respectively
84         plt.setp(sp.get_yticklabels(), visible=False) #making the x and y axes unlabelled
85         plt.setp(sp.get_xticklabels(), visible=False)
86         plt.pcolormesh(X, Y, config, cmap=plt.cm.winter); #the colour of each spin is green and blue respresenting
1 and -1
87         plt.title('Iteration number = %d'%i)
88         plt.show()
89     yo = Ising() #class = Ising
90     yo.simulate() #calling the function inside the class Ising

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