8.5 PROJECTS

Project 8.1 Modeling segregation

In 1971, Thomas Schelling (who in 2005 was co-recipient of the Nobel Prize in Economics) proposed a theoretical model for how racial segregation occurs in urban areas [56]. In the *Schelling model*, as it is now called, individuals belonging to one of two groups live in houses arranged in a grid. Let's call the two groups the Plain-Belly Sneetches and the Star-Belly Sneetches [59]. Each cell in the grid contains a house that is either vacant or inhabited by a Plain-Belly or a Star-Belly. Because each cell represents an individual with its own independent attribute(s), simulations such as these are known as *agent-based simulations*. Contrast this approach with the population models in Chapter 4 in which there were no discernible individuals. Instead, we were concerned there only with aggregate sizes of populations of identical individuals.

In an instance of the Schelling model, the grid is initialized to contain some proportion of Plain-Bellies, Star-Bellies, and unoccupied cells (say 0.45, 0.45, 0.10, respectively) with their locations chosen at random. At each step, a Sneetch looks at each of its eight neighbors. (If a neighbor is off the side of the grid, wrap around to the other side.) If the fraction of a cell's neighbors that are different from itself exceeds some "tolerance threshold," the Sneetch moves to a randomly chosen unoccupied cell. Otherwise, the Sneetch stays put. For example, if the tolerance threshold is 3/8, then a Sneetch will move if more than three of its neighbors are different. We would like to answer the following question.

Question 8.1.1 Are there particular tolerance thresholds at which the two groups always segregate themselves over time?

Create a simulation of the Schelling model to answer this question. Visualize its behavior using the turtle graphics functions provided for the Game of Life. Experiment with different tolerance thresholds, and then answer the following questions, in addition to the one above.

Question 8.1.2 Are there tolerance thresholds at which segregation happens only some of the time? Or does it occur all of the time for some tolerance thresholds and never for others?

Question 8.1.3 In the patterns you observed when answering the previous questions, was there a "tipping point" or "phase transition" in the tolerance threshold? In other words, is there a value of the tolerance threshold that satisfies the following property: if the tolerance threshold is below this value, then one thing is certain to happen and if the tolerance threshold is above this value then another thing is certain to happen?

Question 8.1.4 If the cells become segregated, are there "typical" patterns of segregation or is segregation different every time?

Question 8.1.5 The Schelling model demonstrates how a "macro" (i.e., global) property like segregation can evolve in an unpredictable way out of a sequence of entirely "micro" (i.e., local) events. (Indeed, Schelling even wrote a book titled Micromotives and Macrobehavior [57].) Such properties are called emergent. Can you think of other examples of emergent phenomena?

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Question 8.1.6 Based on the outcome of this model, can you conclude that segregation happens because individuals are racist? Or is it possible that something else is happening?

Project 8.2 Modeling ferromagnetism

The *Ising model* is a model of a ferromagnet at a microscopic scale. Each atom in the magnet has an individual polarity, known as spin up (+1) or spin down (-1). When the spins are random, the material is not magnetic on its own; rather, it is paramagnetic, only becoming magnetic in the presence of an external magnetic field. On the other hand, when the spins all point in the same direction, the material becomes ferromagnetic, with its own magnetic field. Each spin is influenced by neighboring spins and the ambient temperature. At lower temperatures, the spins are more likely to "organize," pointing in the same direction, causing the material to become ferromagnetic.

This situation can be modeled on a grid in which each cell has the value 1 or -1. At each time step, a cell may change its spin, depending on the spins of its four neighbors and the temperature. (To avoid inconvenient boundary conditions, treat your grid as if it wraps around side to side and bottom to top. In other words, use modular arithmetic when determining neighbors.)

Over time, the material will seek the lowest energy state. Therefore, at each step, we will want the spin of an atom to flip if doing so puts the system in a lower energy state. However, we will sometimes also flip the spin even if doing so results in a higher energy state; the probability of doing so will depend on the energy and the ambient temperature. We will model the energy associated with each spin as the number of neighbors with opposing spins. So if the spin of a particular atom is +1 and its neighbors have spins -1, -1, +1, and -1, then the energy is 3. Obviously the lowest energy state results when an atom and all of its neighbors have the same spin.

The most common technique used to decide whether a spin should flip is called the *Metropolis algorithm*. Here is how it works. For a particular particle, let $E_{\rm old}$ denote the energy with the particle's current spin and let $E_{\rm new}$ denote the energy that would result if the particle flipped its spin. If $E_{\rm new} < E_{\rm old}$, then we flip the spin. Otherwise, we flip the spin with probability

$$e^{-(E_{\text{new}}-E_{\text{old}})/T}$$

where e is Euler's number, the base of the natural logarithm, and T is the temperature.

Implement this simulation and visualize it using the turtle graphics functions provided for the Game of Life. Initialize the system with particles pointing in random directions. Once you have it working, try varying the temperature T between 0.1 and 10.0. (The temperature here is in energy units, not Celsius or Kelvin.)

Question 8.2.1 At what temperature (roughly) does the system reach equilibrium, i.e., settle into a consistent state that no longer changes frequently?

Question 8.2.2 As you vary the temperature, does the system change its behavior gradually? Or is the change sudden? In other words, do you observe a "phase transition" or "tipping point?"

Question 8.2.3 In the Ising model, there is no centralized agent controlling which atoms change their polarity and when. Rather, all of the changes occur entirely based on an atom's

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local environment. Therefore, the global property of ferromagnetism occurs as a result of many local changes. Can you think of other examples of this so-called emergent phenomenon?

Project 8.3 Growing dendrites

In this project, you will simulate a phenomenon known as diffusion-limited aggregation (DLA). DLA models the growth of clusters of particles such as snowflakes, soot, and some mineral deposits known as dendrites. In this type of system, we have some particles (or molecules) of a substance in a low concentration in a fluid (liquid or gas). The particles move according to Brownian motion (i.e., a random walk) and "stick" to each other when they come into contact. In two dimensions, this process creates patterns like the one in Figure 1. These structures are known as Brownian trees and they are fractals in a mathematical sense.

To simplify matters, we will model the fluid as a two dimensional grid with integer coordinates. The lower left-hand corner will have coordinates (0,0) and the upper right-hand corner will have coordinates (199,199). We will place an initial seed particle in the middle at (100,100), which we will refer to as the origin. We will only let particles occupy discrete positions in this grid.

In the simulation, we will introduce new particles into the system, one at a time, some distance from the growing cluster. Each of these new particles will follow a random walk on the grid (as in Section 5.1), either eventually sticking to a fixed particle in the cluster or walking far enough away that we abandon it and move on to the next particle. If the particle sticks, it will remain in that position for the remainder of the simulation.

To keep track of the position of each fixed particle in the growing cluster, we will need

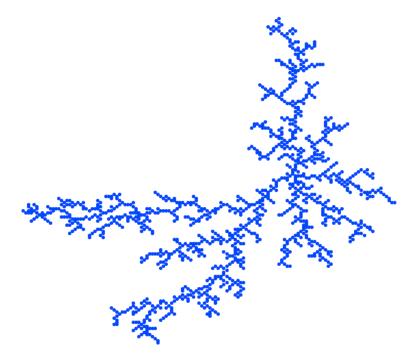


Figure 1 A two-dimensional Brownian tree.

a 200×200 grid. Each element in the grid will be either zero or one, depending upon whether there is a particle fixed in that location. To visualize the growing cluster, you will also set up a turtle graphics window with world coordinates matching the dimensions of your grid. When a particle sticks, place a dot in that location. Over time, you should see the cluster emerge.

The simulation can be described in five steps:

- 1. Initialize your turtle graphics window and your grid.
- 2. Place a seed particle at the origin (both in your grid and graphically), and set the radius R of the cluster to be 0. As your cluster grows, R will keep track of the maximum distance of a fixed particle from the origin.
- 3. Release a new particle in a random position at a distance of R+1 from the origin. (You will need to choose a random angle relative to the origin and then use trigonometry to find the coordinates of the random particle position.)
- 4. Let the new particle perform a random walk on the grid. If, at any step, the particle comes into contact with an existing particle, it "sticks." Update your grid, draw a dot at this location, and update R if this particle is further from the origin than the previous radius. If the particle does not stick within 200 moves, abandon it and create a new particle. (In a more realistic simulation, you would only abandon the particle when it wanders outside of a circle with a radius that is some function of R.)
- 5. Repeat the previous two steps for particles particles.

Write a program that implements this simulation.

Additional challenges

There are several ways in which this model can be enhanced and/or explored further. Here are some ideas:

• Implement a three-dimensional DLA simulation. A video illustrating this can be found on the book website. Most aspects of your program will need to be modified to work on a three-dimensional grid. To visualize the cluster in three dimensions, you can use a module called vpython.

For instructions on how to install VPython, visit http://vpython.org. Once you have vpython installed, you can import it with

```
import vpython as vp
```

Placing a sphere at a particle location looks like this:

```
vp.sphere(pos = vp.vector(0, 0, 0), radius = 1, color = vp.color.blue)
```

This particular call draws a blue sphere with radius 1 at the origin.

At any time, you can zoom the image by dragging while holding down the Option key. You can rotate the image by dragging while holding down the

Control key. There is very good documentation for vpython available on their website.

- Investigate what happens if the particles are "stickier" (i.e., can stick from further away).
- What if you start with a line of seed particles across the bottom instead of a single particle? Or a circle of seed particles and grow inward? (Your definition of distance or radius will need to change, of course, in these cases.)

Project 8.4 Simulating an epidemic
Simulating an epidemic (or pandemic) like COVID-19
Modify the Game of Life program...