Homework 7: Cream in your Coffee Diffusion Part 2

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Introduction

This assignment is divided into two portions. Our first objective is to plot the mug as a bi-variate histogram and to plot its entropy with time (Problem 7.12). The second objective is to represent the loss of particles overtime assuming there is a hole in the mug where particles can be lost (Problem 7.15).

Method

Problem 7.12

We create a bi-variate histogram Pxy of the data of the particles in the mug. Because the data is represented by the edges of the bins, the histogram is 9×9 rather than 8×8. The extra row and column come from the edges representative of $y = 100$ and $x = 100$. These extra bins are discarded for the entropy calculation, whence our histogram is essentially 8×8.

To calculate entropy, the following equation is applied after each step (the loop for the walkers is still nested inside the loop for the steps):

$$S(\text{current step}) = \sum_{x_{bin}}^{8} \sum_{y_{bin}}^{8} -Pxy(x_{bin}, y_{bin}) \log Pxy(x_{bin}, y_{bin}). \tag{1}$$

Problem 7.15

We switch the nesting of the step and walker loops; hence, we are calculating all steps for a walker one walker at a time. There exists a region at $x = 100$ in $-25 \leq y \leq 25$ where if the particle exists here, it is removed from the mug (this is the so-called "hole"). We keep track of the number of particles in the system in the loop for time. Initially, we have an array of the same length as the time array with all values at 400. If a walker is found to be falling out of the hole, then for the time for which this event happens as well as for all subsequent

times, the value of the corresponding position in the array for number of walkers is subtracted by one.

An exp2 nonlinear fit is applied to the resulting walkers versus steps graph.

Verification of program

The data is output as expected. Here, **Figure 1** very closely resembles Figure 7.16 in the textbook.

Data

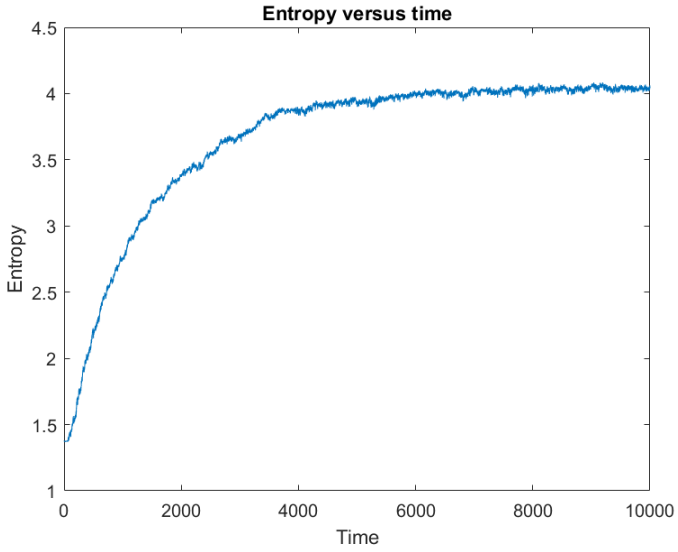

Figure 1: Entropy versus time.

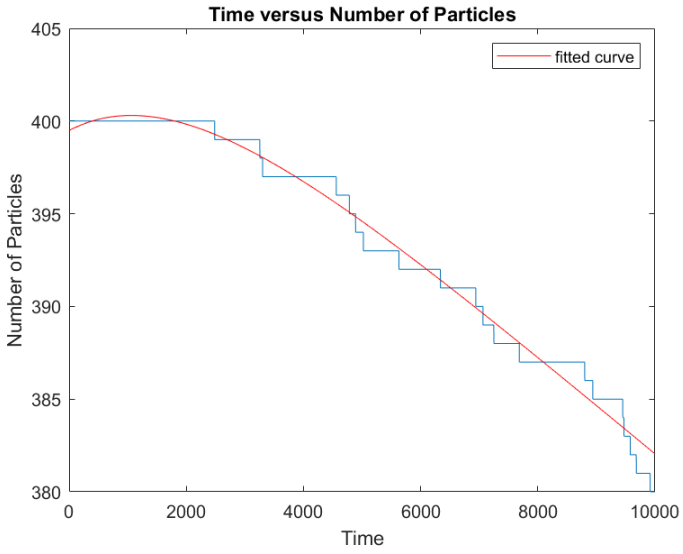

Figure 2: Time versus number of particles with an exp2 nonlinear fit.

Analysis

In **Figure 1**, we note that the entropy flattens off as the diffusion continues. This is to be expected, as the initial level of order is never to be reached again, while the particles continue to be contained in the mug, so the entropy is limited.

In **Figure 2**, we note the exponential curve needed to fit the data. This is due to the fact that it will take at the very least 80 steps for a particle to fall out of the hole. As entropy flattens off, the relationship becomes more linear.

Critique

This assignment has introduced me to exporting data from arrays to files (such as text files), nonlinear fits, and bi-variate histograms (see program).