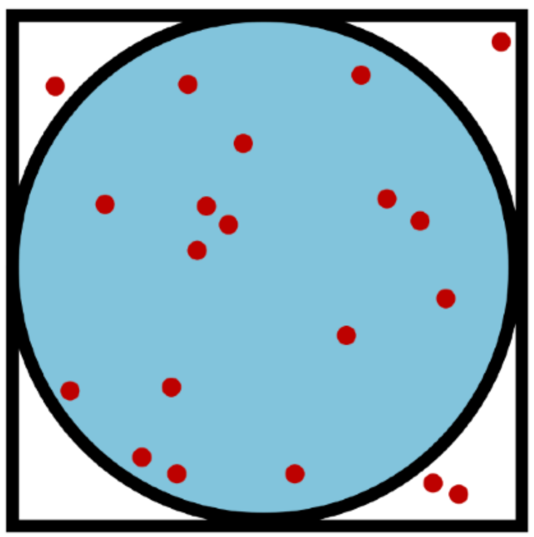
Numerical Methods



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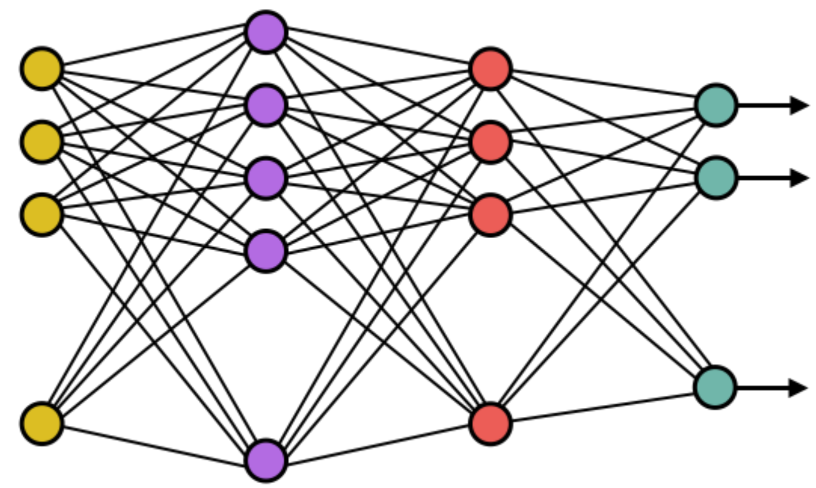

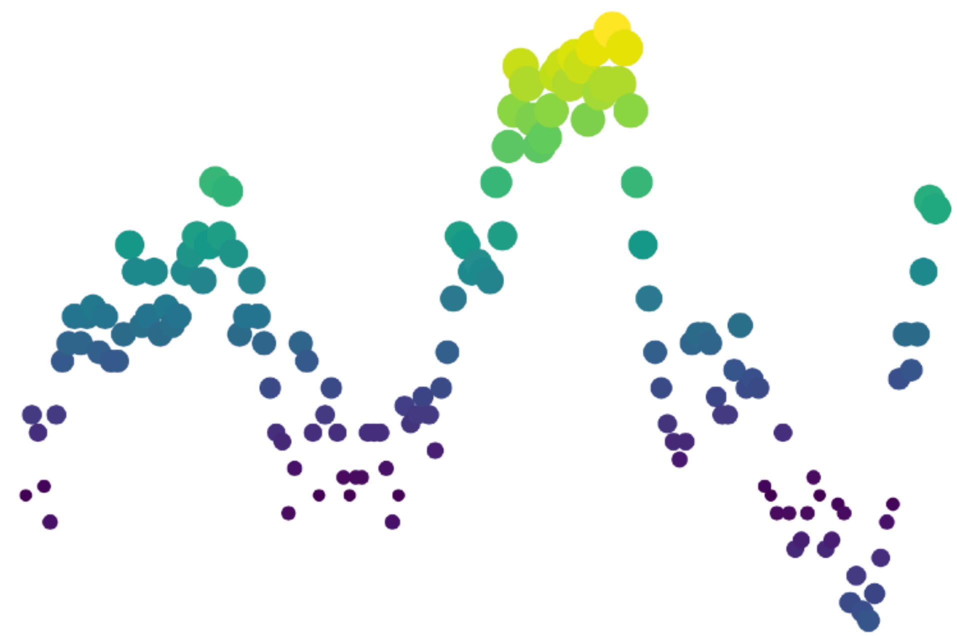

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Continued from last time

Numerical Methods, Lecture 3:

Fitting data and 2D Ising Model

PSI Start Online School 2023

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Lauren Hayward

In this notebook, we will study

1. how to perform fits to data corresponding to random walks in one dimension, and
2. how to calculate properties of a two-dimensional Ising model.

Today's objective is to learn now to perform fits when given numerical data, and to become familiar with the two-dimensional Ising model (which we will revisit in Lecture 4).

Note: Exercises 1 and 2 originally appeared in Lecture 2, but most students did not have enough time to complete them.

1. Fitting data

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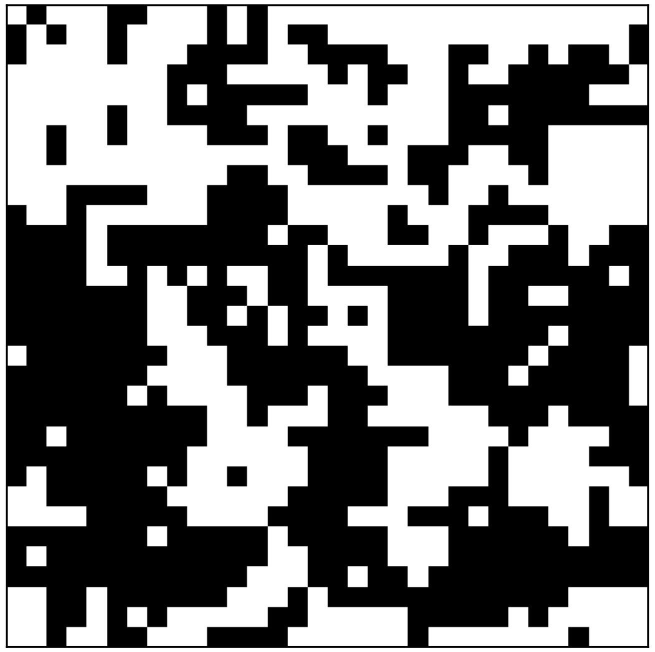
Outline

- Statistical physics and the Ising model
- Monte Carlo methods in statistical physics



Statistical physics

Goal: to study phenomena such as phase transitions for systems of N interacting particles when N is large.

Example: Ising model

$$E = -J \sum_{\langle ij \rangle} s_i s_j \qquad s_i = +1 \text{ or } -1 \quad (\blacksquare \text{ or } \square)$$

Energy

coupling energy

nearest neighbours

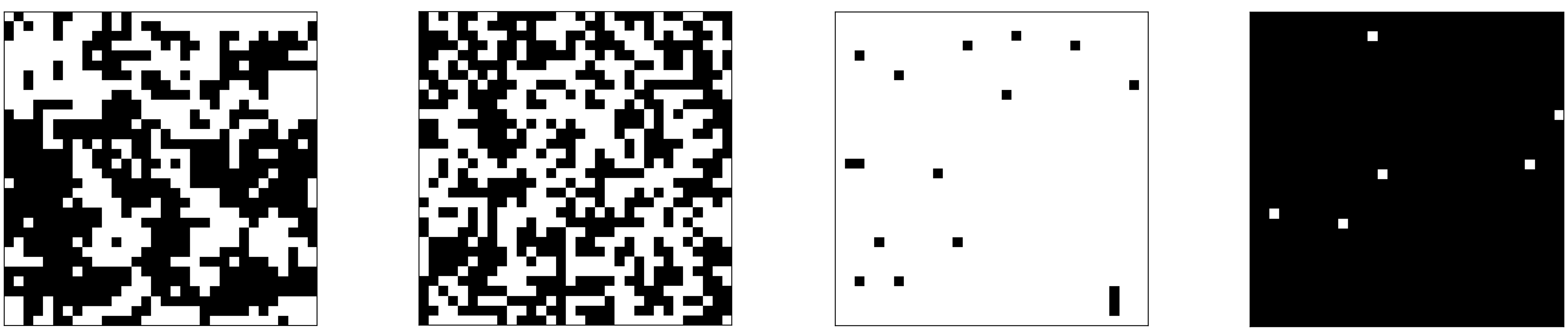
spin state at site i of the lattice

2D Ising model

$$E = -J \sum_{\langle ij \rangle} s_i \, s_j$$

$$s_i = \mathbf{+1} \text{ or } \mathbf{-1}$$

(■ or □)



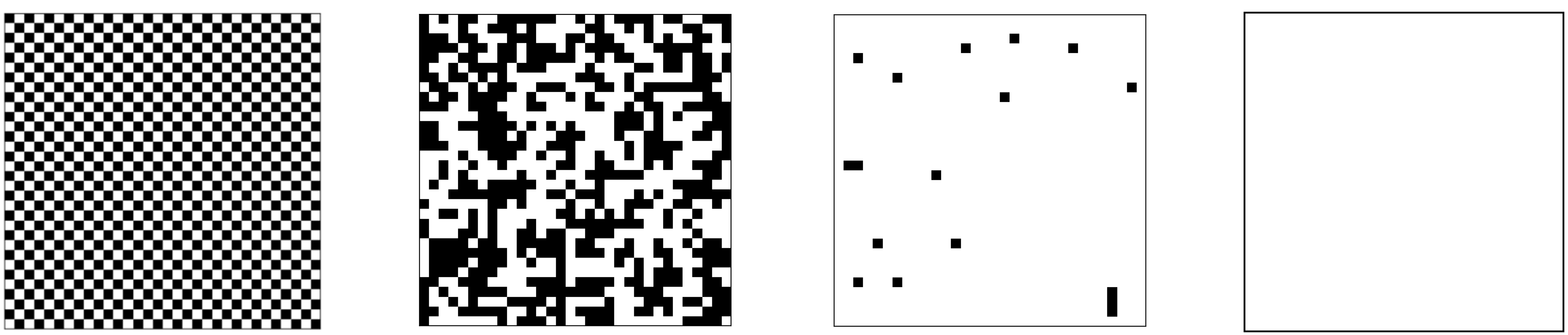
2D Ising model

$$E = -J \sum_{\langle ij \rangle} s_i \, s_j$$

$s_i =$ **+1** or **-1**

(■ or □)

When $J > 0$, which of the following spin configurations minimizes the energy E?



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2D Ising model

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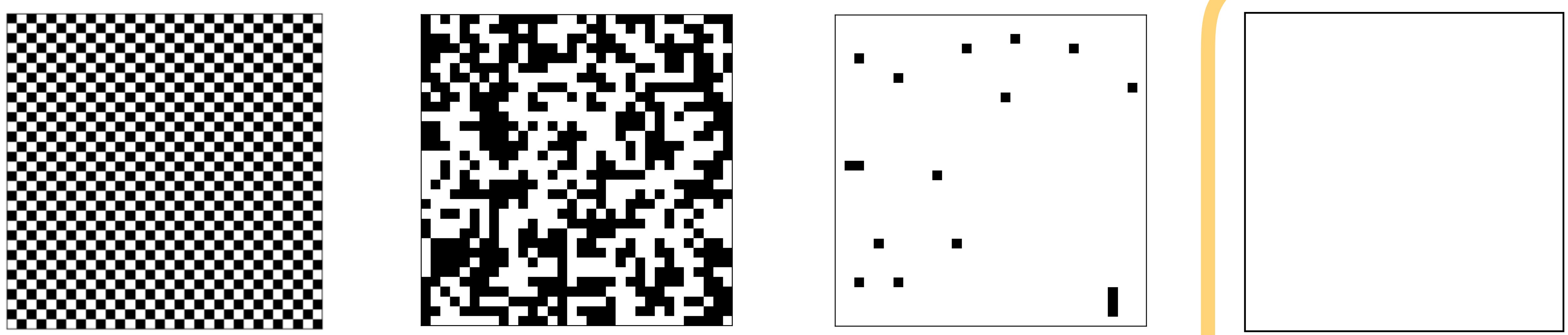

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$$E_{\text{min}} = -J \sum_{\langle ij \rangle} 1 = -J(2N) = -2JL^2$$

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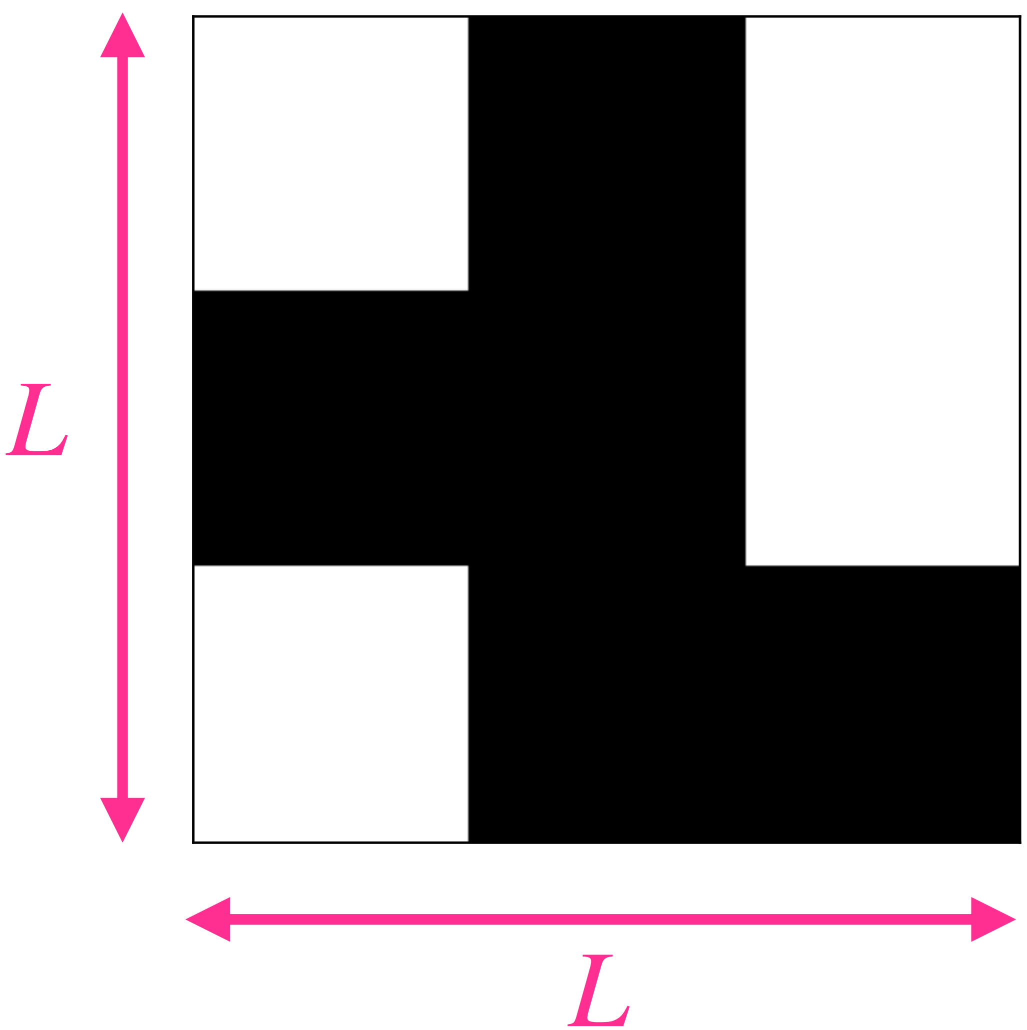
2D Ising model

Consider an Ising model on a two-dimensional lattice with periodic boundaries.



$$s_i = \mathbf{+1} \text{ or } \mathbf{-1}$$

(■ or □)

The configuration of the system can be stored in a two-dimensional array called "spins".

For the example here with L=3:

$$\text{spins} = \begin{bmatrix} -1 & +1 & -1 \\ +1 & +1 & -1 \\ -1 & +1 & +1 \end{bmatrix}$$

Breakout room activities

2. Ising model in two dimensions

Let us consider a classical nearest-neighbour Ising model on a two-dimensional lattice with periodic boundary conditions. The energy of a given spin configuration is given by

$$E = -J \sum_{\langle ij \rangle} s_i s_j,$$

where $J > 0$ is a coupling strength, $s_i = \pm 1$, and $\sum_{\langle ij \rangle}$ denotes a sum over nearest neighbours. We assume that the spins s_i live on the sites of a square $L \times L$ lattice. The total number of spins is then $N = L^2$.

As discussed in the lecture slides, the spins can be stored in a two-dimensional array called `spins`.

Consider the following configuration for $L = 3$: