2024Spring Probability & Statistics for EECS 2024/05/16

Final Project Option 2

Professor: Ziyu Shao *Due: 2024/06/16 10:59pm*

This is the Final Project Option 2 entitled "Phase Transition", which has two parts. Part I is **Percolation**, and Part II is **Ising Model**. This project can be done by a team with no more than three students. Your team is required to use Python for the programming part. Your team needs to submit all things in Jupyter Notebook format, including Python codes, simulation results, analysis, discussions, tables, figures, *etc.* Always keep the **academic integrity** in mind and remember to give credit to any source that inspires you.

- **Part I: Percolation**

  Estimate the value of the percolation threshold via Monte Carlo simulation.

  1. **Percolation**. Given a composite systems comprised of randomly distributed insulating and metallic materials: what fraction of the materials need to be metallic so that the composite system is an electrical conductor? Given a porous landscape with water on the surface (or oil below), under what conditions will the water be able to drain through to the bottom (or the oil to gush through to the surface)? Scientists have defined an abstract process known as percolation to model such situations.
  2. **The model**. We model a percolation system using an $n \times n$ grid of sites. Each site is either open or blocked, where open means the water or other materials can flow through such site. Open sites can be further classified into two categories: full open sites and empty open sites. A full open site is an open site that can be connected to an open site in the top row via a chain of neighboring (left, right, up, down) open sites. An empty open site is an open site that is NOT full. We say the system percolates if there is a full open site in the bottom row. In other words, a system percolates if we could find a path of open sites from the top row to the bottom row. (For the insulating/metallic materials example, the open sites correspond to metallic materials, so that a system that percolates has a metallic path from top to bottom, with full sites conducting. For the porous substance example, the open sites correspond to empty space through which water might flow, so that a system that percolates lets water fill open sites, flowing from top to bottom.)

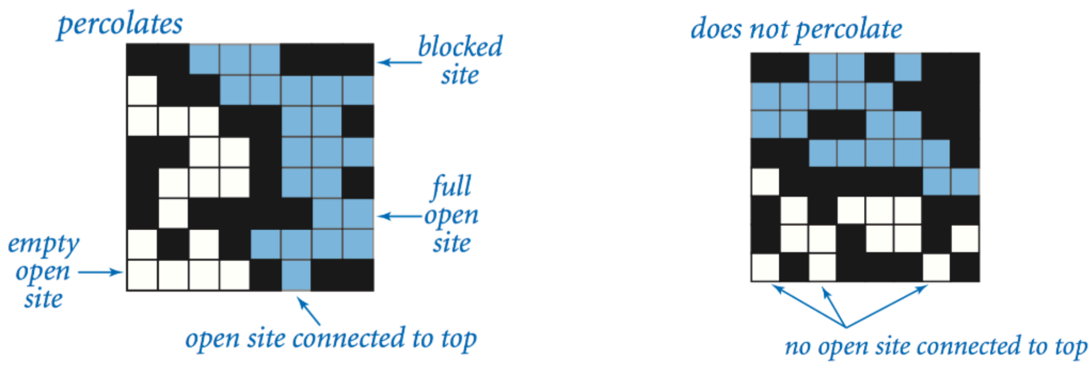
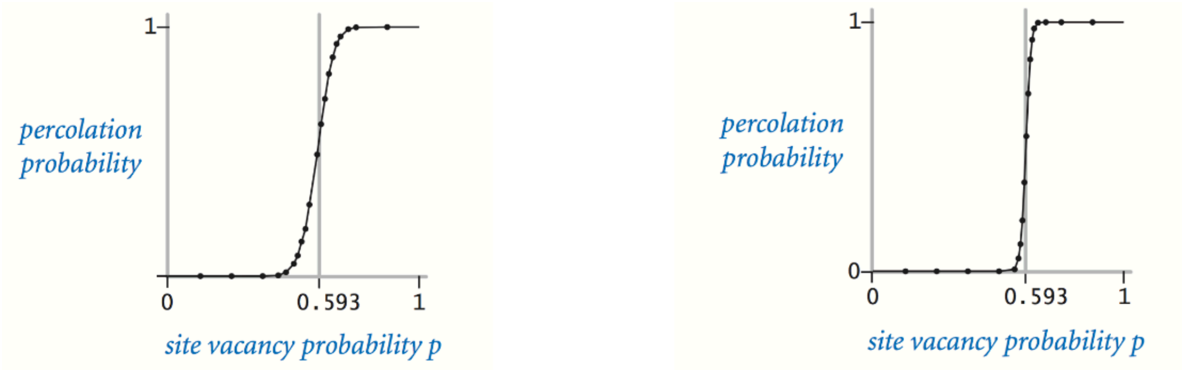


Figure 1: The blocked sites are displayed in black. The full open sites are displayed in cyan. The empty open sites are displayed in white.

3. **The problem**. In a famous scientific problem, researchers are interested in the following question: given an $n \times n$ random grid, if sites are independently set to be open with probability p (and therefore blocked with probability $1 - p$), what is the probability that the system percolates? When $p = 0$, the system does not percolate; when $p = 1$, the system percolates. The plots below show the site vacancy probability p versus the percolation probability for 20×20 random grid (left) and 100×100 random grid (right).

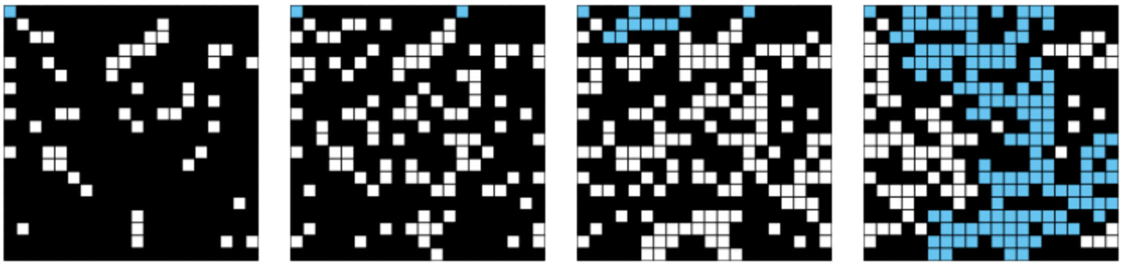


When n is sufficiently large, there is a threshold value p^* such that when $p < p^*$ a random n-by-n grid almost never percolates, and when $p > p^*$, a random n-by-n grid almost always percolates. No mathematical solution for determining the percolation threshold p^* has yet been derived. Your task is to write a computer program to estimate p^*.

4. **Monte Carlo simulation**. To estimate the percolation threshold, consider the following computational experiment:
   - Initialize all sites to be blocked and black.

  - Repeat the following until the system percolates:
    * Choose a site uniformly at random among all blocked sites.
    * Open the site.
  - The fraction of sites that are opened when the system percolates provides an estimate of the percolation threshold.

  For example, if sites are opened in a 20-by-20 lattice according to the snapshots below, then our estimate of the percolation threshold is $204/400 = 0.51$ because the system percolates when the 204th site is opened.



50 open sites *100 open sites* *150 open sites* *204 open sites*

  By repeating this computation experiment T times and averaging the results, we obtain a more accurate estimate of the percolation threshold. Let x_t be the fraction of open sites in computational experiment t. The sample mean $\bar{x}$ provides an estimate of the percolation threshold:

$$\bar{x} = \frac{x_1 + x_2 + \cdots + x_T}{T}.$$

5. **The task**. Estimate the percolation threshold for $20 - by - 20$ grid, $50 - by - 50$ grid, and $100 - by - 100$ grid via Monte Carlo simulation.

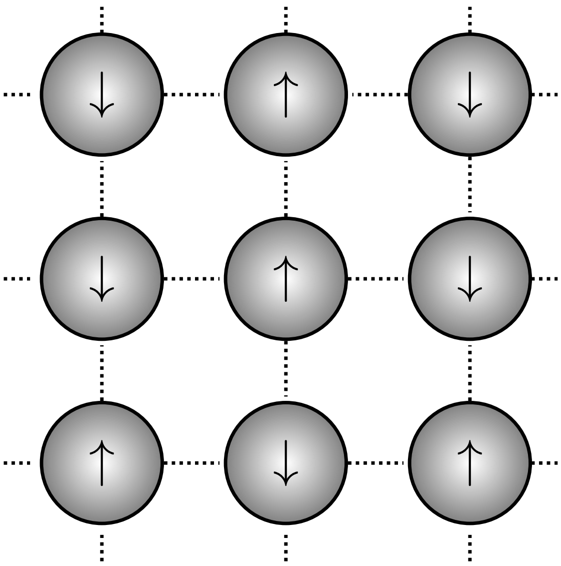
- **Part II: Ising Model**

  In certain alloys, particularly those containing Fe, Co or Ni, the electrons have a tendency to align their spins in a common direction. This phenomenon is called **ferromagnetism** and is characterized by the existence of a finite magnetization even in the absence of a magnetic field. It has its origin in a genuinely quantum mechanical effect known as the exchange interaction and related to the overlap between the wave functions of neighboring electrons.

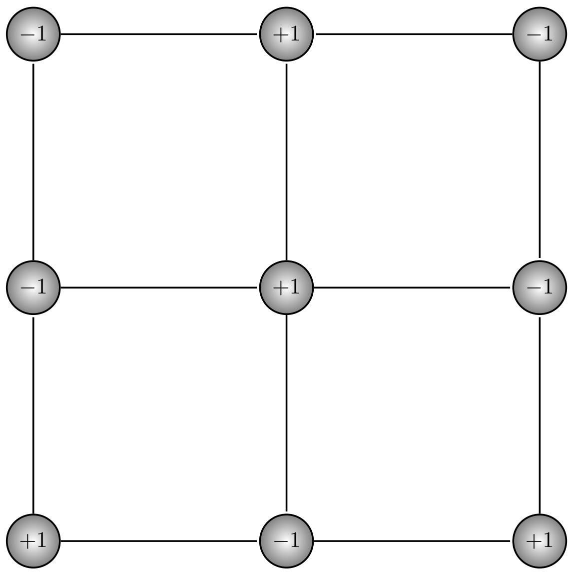
  The spin ordering diminishes as the temperature of the sample increases and, above a certain temperature T_c, the magnetization vanishes entirely. This is a **phase transition** and T_c is called the **critical temperature** or the **Curie temperature**. The Curie temperature is named after Pierre Curie, who received the Nobel Prize in Physics with his wife, Marie Curie. With their win, the Curies became the first ever married couple to win the Nobel Prize, launching the Curie family legacy of five Nobel Prizes.

The Ising model is a mathematical model of ferromagnetism in statistical physics. The Ising model was invented by the physicist Wilhelm Lenz in 1920, who gave it as a problem to his student Ernst Ising. The one-dimensional Ising model was solved by Ising alone in his 1924 thesis; however it has no phase transition. The two-dimensional Ising model is much harder and was only given an analytic description much later, by Lars Onsager in 1944. The two-dimensional Ising model is one of the simplest statistical models to show a phase transition.

1. Now we describe a two-dimensional square-lattice Ising model: given an undirected graph $G = (V, E)$, where V is the set of vertex (site) and E is the set of edges. If $(v, w) \in E$, then we say vertex v is the neighbor of vertex w, i.e., $v \sim w$, and vice versa. G is an $n \times n$ grid graph with $|V| = n^2$. Each vertex $v \in V$ is associated with a discrete variable σ_v such that $\sigma_k \in \{-1, +1\}$, representing the vertex's spin. An example of two-dimensional Ising model with $n = 3$ is illustrated as follows:



(a) Physical Model



(b) Mathematical Model

Figure 2: An example of two-dimensional Ising model with 3×3 grid graph

2. Define the spin configuration as $\boldsymbol{\sigma} = \{\sigma_v, v \in V\}$. The corresponding energy is

$$H(\boldsymbol{\sigma}) = -\sum_{(v,w)\in E} \sigma_v \sigma_w.$$

Define the set of all possible spin configurations as Ω, and define the Gibbs distribution(or called Boltzmann Distribution) over Ω as follows:

$$\pi_{\boldsymbol{\sigma}} = \frac{e^{-\beta H(\boldsymbol{\sigma})}}{Z}, \forall \boldsymbol{\sigma} \in \Omega.$$

where β is the constant representing the inverse of the temperature, and Z is the normalization constant (also called the partition function).

3. **Task A**: Show that given all other vertexes' spin value, the conditional distribution of vertex k 's spin is:

$$P(\sigma_k = +1|\boldsymbol{\sigma}_{-k}) = \frac{1}{1 + e^{-2\beta\left(\sum_{v\sim k}\sigma_v\right)}}$$
$$P(\sigma_k = -1|\boldsymbol{\sigma}_{-k}) = \frac{1}{1 + e^{2\beta\left(\sum_{v\sim k}\sigma_v\right)}}.$$

   where

$$\boldsymbol{\sigma}_{-k} = (\sigma_1, \ldots, \sigma_{k-1}, \sigma_{k+1}, \ldots, \sigma_{|V|}).$$

4. **Task B**: Simulate the two-dimensional Ising model with parameters as follows: $n = 100$, $\beta = -1, 0, 0.441, 0.8$. Illustrate the observed phase transition phenomenon and find the corresponding physical explanation.

5. **Task C**: Simulate the two-dimensional Ising model with parameters as follows: $n = 300$, $\beta = -5, 0.2, 0.441, 0.6$. Illustrate the observed phase transition phenomenon and find the corresponding physical explanation.