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1. Generalize the provided code for the one-dimensional Ising model to two dimensions, where the spins are arranged in a square lattice and interact with the nearest neighbours only. Impose periodic boundary conditions in both directions.

The general code for the 2D Ising model was obtained from the provided code for the 1D Ising model at http://www.phas.ubc.ca/~rozali/ising1D.m.

- The first change was the initialization of the grid initialization so that the lattice was represented by a 2D array instead of a 1D array.
- The number of steps needed to be changed too be related the number of elements inside the 'grid' or Ising Model.
- The calculation for the 2D model was slightly different than the calculation for the 1D model. The following steps were taken for calculating the initial energy of the model.

$$E_m = -J\sigma_m \sum_n \sigma_n.$$

  - Calculation for the sum of neighbours. In the 2D model there were neighbours in the 'up', 'down', 'left' and 'right' position.

```
sumOfNeighbors = ...
      circshift(grid, [ 0  1]) ...
    + circshift(grid, [ 0 -1]) ...
    + circshift(grid, [ 1  0]) ...
    + circshift(grid, [-1  0]);
```

  - Include the coupling constant in the sum of all the neighbors and all the energies.

```
Em = -J*grid.*sumOfNeighbors;
Energy = 0.5 * sum(sum(Em));%initial Energy
```

- Two sets of random integers between 1 and N needed to be generated for the 2D model because both the index for the row and column needed to be chosen.

- In addition to the periodic boundary condition for the rows, the periodic boundary conditions for the columns were implemented.

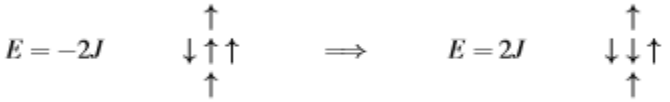
```
if x~=1; left=grid(y,x-1);else left=grid(y,N);end
if x~=N; right=grid(y,x+1);else right=grid(y,1);end
if y~=1; down=grid(y-1,x);else down=grid(N,x);end
if y~=N; up=grid(y+1,x);else up=grid(1,x);
```

- For efficiency we predetermined all the possible probabilities for the Metropolis algorithm. This way the code does not have to execute the relatively taxing 'exp' function every iteration.
    - Calculation for p:

```
p = exp(-dE/T);
```

    - For a 2D Ising model we know that there are 5 possibilities for change in energy based on the possible spin orientations since we are treating the coupling factor J as a constant:
        - dE = 8J

        - dE = 4J



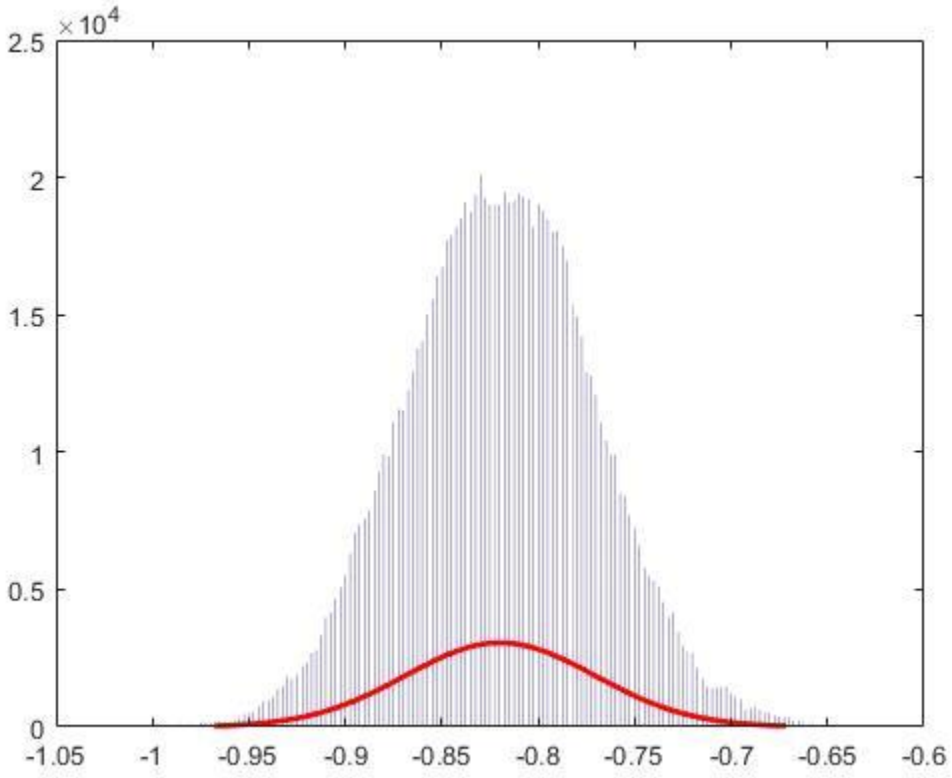
        - dE = 0

        - dE = -4J

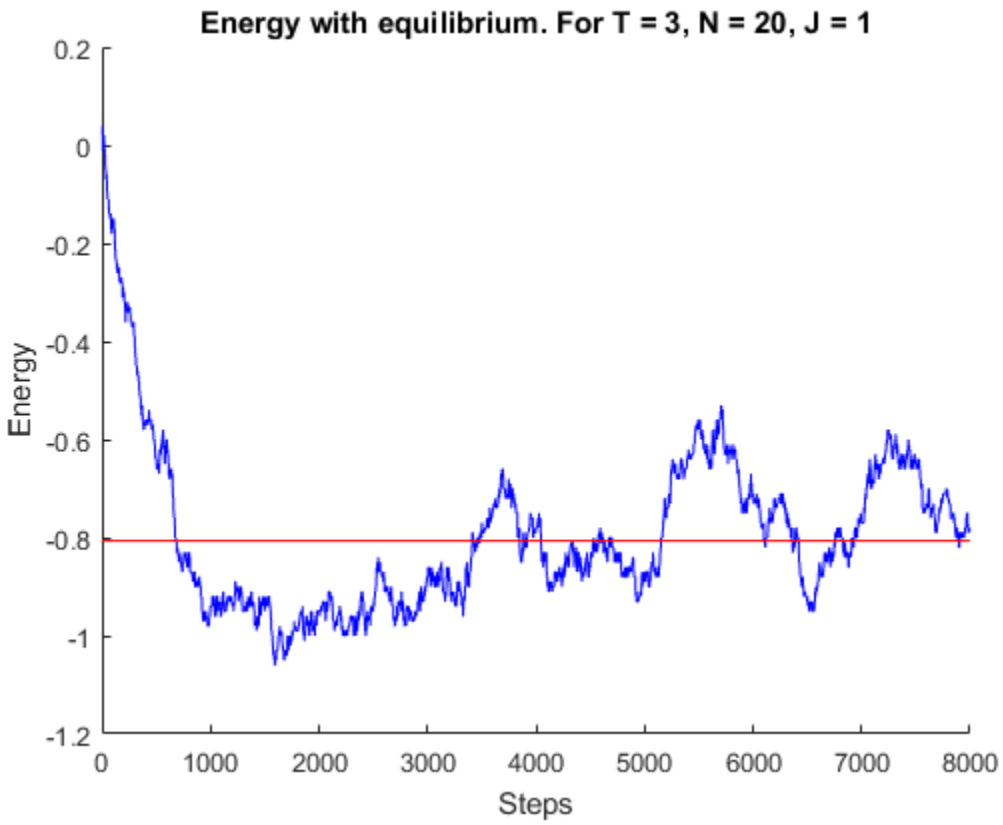
        - dE = -8J

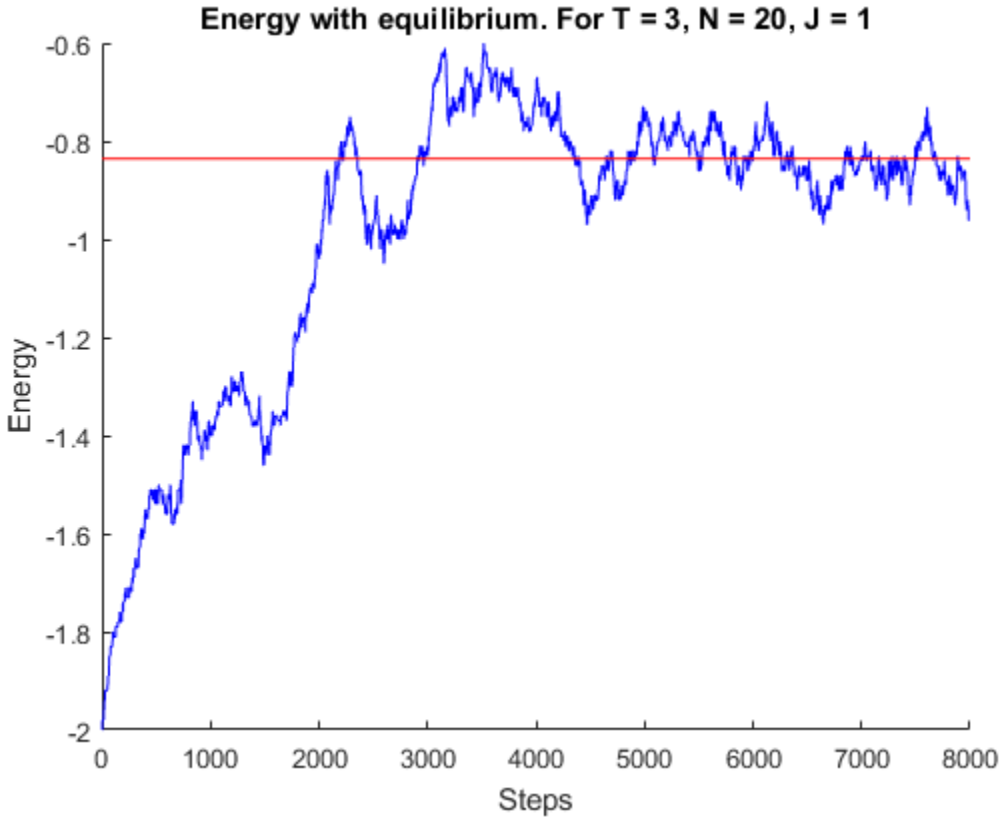
2. For the coupling J = 1 and temperature T = 3 plot the total energy of generated configurations as function of time, and determine the approximate time when thermalization occurs. Study this for two lattices with N ×N spins, where N = 20 and N = 40; how does the thermalization time depend on the lattice size?

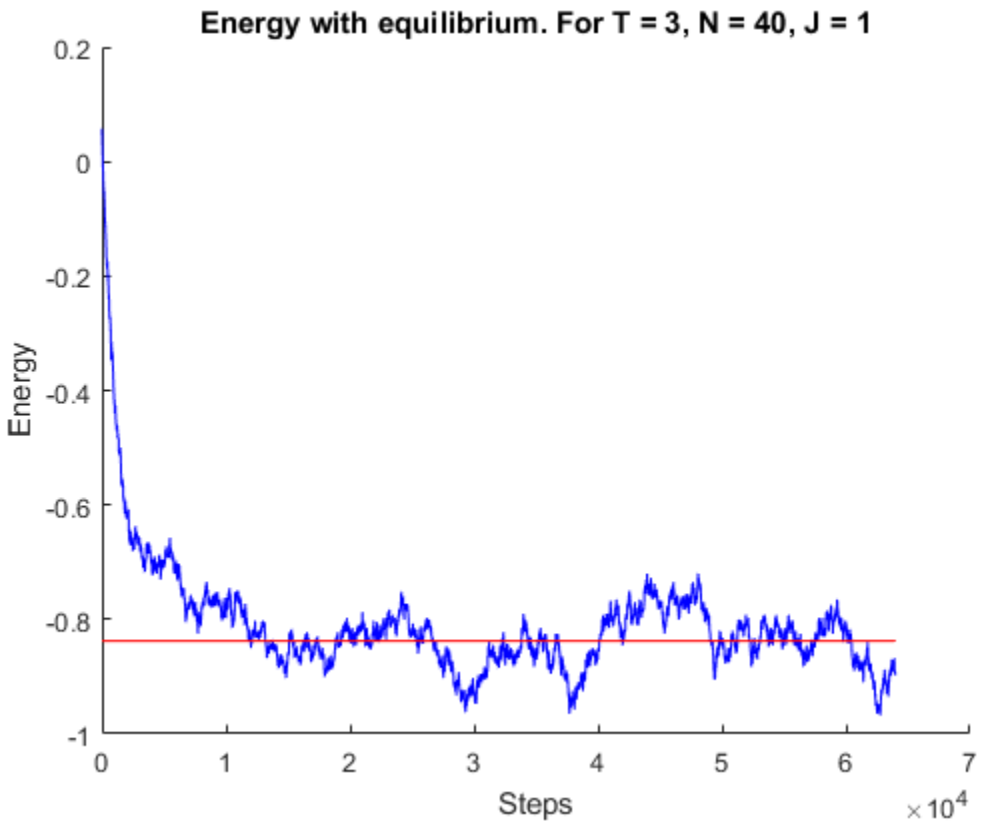
- A way to check whether the system has had enough time to reach equilibrium is to graph the energy points in an histogram style (cutting off initial pre thermalization points).
    - If the graph is in the shape of a gaussian distribution, then we know that it has reached equilibrium.
    - The system is oscillating about its thermalization energy as a gaussian distribution after reaching equilibrium.

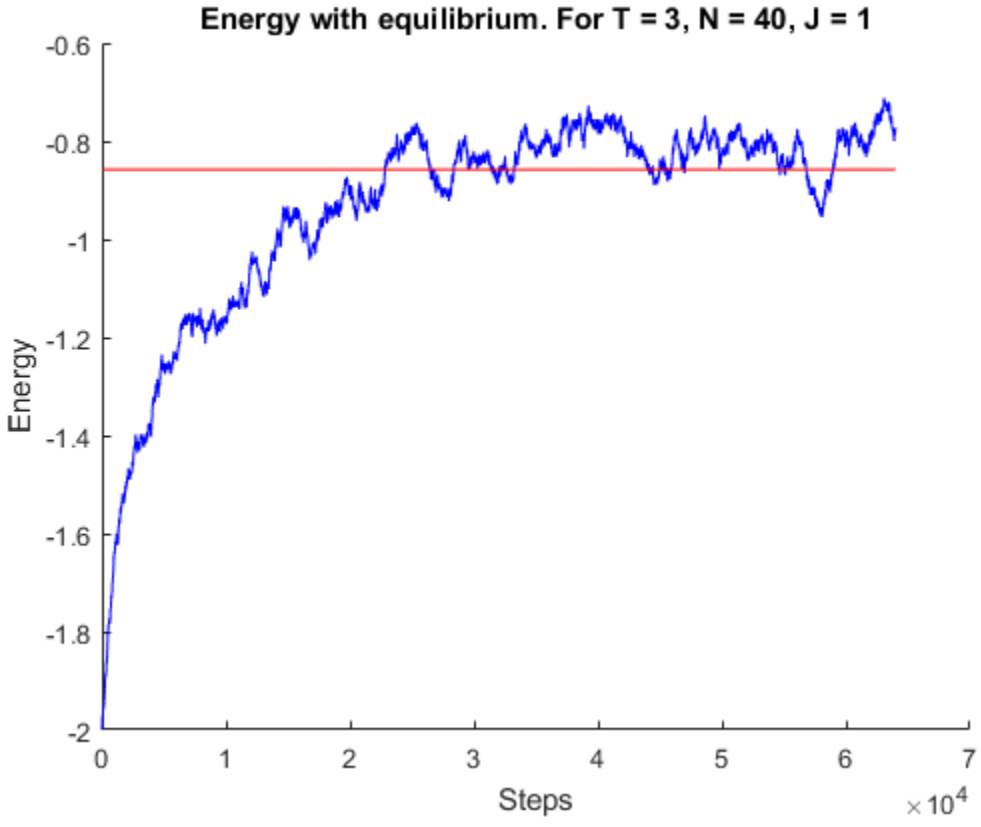


- Another quick way to check if the system has had sufficient time to thermalize, the function was started from two different states to see if they would converge to approximately the same energy.
    - To execute the above method, the system was started in a random disordered state and a known state where all the spins are in the same direction.


Energy with equilibrium. For T = 3, N = 20, J = 1
0.2
0
-0.2
-0.4
-0.6
-0.8
-1
-1.2
Energy
0
1000
2000
3000
4000
5000
6000
7000
8000
Steps


Energy with equilibrium. For T = 3, N = 20, J = 1
-0.6
-0.8
-1
-1.2
-1.4
-1.6
-1.8
-2
Energy
0
1000
2000
3000
4000
5000
6000
7000
8000
Steps

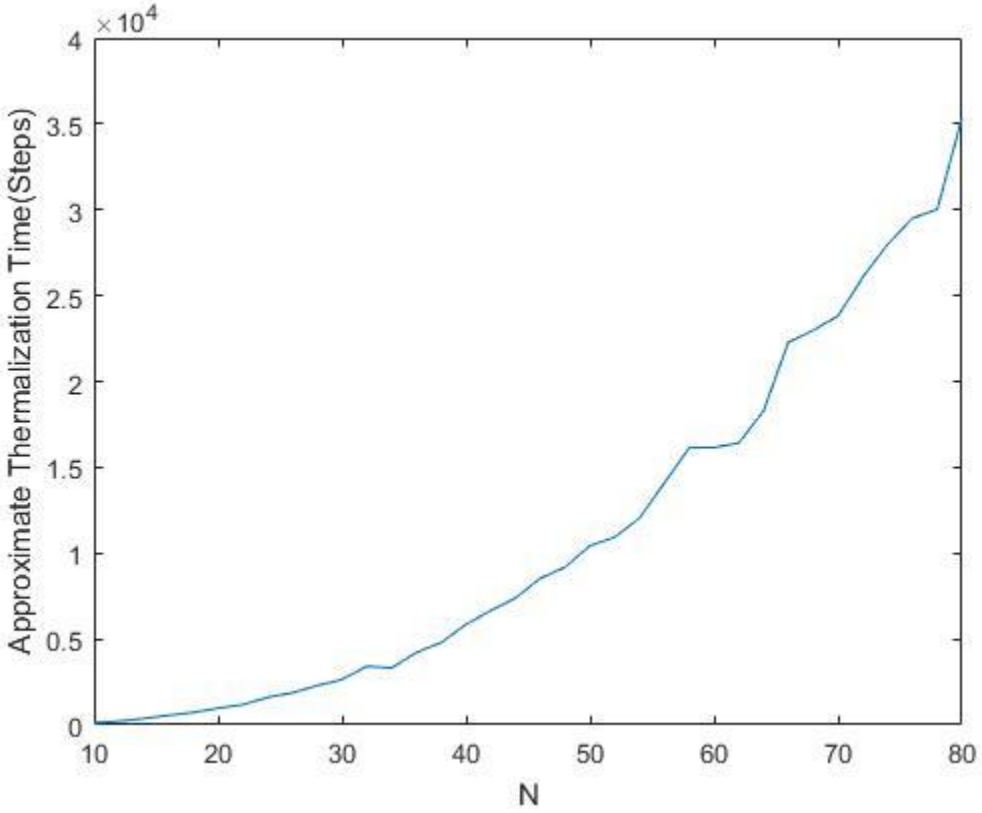

Energy with equilibrium. For T = 3, N = 40, J = 1
0.2
0
-0.2
-0.4
-0.6
-0.8
-1
Energy
0
1
2
3
4
5
6
7
Steps
×10^4


Energy with equilibrium. For T = 3, N = 40, J = 1
-0.6
-0.8
-1
-1.2
-1.4
-1.6
-1.8
-2
Energy
0
1
2
3
4
5
6
7
Steps
×10^4

- The thermalization time can be approximated by taking points where the equilibrium has clearly been reached and finding the mean and the standard deviation. The approximate time of thermalization is when the energy first gets into his energy range.

```
thermalization_time = find(E<mean(Ee)+std(Ee) & E > mean(Ee)-std(Ee), 1,
'first')
```

    - Using this approximation for thermalization time we can discern roughly the relationship between N and thermalization time of the system.
    - Below is the graph of the thermalization times for N = 10 to N = 80 incrementing by 2.
        - The value of each thermalization time is the average of 30 tries to get as close to the center of the distribution as possible.



- As we can see from the graph the shape is roughly parabolic, for a temperature of 3 and a coupling of 1.
    - The artefacts of the graph are due to the random nature of the modelling of the Ising system. One way that this can improving is increasing the number of steps that the equilibrium is averaged for.
        - The example graph above allowed for 1000000 steps for each system and averaged 30 systems for each N.
        - N was incremented by 2.
    - The code for question 2 is found in the file thermalization.m, thermalization_relationship.m and ising2D.m

- This scaling makes sense because as N increases for the 2D model the number of spins that can change in the system changes in relation to ~N^2.

3. For each one of the following quantities, determine and plot their dependence on temperature (for T between 2 and 2.6, in steps of 0.02). Use an N×N lattice (for N=10,20,50) and calculate the average using 5×104N^2 thermalized configurations (i.e. that number of Monte-Carlo steps, past thermalization). The quantities to determine are: energy, magnetization, heat capacity, magnetic susceptibility.

The equation for calculating magnetic susceptibility:

$$\chi = \frac{< M^2 > - < M >^2}{T}$$

The equation for calculating heat capacity:

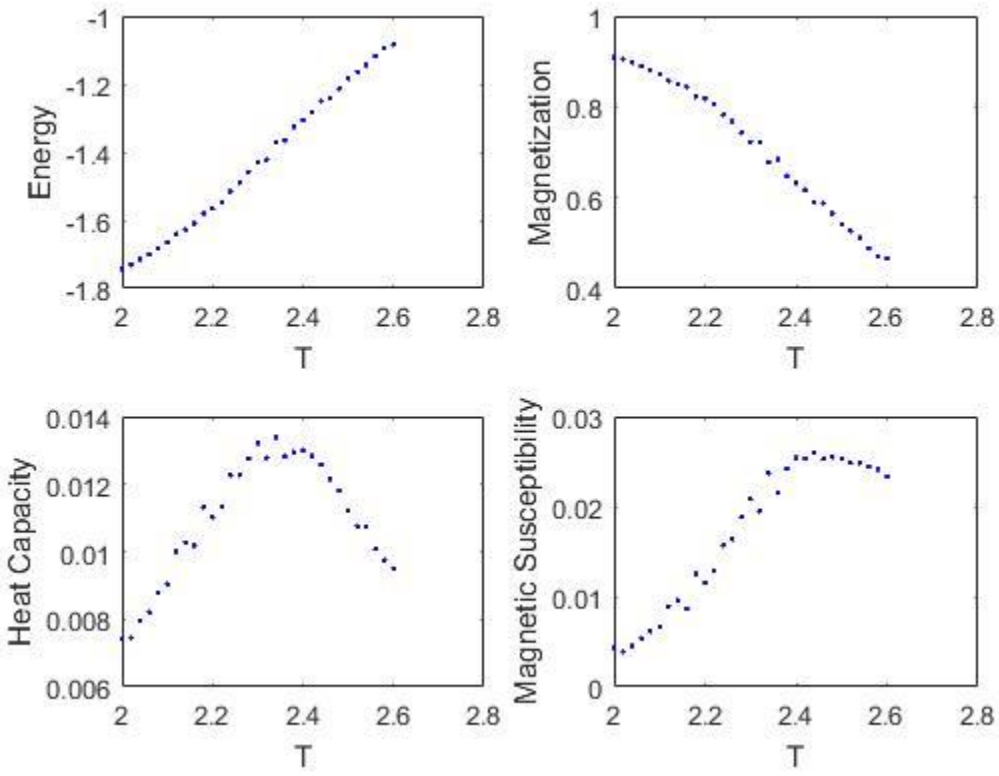
$$C_v = \frac{< E^2 > - < E >^2}{T^2}$$

For each of the graphs, the behaviour of the plot was related to the distance from T_c.

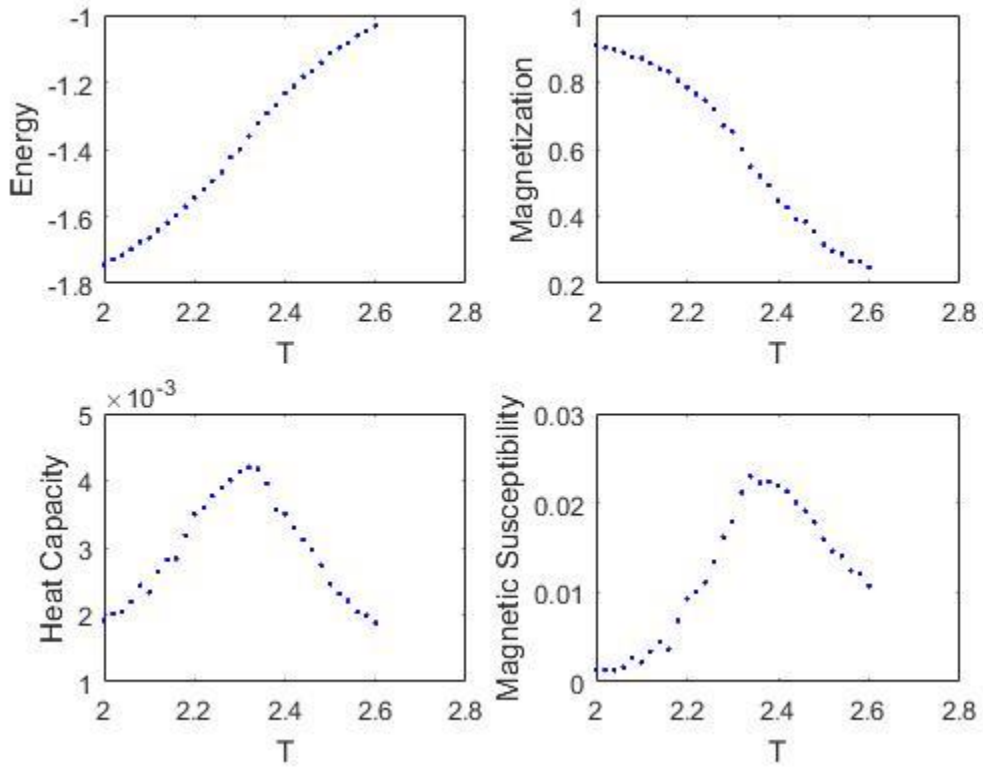
- Energy
    - The difference in temperature from T_c is related to the slope of the plot. On either side of T_c the closer the temperature was to the critical temperature, the steeper the slope became.
- Magnetization
    - The difference in temperature from T_c is related to the *negative* slope of the plot. On either side of T_c the closer the temperature was to the critical temperature, the steeper the slope became.
    - For magnetization the average absolute value is graphed because below the critical temperature magnetisation may oscillate between negative and positive values since the system could either be majority pointing up or majority pointing down.
    - The amount above or below 0 this number of spins is depends on the coupling.
- For both the heat capacity and the magnetic susceptibility, the magnitude was related to the distance from T_c. As shown in the plots, the plots peak at T_c.

- The above relationships/patterns are becoming more vivid as N increases.
    - A possible sign of a phase transition, from a state where most spins align in a specific direction to a phase where both spin directions are equally and result in zero net magnetisation.
        - Transition from a ferromagnetic phase to a paramagnetic phase.
    - Increased temperature increases the randomness of the system.
- To estimate the critical temperature, the quantities of heat capacity and magnetic susceptibility are the best because they have vivid peaks.
- The files containing the code producing the below graphs are ising2D2.m and tempChange.m

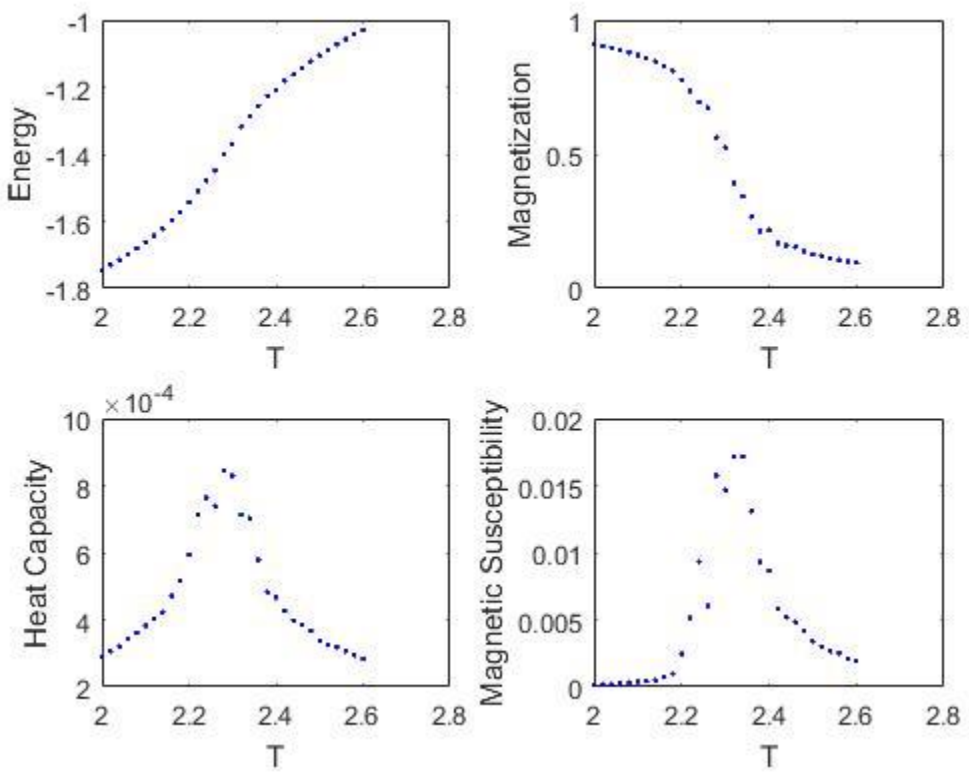
- N = 10


Energy
-1
-1.2
-1.4
-1.6
-1.8
2
2.2
2.4
2.6
2.8
T
Magnetization
1
0.8
0.6
0.4
2
2.2
2.4
2.6
2.8
T
Heat Capacity
0.014
0.012
0.01
0.008
0.006
2
2.2
2.4
2.6
2.8
T
Magnetic Susceptibility
0.03
0.02
0.01
0
2
2.2
2.4
2.6
2.8
T

- N = 20


Energy
-1
-1.2
-1.4
-1.6
-1.8
2
2.2
2.4
2.6
2.8
T
Magnetization
1
0.8
0.6
0.4
0.2
2
2.2
2.4
2.6
2.8
T
Heat Capacity
×10^-3
5
4
3
2
1
2
2.2
2.4
2.6
2.8
T
Magnetic Susceptibility
0.03
0.02
0.01
0
2
2.2
2.4
2.6
2.8
T

- N = 50



  - In the above graphs we can see that there is disfigurement near T_c. This is because the thermalization time increases as T gets closer to T_c.
  - To fix the above issue code for the system is altered to:
    - Focus more closely on the critical temperature to save computation time.
    - Increase frequency of temperatures taken to a increment of 0.005.
    - Increase the anticipated number of steps before thermalization from N^3 to N^4.5.
      - Referencing the notes from http://www.phas.ubc.ca/~rozali/lectures2015.pdf in section "13.7.1 Thermalization" it states that the time for thermalization around the critical temperature is approximately:

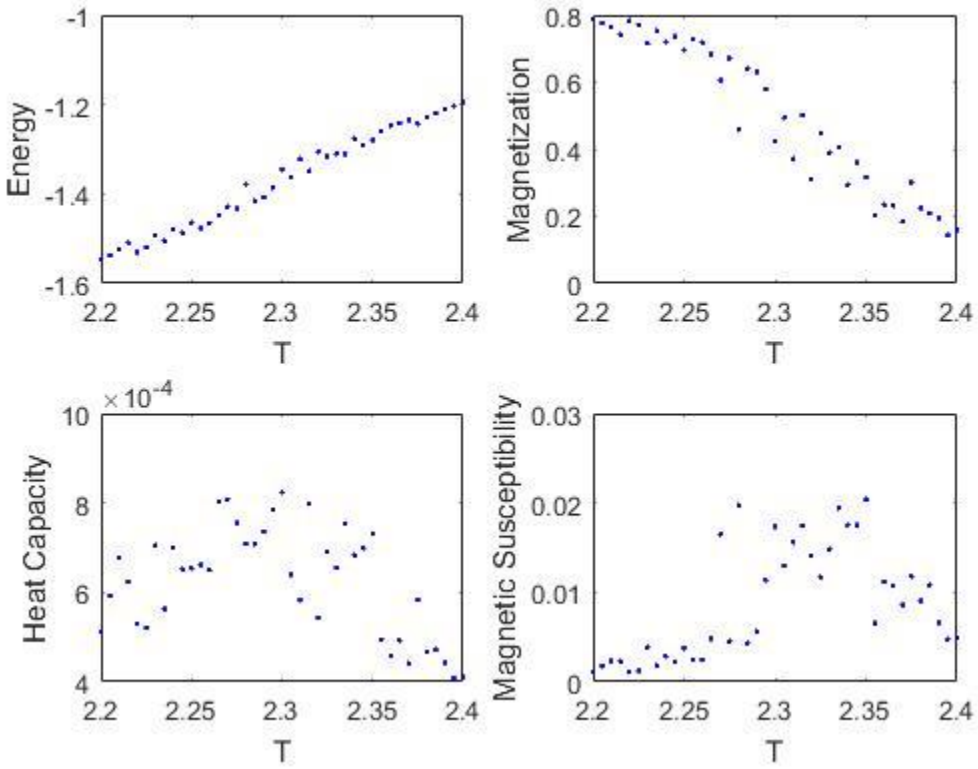
$$\tau \sim N^{d+z}$$

$$d = Dimensions\ in\ system = 2$$

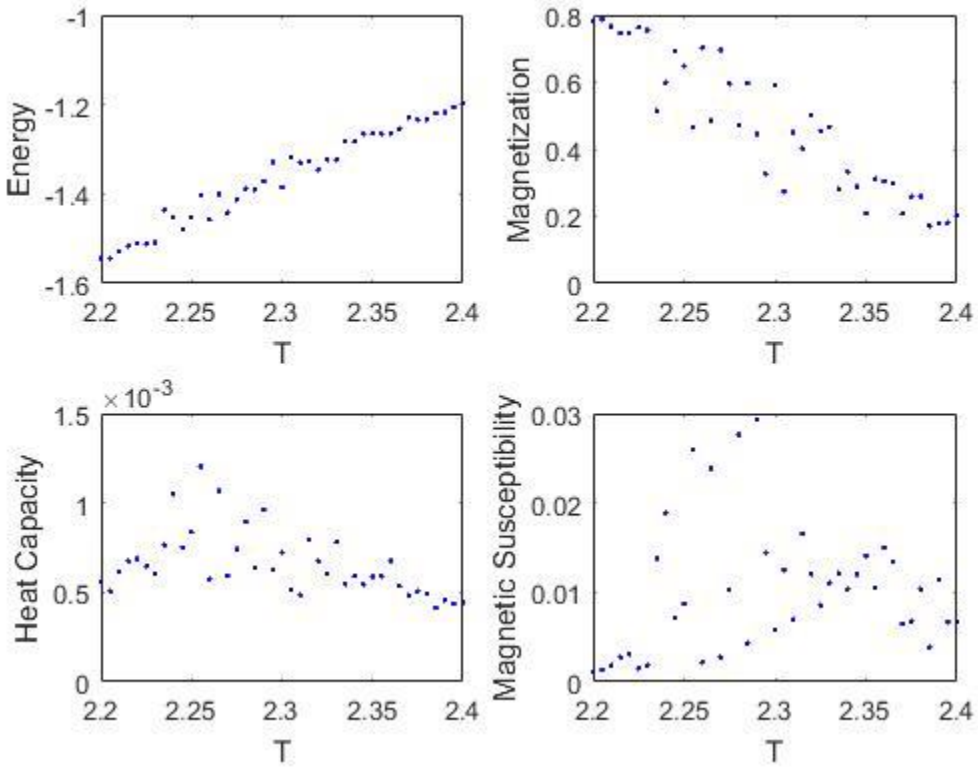
$$z = \ 2.1665 \pm 0.0012$$

- The above equation is confirmed by the graphs below as the trend stopped improving around a thermalization time of 4.2
  - Note: all the graphs below are for a 2D Ising Model of 50x50 spins.
- The scripts for the plots below are in ising2D3.m and T_C_investigation.m

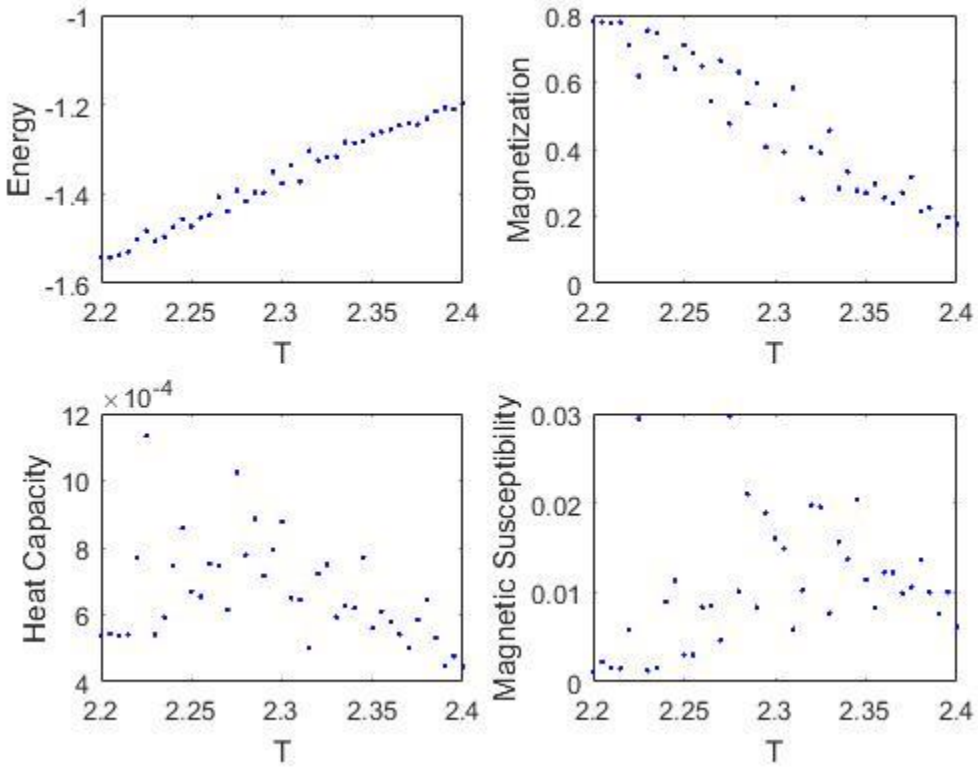
- Thermalization time of N^4 steps:



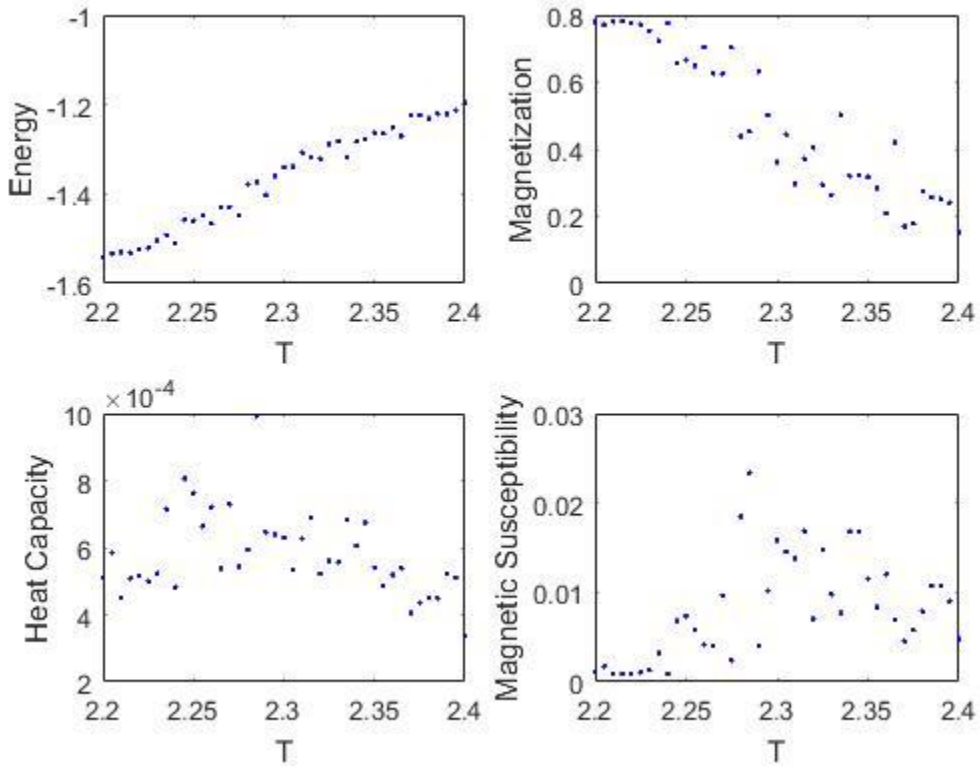
- Thermalization time of N^4.1 steps:



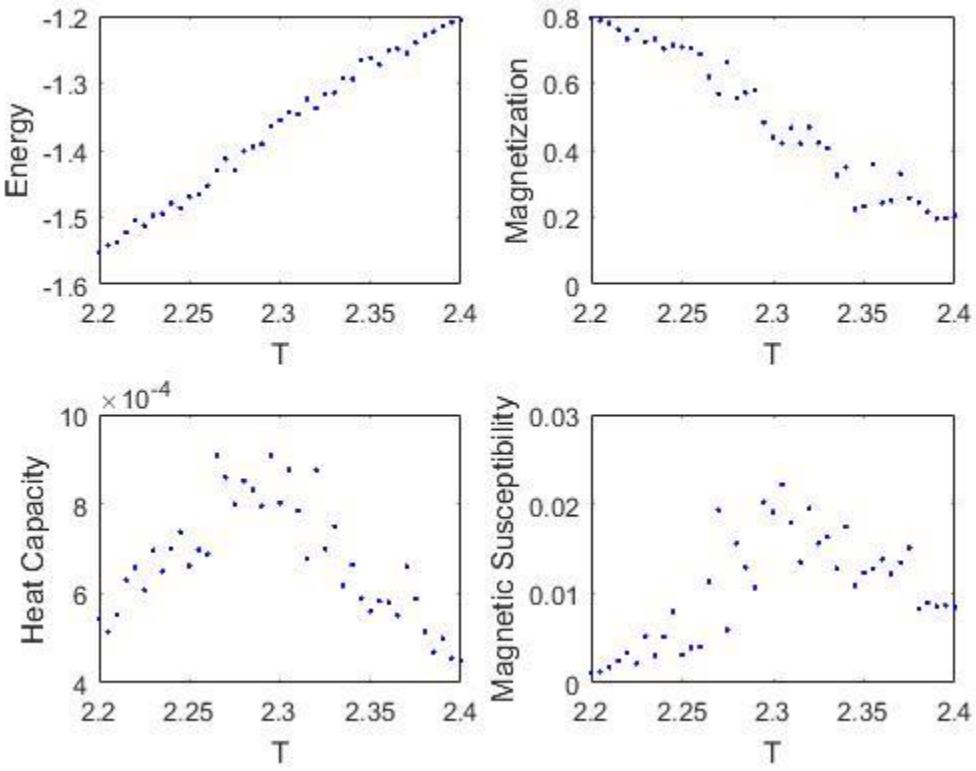
- Thermalization time of N^4.2 steps:



- Thermalization time of N^4.5 steps:



- Thermalization time of N^4.5 steps, increased points for equilibrium:



- From the above graphs we can estimate that the thermalization time is around 2.3.
- That estimation is based off the peaks of heat capacity and magnetic susceptibility since at N = 50, the graphs for energy and magnetization do not have a clear enough phase change.