Mathematical Sciences Exercise

Topics in Nonlinear Dynamics and Statistical Mechanics

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0 About This Exercise

Overview

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This document is a **reorganized version** of the assignment materials for Mathematical Science Exercise I conducted in the Winter Semester of 2023.

Contents

We will conduct simulations of problems related to statistical physics and nonlinear science. The following three topics will be addressed in order:

1. **Nonlinear Dynamical Systems**: approximately 4 weeks
   Specifically, we will explore bifurcation phenomena, attractor phenomena, and chaos.
2. **Monte Carlo Methods**: approximately 4 weeks
   Specifically, we will work on the Ising model and percolation.
3. **Modeling Various Phenomena (Independent Study)**: approximately 4 weeks
   We will apply what we have learned so far to many-degree-of-freedom dynamical systems, statistical physics, non-equilibrium phenomena, and biological phenomena by creating and researching actual models.

1 Nonlinear Dynamical Systems

Linear differential equations, such as the simple harmonic oscillator, can be solved by hand. However, in general, nonlinear equations cannot be solved analytically (with current mathematical capabilities). One approach to studying them is to use numerical calculations to observe the behavior of their solutions.

In this exercise, there will be no lectures on the theoretical foundations of nonlinear dynamical systems. Often, understanding a significant portion of nonlinear differential equation systems only progresses through actual numerical computations. This exercise will focus on such aspects.

Contents

- Linear stability analysis and nonlinear oscillations
- Synchronization phenomena of nonlinear oscillators
- Excitation phenomena in neurons
- Analysis of chaotic systems

Recommended References

1. Berje, Pomow, Bidal, *Order Within Chaos*, Sangyō Tosho
2. Ott, *Chaos in Dynamical Systems*, Cambridge University Press
3. Nicolis, Prigogine, *Dissipative Structures*, Iwanami Shoten
4. Hatsuo Hayashi, *Nonlinear Phenomena in Neural Systems*, Corona Publishing
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1.0 Numerical Integration Methods for Ordinary Differential Equations

In this chapter, we aim to numerically solve differential equations expressed as follows:

$$\frac{dx}{dt} = f(t, \boldsymbol{x}) \tag{1}$$

Generally, it is not possible to find analytical solutions to nonlinear differential equations, so it is necessary to compute numerical solutions using computers. Handling differential and integral calculus rigorously requires limit operations, but since infinite computational resources are impossible, we must approximate the differential equations to obtain recursive formulas when solving them numerically. The numerical methods commonly used for solving differential equations include the following (in practice, infinitely many methods are possible, but the ones listed below are typically used for standard applications):

Euler Method

The accuracy is first order in Δt (time step). Let Δt be denoted by h.

$$x_{n+1} = x_n + f(t_n, x_n)h \tag{2a}$$
$$t_{n+1} = t_n + h \tag{2b}$$

Second-Order Runge-Kutta Methods

The accuracy is second order in h.

Heun's Method

$$\boldsymbol{k}_1 = f(t_n, x_n)h \tag{3a}$$
$$\boldsymbol{k}_2 = f\left(t_n + h, x_n + \boldsymbol{k}_1\right)h \tag{3b}$$
$$x_{n+1} = x_n + \frac{1}{2}(\boldsymbol{k}_1 + \boldsymbol{k}_2) \tag{3c}$$
$$t_{n+1} = t_n + h \tag{3d}$$

Midpoint Method

$$\boldsymbol{k}_1 = f(t_n, x_n)h \tag{4a}$$
$$\boldsymbol{k}_2 = f\left(t_n + \frac{h}{2}, x_n + \frac{\boldsymbol{k}_1}{2}\right)h \tag{4b}$$
$$x_{n+1} = x_n + \boldsymbol{k}_2 \tag{4c}$$
$$t_{n+1} = t_n + h \tag{4d}$$

Fourth-Order Runge-Kutta Method

The accuracy is fourth order in h. Due to its high accuracy and reasonable computational cost, it is the most commonly used method in practice. In this exercise, it is preferable to use the fourth-order Runge-Kutta method as a standard approach.

$$\boldsymbol{k}_1 = f(t_n, x_n)h \tag{5a}$$
$$\boldsymbol{k}_2 = f\left(t_n + \frac{h}{2}, x_n + \frac{\boldsymbol{k}_1}{2}\right)h \tag{5b}$$
$$\boldsymbol{k}_3 = f\left(t_n + \frac{h}{2}, x_n + \frac{\boldsymbol{k}_2}{2}\right)h \tag{5c}$$

$$\boldsymbol{k}_4 = f\left(t_n + h, x_n + \boldsymbol{k}_3\right) h \tag{5d}$$

$$x_{n+1} = x_n + \frac{1}{6}(\boldsymbol{k}_1 + 2\boldsymbol{k}_2 + 2\boldsymbol{k}_3 + \boldsymbol{k}_4) \tag{5e}$$

$$t_{n+1} = t_n + h \tag{5f}$$

(Note: When numerically integrating a system of multivariable differential equations, all variables must be calculated and updated simultaneously. The same applies to numerical methods for partial differential equations.)

Exercise 1.0.0

Numerically solve the following harmonic oscillator using both the Euler method and the fourth-order Runge-Kutta method:

$$\frac{d^2x}{dt^2} = -x \tag{6}$$

Vary the time step and compare how the trajectories in phase space change for each numerical method. Additionally, verify how the value of $x^2 + \left(\frac{dx}{dt}\right)^2$ changes over time.

1.1 Linear Stability Analysis and Nonlinear Oscillations

It is generally not possible to find analytical solutions to nonlinear differential equations. Therefore, to understand the targeted nonlinear phenomena, it is important to comprehend the stable behavior of their solutions. Here, we will learn the basics of observing the behavior of solutions in phase space.

1.1.1 Linear Stability Analysis

Consider the following two-variable nonlinear differential equations:

$$\begin{cases} \frac{dX}{dt} = f(X, Y), \\ \frac{dY}{dt} = g(X, Y) \end{cases} \tag{7}$$

If this system has a fixed point (X_0, Y_0) that satisfies $\dot{X} = \dot{Y} = 0$, we can expand around the fixed point to obtain the following linearized differential equations:

$$\begin{cases} \frac{dx}{dt} = Ax + By, \\ \frac{dy}{dt} = Cx + Dy \end{cases} \tag{8}$$

Here, (x, y) represents small deviations from the fixed point, such that $(X, Y) = (X_0 + x, Y_0 + y)$. By examining the behavior of the linearized equations, we can understand the local properties of the original nonlinear differential equations around the fixed point. This method is called **Linear Stability Analysis**.

Classification of Equilibrium Points Equation (8) can also be rewritten as the following linear second-order differential equation:

$$\frac{d^2x}{dt^2} - (A + D)\frac{dx}{dt} + (AD - BC)x = 0 \tag{9}$$

The solutions to this differential equation can be interpreted as points moving over time in the (x, y) plane. In general, the collection of these points is called an **orbit**, and the space in which the orbit moves is called **phase space**.

The behavior of the solutions around the fixed point $(x, y) = (0, 0)$ depends on the values of the parameters A, B, C, D. The nature of the fixed point can be classified based on the roots of the characteristic equation

$$\lambda^2 - (A + D)\lambda + (AD - BC) = 0 \tag{10}$$

into **Stable Focus**, **Unstable Focus**, **Stable Node**, **Unstable Node**, **Center**, and **Saddle**.

Exercise 1.1.1

1. Organize the conditions on the parameters A, B, C, D under which each of the six types of fixed points is obtained (homework).
2. Create differential equations that satisfy each of these conditions, solve them numerically using a computer, and plot the trajectories in phase space.
3. Classify the harmonic oscillator and the damped oscillator accordingly.

1.1.2 Nonlinear Oscillations

A typical example of nonlinear oscillations is the van der Pol equation:

$$\frac{d^2x}{dt^2} - \mu(1 - x^2)\frac{dx}{dt} + x = 0 \tag{11}$$

where $\mu > 0$. Here, we consider the following equation obtained by a variable transformation of the van der Pol equation:

$$\frac{d^2x}{dt^2} - (\epsilon - x^2)\frac{dx}{dt} + x = 0 \tag{12}$$

(Note: While μ is a positive number, ϵ is a real number, so the variable transformation is valid only in the region where $\epsilon > 0$.)

Exercise 1.1.2

For the van der Pol equation (12),

1. Perform a linear stability analysis to investigate the stability of the fixed points.
2. Solve the equation numerically using a computer. Plot the time evolution and the solution trajectories in phase space. Observe the behavior of the trajectories starting from various initial conditions. How does the qualitative behavior of the solutions change with different values of ϵ?
3. By taking a suitable cross-section of the phase space and tracking the points where the trajectories intersect this cross-section (such a plane is called a **Poincaré Section**), you can effectively capture the characteristics of the phase space structure. Take the Poincaré section at $x = 0$ (which, in this case, is a straight line) and observe the behavior of the trajectories for various initial conditions.
4. Let the discrete orbit on the Poincaré section (Poincaré map) be denoted as $x_1, x_2, \ldots, x_n, \ldots$ (where the sequence consists of points where the orbit crosses the Poincaré section in the same direction). Plot x_n on the horizontal axis and x_{n+1} on the vertical axis (**Return Map**), and numerically observe the shape of this function and the asymptotic behavior of the points as $n \to \infty$ for various initial conditions. Consider what these asymptotic states correspond to and numerically explain their linear stability and uniqueness.
5. When $\epsilon = 0$, a stable limit cycle appears (a **Hopf Bifurcation**). When ϵ is sufficiently small, evaluate how the amplitude of the limit cycle depends on the parameter ϵ and determine the order of this dependence. Additionally, provide an analytical explanation for this dependency.

1.2 Attractor Phenomena in Nonlinear Oscillators

An interesting behavior of nonlinear oscillators is observed when a periodic external force is applied. For example, consider adding a periodic external force to the van der Pol equation as follows:

$$\frac{d^2x}{dt^2} - \mu(1-x^2)\frac{dx}{dt} + x = F\sin\omega t \tag{13}$$

Consider $\epsilon > 0$. Here, the left-hand side can be obtained by appropriately transforming equation (11). Under certain conditions, even if the natural frequency of the nonlinear oscillator is slightly different from the frequency of the external force, the oscillator will synchronize with the frequency of the external force. This phenomenon is called **Attractor Phenomena** or specifically **Forced Synchronization**. In the case of a linear oscillator with a periodic external force, a beat phenomenon occurs, but synchronization does not occur. Synchronization is an important characteristic of nonlinear oscillators.

Exercise 1.2.0

1. For a suitable value of μ, vary F and ω and observe the behavior.
2. Characterize synchronization by the relative period of the limit cycle with respect to the external force. For a suitable F, observe how the relative period of the limit cycle changes with ω.
3. Plot the parameter regions where synchronization occurs by setting the horizontal axis to F and the vertical axis to ω (observe the **Arnold Tongues**).
4. Observe how the dependencies on F and ω change with μ.
5. Introduce a variable $u = \omega t$, which transforms the system into a first-order differential equation with one variable. By setting $u(t + 2\pi/\omega) = u(t)$, forced synchronization can be regarded as motion on a T^2 torus. Take suitable upper and lower Poincaré sections and observe the behavior of the solutions. Construct a return map and discuss the behavior of the attractors with respect to ω based on the behavior of the obtained map. Also, discuss how the behavior of this map corresponds to the solution trajectories on the torus.
6. The following map is a model of the synchronization phenomenon of oscillators using a one-dimensional map:
$$\theta_{n+1} = \theta_n + \Omega - \frac{K}{2\pi}\sin(2\pi\theta_n) \tag{14}$$
This map is called the **Circle Map**. It represents the synchronization of two oscillators with phases represented by ϕ, where the natural frequencies when uncoupled are $P(\phi)$ and Ω, with $P(\phi) = P(\psi)$ and $\theta_n = \phi/2\pi$.
By considering the oscillators as periodic external forces, you can relate the results analyzed in the previous sections.
Focus on the region where $K < 1$ and investigate the behavior of the system with respect to the parameters Ω and K. Compare this with the return map constructed in the previous question and consider the physical correspondence (observe the **Arnold Tongues** and the **Devil's Staircase**).

1.3 Neuronal Excitation Phenomena and the Hodgkin-Huxley Equations

1.3.1 Analysis of the Hodgkin-Huxley Equations

The Hodgkin-Huxley equations (HH equations) are expressed as follows:

$$\begin{cases} I & = C_M \frac{dV}{dt} + \bar{g}_K n^4 (V - V_K) + \bar{g}_{\mathrm{Na}} m^3 h (V - V_{\mathrm{Na}}) + \bar{g}_L (V - V_L), \\ \frac{dn}{dt} & = \alpha_n (1 - n) - \beta_n n, \\ \frac{dm}{dt} & = \alpha_m (1 - m) - \beta_m m, \\ \frac{dh}{dt} & = \alpha_h (1 - h) - \beta_h h, \\ \alpha_n & = \frac{0.01(V+55)}{\exp\left(\frac{V+55}{10}\right)-1}, \quad \beta_n = 0.125 \exp\left(\frac{-V-65}{80}\right), \\ \alpha_m & = \frac{0.1(V+40)}{\exp\left(\frac{V+40}{10}\right)-1}, \quad \beta_m = 4 \exp\left(\frac{-V-65}{18}\right), \\ \alpha_h & = 0.07 \exp\left(\frac{-V-65}{20}\right), \quad \beta_h = \frac{1}{\exp\left(\frac{V-35}{10}\right)+1}. \end{cases} \tag{15}$$

Where $C_M = 1.0\,[\mu\mathrm{F/cm^2}]$, $V_{\mathrm{Na}} = 50\,[\mathrm{mV}]$, $V_K = -77\,[\mathrm{mV}]$, $V_L = -54.4\,[\mathrm{mV}]$, $\bar{g}_{\mathrm{Na}} = 120\,[\mathrm{mS/cm^2}]$, $\bar{g}_K = 36\,[\mathrm{mS/cm^2}]$, $\bar{g}_L = 0.3\,[\mathrm{mS/cm^2}]$.

Exercise 1.3.1

Simulate the HH equations to reproduce neuronal excitation phenomena.

1. Observe properties such as thresholds, action potentials, and refractory periods as seen in actual neurons. When slightly varying the initial conditions, how do the temporal changes in membrane potential differ? Plot the trajectories on the V-t plane. How does the membrane potential V behave in response to a step-like stimulus $I(t)$ applied at regular intervals?

2. Observe changes in variables other than the membrane potential and consider how the behavior of the membrane potential arises.

3. When the membrane current $I = 0$, regardless of whether an action potential occurs, the membrane potential eventually stabilizes to its resting value, making the state stable. However, if a membrane current of a certain magnitude is continuously applied, a periodic solution with a constant rhythm of action potentials should emerge. Investigate the range of the parameter I for which such periodic solutions are found. Specifically, to grasp the qualitative changes in solutions corresponding to changes in membrane potential, plot a bifurcation diagram. For instance, when the potential settles to a constant value, plot the resting membrane potential value against the parameter I, and when periodic solutions are obtained, plot the maximum and minimum values of the potential against I. Pay special attention to bifurcation points where the nature of the solutions changes by taking finer increments of I.

1.3.2 Reduction of the Hodgkin-Huxley Equations

The HH equations consist of four variables, but they do not capture all properties of neurons. For example, to reproduce the slow changes in membrane potential observed in specific neurons, additional ion channels other than Na and K must be considered, necessitating more variables. Furthermore, the morphology of the cell may significantly influence neuronal activity, requiring extensions to spatial models. This constructive approach aims to understand the behavior of real neurons by incrementally increasing the number of variables in the model.

On the other hand, from a theoretical standpoint, it is desirable to understand the essence of phenomena using models with as few variables as possible. For instance, can we simplify (reduce) equations like the HH equations, which consist of numerous variables and parameters, while retaining their essential properties?

Exercise 1.3.2

Attempt to reduce the four-variable HH equations to two variables. To achieve this, assume that the variable m changes much more rapidly compared to the variables n and h, quickly reaching a steady state. Additionally, assume that the sum of the slowly changing variables n and h remains constant ($n + h = K$, where K is a constant).

1. Evaluate the validity of the two assumptions by numerically examining the behavior of the variables m, n, and h in the HH equations.
2. Eliminate m and h from the equations based on the two assumptions to derive differential equations involving only V and n.
3. Simulate the derived equations (set $K = 0.75$). Examine the solution trajectories and bifurcation diagrams. When analyzing two-dimensional dynamical systems, drawing nullclines is a useful method for understanding the system. Investigate how the nullclines change with bifurcations. When drawing nullclines, using the **Newton Method** is recommended.
4. Compare the results obtained with the reduced equations to those obtained from the Hodgkin-Huxley equations.
5. Simulate the following FitzHugh-Nagumo equations and examine their nullclines, comparing them with the reduced HH equations:

$$\begin{aligned} \dot{v} &= v - \frac{v^3}{3} - w + I, \\ \tau \dot{w} &= v + a - bw. \end{aligned} \tag{16-17}$$

1.4 Chaos

In the previous chapters, we have examined two types of steady-state behaviors in nonlinear dynamical systems: fixed points and limit cycles. Additionally, as examples of transient behaviors leading up to steady states, excitation systems were discussed, which effectively represent the behavior of neurons. But are fixed points and limit cycles, along with the transient processes leading to them, the only behaviors exhibited by nonlinear dynamical systems? The answer is no. Another typical behavior observed in nonlinear dynamical systems is chaos, which demonstrates a perpetually irregular time evolution. Here, we will learn how to analyze chaos.

Exercise 1.4.0

Experience chaos firsthand and compare it with rhythmic phenomena (van der Pol equation).

1. Observe the time series and trajectories of the following systems.

   (a) **Hénon Map**

   $$\begin{cases} x_{n+1} &= y_n + 1 - a x_n^2, \\ y_{n+1} &= b x_n. \end{cases} \tag{18}$$

   First, try $a = 1.4$ and $b = 0.3$. Zoom in on a portion of the phase space to confirm the fractal nature of the attractor.

   (b) **Lorenz Equations (Meteorological Model)**

   $$\begin{cases} \dot{x} &= -\sigma x + \sigma y, \\ \dot{y} &= -xz + rx - y, \\ \dot{z} &= xy - bz. \end{cases} \tag{19}$$

   First, use $\sigma = 10$, $r = 28$, and $b = \frac{8}{3}$. Observe the chaotic behavior characteristic of the Lorenz attractor.

   (c) **Rössler Equations (Chemical Reaction Model)**

   $$\begin{cases} \dot{x} &= -y - z, \\ \dot{y} &= x + ay, \\ \dot{z} &= b + xz - cz. \end{cases} \tag{20}$$

   First, try $a = 0.2$, $b = 0.2$, and $c = 5.7$. Examine the emergence of chaos in the Rössler attractor.

2. A universal property observed in chaos is the sensitive dependence on initial conditions (initial condition sensitivity). Investigate the time evolution of the distance between two trajectories in phase space that start with slightly different initial conditions.

3. Choose a sufficiently small region and select many initial conditions within it. Observe the time evolution of the distribution of these points. Notice how the shape and area (volume) of this small region change over time, with the set of points being attracted, merged, and folded repeatedly.

Characterizing Chaos

Exercise 1.4.1

1. For the three models mentioned earlier, analytically calculate the rate of decrease of phase space volume and verify the results through numerical computations.

2. Strange attractors that generate chaos exhibit stretching and folding structures in phase space. This is a crucial property of chaos and is responsible for the fractal structures observed, such as those in the Hénon map. Consider calculating the dimension of such fractal structures.
Compute the box-counting dimension (capacity dimension), information dimension, and correlation dimension for the Hénon map.

Dimensions of Sets Consider dividing a d-dimensional phase space into a grid with width ϵ. Sample the solution trajectories at appropriate time intervals τ to create a total of N points $(x(t), x(t+\tau), \ldots, x(t+(\mathrm{N}-1)\tau))$. Number the grid cells that contain at least one of these points and denote the total number of such cells as $\tilde{N}(\epsilon)$. Count the number of points in each grid cell and define the probability for each cell as $p_i = N_i/N$ for $i = 1, \cdots, \tilde{N}(\epsilon)$. The dimensions are defined as follows:

Box-Counting Dimension (Capacity Dimension): D_0

$$D_0 = \lim_{\epsilon \to 0} \frac{\log \tilde{N}(\epsilon)}{\log(1/\epsilon)}.$$

Information Dimension: D_1

$$D_1 = \lim_{\epsilon \to 0} \frac{I(\epsilon)}{\log(1/\epsilon)}, \quad I(\epsilon) = -\sum_{i=1}^{\tilde{N}(\epsilon)} p_i \log p_i.$$

Correlation Dimension: D_2

$$D_2 = \lim_{\epsilon \to 0} \frac{\log\left(\sum_{i=1}^{\tilde{N}(\epsilon)} p_i^2\right)}{\log(1/\epsilon)} = \lim_{\epsilon \to 0} \frac{\log C(\epsilon)}{\log(1/\epsilon)},$$

where $C(\epsilon)$ is

$$C(\epsilon) = \frac{1}{N^2} \sum_{i=1}^{N} \sum_{j=1}^{N} \Theta(\epsilon - |x_i - x_j|).$$

$\Theta(x)$ is the step function defined as $\Theta(x) = 1$ for $x \geq 0$ and $\Theta(x) = 0$ for $x < 0$. When calculating the correlation dimension, it is advisable to sample M points from the N points and use the following formula:

$$C(\epsilon) = \frac{1}{NM} \sum_{i=1}^{N} \sum_{j=1}^{M} \Theta(\epsilon - |x_i - x_j|).$$

3. The logistic map is one of the simplest examples that exhibit chaos:

$$x_{n+1} = a x_n (1 - x_n) \tag{21}$$

Observe the trajectories for various parameters ($0 < a < 4$). How does the distance between two trajectories with slightly different initial conditions evolve over time for each parameter?

4. For the Rössler equations, take a Poincaré section at $x < 0$, $y = 0$, and construct a return map. Compare the results with the logistic map. Additionally, how is the stretching and folding structure observed in the Rössler attractor reflected in the properties of the map?

5. Draw bifurcation diagrams for both the logistic map and the Rössler equations (for the Rössler equations, investigate the region where $c^2 > 4ab$). What are the common features between the two?

6. As observed, the expansion rate of a small difference in initial conditions is an indicator of chaos. The Lyapunov exponent characterizes this expansion rate. Calculate the Lyapunov exponent for the logistic map and compare it with the bifurcation diagram.

2 Monte Carlo Methods

2.1 Random Number Generation

2.1.1 What are Random Numbers?

Monte Carlo methods utilize various random numbers. Consider N independent random variables $X_1, \cdots, X_N$ following the same probability distribution $P(X)$. For any subset A_i of the space of X,

$$P(V_i, X_i \in A_i) = \prod_i P(X_i \in A_i) \tag{25}$$

holds true. In this case, the random variables X_i are said to be independent. The realization values of independent random variables following the same probability distribution are called random numbers.

Computers cannot generate true random numbers. However, they can generate pseudorandom numbers with sufficiently long periodic sequences that exhibit the same distribution and statistical properties as random numbers within the range of N. Below, we will learn methods for generating pseudorandom numbers (for example, see [1, Volume 2], [2] Ch12). In practice, once you can generate uniform pseudorandom numbers in the interval [0,1], you can generate random numbers with any probability distribution (see the following exercises).

Linear Congruential Method Consider the sequence defined by the following recurrence relations for a set of integers (a, c, m, r):

$$r_0 = r, \tag{26}$$

$$r_{k+1} = ar_k + c \mod m. \tag{27}$$

In this case, the sequence $\{r_k\}$ takes on integer values "irregularly" within $0, 1, \cdots, m-1$. The degree of irregularity depends on (a, r, c, m) (ideally repeating with a period of m). Good combinations for generating random numbers include, for example:

$$(a, c, m) = (1229, 351750, 1664501), \tag{28}$$

$$(a, c, m) = (5^{11}, 0, 2^{31}), \tag{29}$$

$$(a, c, m) = (16807, 0, 2^{31} - 1), \tag{30}$$

$$(a, c, m) = (11^{13}, 0, 2^{48}). \tag{31}$$

Among these, the sequence $s_k = r_k/m$ yields a (pseudo) uniformly distributed random number in the interval $[0, 1)$, provided the parameters are chosen appropriately.

Exercise 2.1.1

1. Implement the above algorithm to generate uniformly distributed random numbers in $[0, 1)$.
2. Plot a histogram of the generated random numbers.
3. Calculate the mean, standard deviation, and the correlation between consecutive pairs of random numbers (be mindful of the precision and data type size of the programming language used).
4. Generate random numbers following the probability density function

$$\rho(x) = \begin{cases} 1 - |x| & (|x| \leq 1), \\ 0 & (|x| > 1) \end{cases} \tag{32}$$

5. Devise an algorithm to generate random numbers following any (with finite support) probability density function of your choice (a simple method is sufficient).

6. Use random numbers to numerically compute the value of an integral. As an example, write a program to approximate the value of π using random numbers.

7. Currently, one of the most effective pseudorandom number generation methods is the Mersenne Twister. Refer to `http://www.math.sci.hiroshima-u.ac.jp/ m-mat/MT/mt.html`, and use this algorithm to create a histogram of uniformly distributed random numbers.

2.2 Random Walk

2.2.1 What is a Random Walk?

A random walk, also known as a drunkard's walk, is one of the most fundamental models of random motion. Here, consider the problem of whether a drunkard can safely reach home by following a straight path. Assume the drunkard starts at position 0. At any given step, the drunkard only remembers that they are 100 steps away from their starting point but does not know whether to move left or right. The drunkard will take one step to the left or right with equal probability. Being extremely drunk, upon taking a step, they completely forget the direction from which they came, so they again move left or right with equal probability. The only thing the drunkard vaguely remembers is that taking 100 steps will allow them to reach home. The question is: after taking 100 steps, will the drunkard successfully reach home?

Exercise 2.2.1

1. Implement the random walk as described above and observe how the drunkard moves. Additionally, calculate the probability $p(m, 100)$ that the drunkard is at a certain position after m steps (plot $\log(p)$ against m^2). How do the mean and mean squared displacement behave as functions of m?

2. A simple and approximate method for generating Gaussian distributions is to generate k uniformly distributed random numbers in $[0, 1)$, sum them, and divide by k (commonly, $k = 12$ is used). Generate Gaussian-distributed random numbers using this method and compare the distribution of $p(m, 100)$ with it (how does the shape of the distribution change as k increases?). Additionally, discuss why this method approximates a Gaussian distribution.

3. Let x and y be uniformly distributed random numbers in $[0, 1)$. Then,

$$X = \sqrt{-2\log(1-x)}\cos 2\pi y, \tag{33}$$

$$Y = \sqrt{-2\log(1-x)}\sin 2\pi y, \tag{34}$$

   both follow the Gaussian distribution

$$\rho(X) = (2\pi)^{-1/2}\exp\left(-\frac{X^2}{2}\right) \tag{35}$$

   analytically (Box-Muller Method).
   (*Hint: Recall the trick for computing Gaussian integrals.*) Also, actually generate random numbers using the Box-Muller method and compare them with those generated by the summation method and the distribution of $p(m, 100)$.

4. Consider the difference equation where a particle moves either left or right by Δx after a time step Δt:

$$p(x, t+\Delta t) = \frac{p(x-\Delta x, t)}{2} + \frac{p(x+\Delta x, t)}{2} \tag{36}$$

   Expand the left-hand side with respect to Δt and the right-hand side with respect to Δx. What equation do you obtain? Using this result, numerically solve the diffusion equation.

2.3 Langevin Equation

Consider a single particle moving along a one-dimensional axis, with its position at time t denoted by $x(t)$. This particle is subject to a potential $U(x)$ and is in contact with a thermal bath at temperature T. The time evolution of the particle's position is governed by the Langevin equations:

$$\frac{dx}{dt} = \frac{p}{m}, \tag{37}$$

$$\frac{dp}{dt} = -\gamma p - \frac{\partial U(x)}{\partial x} + \xi(t) \tag{38}$$

Here, γ is the viscosity coefficient representing energy dissipation due to friction with the thermal bath, and $\xi(t)$ represents the random fluctuating force exerted by the thermal bath. The noise term ξ has the statistical properties of white Gaussian noise:

$$\langle \xi(t) \rangle = 0, \tag{39}$$

$$\langle \xi(t)\xi(t') \rangle = 2\gamma T \delta(t - t') \tag{40}$$

The appearance of T and γ in the noise term arises from the requirement that the system reaches the canonical distribution in equilibrium:

$$P(p, x) \propto \exp\left(-\frac{p^2}{2T} - \frac{U(x)}{T}\right) \tag{42}$$

(This follows from the fluctuation-dissipation theorem.)

Exercise 2.3.0

1. Implement the Langevin equations for the case where $U(x) = 0$. When discretizing time, consider how the noise term ξ scales with the time step Δt. In this case, the particle undergoes simple diffusion, and the probability density function $P(x)$ for the particle's position follows the diffusion equation
$$\frac{\partial P(x)}{\partial t} = D\frac{\partial^2 P(x)}{\partial x^2} \tag{43}$$
Perform numerical calculations to solve this equation (you can also solve it analytically). How does the diffusion coefficient D relate to the parameters in the Langevin equation?

2. Vary the potential $U(x)$ and verify that the system follows the canonical distribution as given in equation (42).

2.4 [Free Assignment] Percolation

2.5 Ising Model

Consider the Ising model, which is the simplest lattice model. On each site $i \in \Lambda$ of a lattice Λ, there is a spin $S_i = \pm 1$. The Hamiltonian is given by

$$H(\{S_i\}) = -J \sum_{\langle i,j \rangle} S_i S_j - h \sum_i S_i \tag{58}$$

Here, the first term represents the sum over nearest-neighbor spin pairs, indicating the interaction between spins. The second term represents the effect of a uniform external field h. The coupling constant $J > 0$ corresponds to ferromagnetic interactions (favoring alignment of neighboring spins). Its magnitude can be absorbed into the temperature units, so we set $J = 1$ below. The partition function is defined as

$$Z = \sum_{\{S_i\} \in C} e^{-\beta H(\{S_i\})}, \tag{59}$$

where $\beta = \frac{1}{k_B T}$, and the physical quantity A has an expectation value

$$\langle A \rangle = Z^{-1} \sum_{\{S_i\} \in C} A(\{S_i\}) e^{-\beta H(\{S_i\})} \tag{60}$$

The set C represents all possible spin configurations (if the number of sites is $N := |\Lambda|$, then $|C| = 2^N$). Important physical quantities include:

$$\text{Magnetization per site } M = \langle s \rangle, \tag{61}$$

$$\text{Energy per site } u = \frac{1}{N}\langle H \rangle = \frac{1}{N}\left(-\frac{1}{Z}\frac{\partial Z}{\partial \beta}\right), \tag{62}$$

$$\text{Specific Heat per site } c = \frac{\partial \langle u \rangle}{\partial T} = \frac{1}{k_B T^2}(\langle H^2 \rangle - \langle H \rangle^2), \tag{63}$$

$$\text{Susceptibility per site } \chi = \frac{\partial \langle s \rangle}{\partial h} = \frac{N}{k_B T}(\langle s^2 \rangle - \langle s \rangle^2), \tag{64}$$

where

$$s := \frac{1}{N} \sum_{j=1}^{N} S_j. \tag{65}$$

Exercise 2.5.0

Demonstrate the non-trivial equality in the above equations. Additionally, the correlation between two distant spins is given by

$$G(i,j) = \langle S_i S_j \rangle \tag{66}$$

which typically behaves as

$$G(i,j) \sim \exp\left(-\frac{|i-j|}{\xi}\right) \tag{67}$$

Here, ξ, which has the dimension of length, is referred to as the correlation length.

Consider the qualitative behavior of this system when $h = 0$. At high temperatures, the influence of the interaction term is small, and entropy dominates, making it likely that each spin points in a random direction. In other words, $M \simeq 0$. This state is called **paramagnetic** and does not exhibit magnetic properties. At low temperatures, the effect of the interaction term becomes significant, and even slight impurities or external fields can break the symmetry, resulting in all spins aligning in the same direction. Thus, $|M| > 0$. This state is called **ferromagnetic** and behaves as a magnet.

The definition of $\langle s \rangle$ considered above is symmetric under the transformation $S_i \leftrightarrow -S_i$ when $h = 0$. Therefore, $\langle s \rangle$ should inherently be 0. In reality, for finite systems, $\langle s \rangle = 0$ always holds. The spontaneous magnetization in the sense described above for infinite systems is defined as

$$M_{sp} = \lim_{h \to 0} \lim_{N \to \infty} M, \quad \chi_{sp} = \lim_{h \to 0} \lim_{N \to \infty} \chi$$

When considering the process of continuously changing the temperature from high to low, a phase transition point between the two phases occurs at the critical temperature $T = T_c$. In statistical mechanics, determining this transition point T_c and understanding the (singular) behavior of physical quantities at the transition point is of great interest. Specifically, at $T = T_c$,

$$\begin{aligned} M &\propto |T - T_c|^{\beta}, \\ \chi &\propto |T - T_c|^{-\gamma}, \\ \xi &\propto |T - T_c|^{-\nu} \end{aligned}$$

exhibit critical singularities (note that this β is different from the inverse temperature β). Just above the transition point $T = T_c$, the correlation length diverges, and the correlation between two points becomes moderate:

$$G(i, j) \sim |i - j|^{-(d-2+\eta)}. \tag{68}$$

We aim to determine these exponents β, γ, ν, etc. They are related through *hyperscaling* relations:

$$d\nu = 2\beta + \gamma \tag{69}$$

$$2 - \eta = \frac{\gamma}{\nu} \tag{70}$$

The Ising model on one- and two-dimensional square lattices has exact solutions (see [5, Chapter 2]). However, such exact solutions are limited, and methods like Monte Carlo simulations are typically employed to study other cases.

2.5.1 Metropolis Method

What follows is the Monte Carlo method for the canonical ensemble. We aim to reach the thermodynamic limit $N \to \infty$, but the sum in equation (60) consists of 2^N terms, which grows exponentially with N, making the computation infeasible. Therefore, we consider approximating the expectation value $\langle A \rangle$ using random numbers. For simplicity, we denote the spin configuration $\{S_i\} \in C$ as $x_a = \{S_i\} \in C$.

Simple Sampling The most straightforward approach is simple sampling. That is, randomly select n configurations $\{x_a\}_{a=1,\dots,n}$ from the 2^N possible configurations with equal probability, and approximate the expectation value of the physical quantity A as

$$\langle A \rangle \simeq \frac{\sum_{a=1}^{n} A(x_a) e^{-\beta H(x_a)}}{\sum_{a=1}^{n} e^{-\beta H(x_a)}} \tag{71}$$

Weighted Sampling Generalizing the above, instead of equal probability, sample configurations $\{x_a\}_{a=1,\dots,n}$ according to a probability density $\rho(x)$, and approximate the expectation value of A as

$$\langle A \rangle \simeq \frac{\sum_{a=1}^{n} \rho(x_a)^{-1} A(x_a) e^{-\beta H(x_a)}}{\sum_{a=1}^{n} \rho(x_a)^{-1} e^{-\beta H(x_a)}} \tag{72}$$

Notice that dividing by $\rho(x_a)$ allows us to write the sum as

$$\int f(x) dx = \int \frac{f(x)}{\rho(x)} \rho(x) dx \tag{73}$$

Error When calculating $\langle A \rangle$ from a finite number of samples, statistical errors are inevitable. According to the Central Limit Theorem, for a sequence of random variables $\{x_a\}_{a=1,\dots,n}$ following the probability density $\rho(x)$, the quantity

$$\frac{1}{n} \sum_{a=1}^{n} g(x_a) \tag{74}$$

approaches a normal distribution with mean and variance given by

$$\text{Mean } I := \int dx\rho(x)g(x), \tag{75}$$

$$\text{Variance } \frac{\sigma^2}{n} = \frac{1}{n}\left(\int dx\rho(x)g(x)^2 - \left(\int dx\rho(x)g(x)\right)^2\right) \tag{76}$$

Hence, in method (72), the error in the denominator is approximately

$$\frac{\sigma}{\sqrt{n}} = \frac{1}{\sqrt{n}}\left[\frac{\sum_{a=1}^n \left(\rho(x_a)^{-1}e^{-\beta H(x_a)}\right)^2}{\left(\sum_{a=1}^n \rho(x_a)^{-1}e^{-\beta H(x_a)}\right)^2}\right]^{1/2} \tag{77}$$

To minimize this error, not only can we increase n, but we can also cleverly choose $\rho(x)$ to reduce σ. In fact, by selecting

$$\rho(x) = Z^{-1}e^{-\beta H(x)} \tag{78}$$

the variance σ becomes 0. In this case, the right-hand side of equation (72) simplifies to

$$\frac{1}{n}\sum_{a=1}^n A(x_a) \tag{79}$$

(where $\{x_a\}$ is a random sequence following the probability density $\rho(x)$). In Monte Carlo simulations, this is typically how $\langle A\rangle$ is calculated. That is, generate a random sequence $\{x_a\}$ following the probability density $\rho(x)$, measure the physical quantity for each configuration, and take the simple average.

Exercise 2.5.1

1. Explain intuitively why simple sampling is inefficient.

Metropolis Method Consider generating a random sequence that follows the probability distribution $\rho(x)$. Here, x is not necessarily a number but a point in the event space. In the case of the Ising model discussed below, x represents a single spin configuration.

A Markov chain with transition probabilities $W(x, x')$ is a sequence of random variables $\{x_a\}$ where the conditional probability of $x_{i+1} = x'$ given $x_i = x$ is $W(x, x')$. By choosing appropriate transition probabilities $W(x, x')$, it can be shown as follows that, for sufficiently large a, the sequence $\{x_a\}$ follows the distribution $\rho(x)$.

Let us treat the index a as time t and denote the probability distribution at time t as $\rho(x, t)$ for a Markov chain with transition probabilities $W(x, x')$. The time evolution of $\rho(x, t)$ is given by

$$\frac{d\rho(x,t)}{dt} = -\sum_{x'} W(x,x')\rho(x,t) + \sum_{x'} W(x',x)\rho(x',t) \tag{80}$$

After sufficient transitions, when $\rho(x, t)$ reaches a steady state $\rho(x, t) = \rho(x)$, the following condition holds:

$$\sum_{x'} W(x,x')\rho(x) = \sum_{x'} W(x',x)\rho(x') \tag{81}$$

Therefore, by choosing $W(x, x')$ such that equation (81) is satisfied for the desired $\rho(x)$, the equilibrium distribution $\rho(x)$ can be achieved. To satisfy equation (81), especially, choose $W(x, x')$ such that for any $x, x' \in C$,

$$W(x,x')\rho(x) = W(x',x)\rho(x') \tag{82}$$

This condition is known as the **detailed balance condition**. A suitable choice of $W(x, x')$ that satisfies this condition is

$$W(x,x') = \min\{1, \rho(x')/\rho(x)\}. \tag{83}$$

Exercise 2.5.1

2. Show that equation (83) satisfies equation (82).

   The steps of the Metropolis method are as follows:

   (a) Use a random number to generate a nearby event x' from x.

   (b) Calculate $w = \frac{\rho(x')}{\rho(x)}$.

   (c) If $w \geq 1$, accept the new event x'.

   (d) If $w < 1$, generate another random number and accept x' if $r \leq w$, otherwise reject x' and retain x.

Metropolis Method for the Ising Model The transition probability is given by

$$W(x, x') = \min\{1, \exp(-\beta(H(x') - H(x)))\} \times (\text{normalization constant}) \tag{84}$$

Algorithm For the Ising model, the Monte Carlo method proceeds as follows:

1. Choose an initial configuration $x_0 \in C$ randomly.
2. From the configuration x_a, generate a new configuration x_{a+1} as follows:
   (a) Let $x_a = x_{a,0}$.
   (b) Flip one spin in x_a to obtain a tentative configuration $x_{a,1}$.
   (c) Generate a uniform random number r in $[0, 1]$.
   (d) If $r < \min\{1, \exp(-\beta(H(x_{a,1}) - H(x_{a,0}))\}$, accept the tentative configuration by setting $x_a = x_{a,1}$. Otherwise, reject the tentative configuration and retain $x_a = x_{a,0}$.
   (e) Repeat step (b), changing the location of the spin to be flipped. Continue this process until, on average, each spin has been attempted to be flipped once. Once completed, set $x_a = x_{a+1}$.
3. Measure the physical quantities.
4. Return to step 2.
5. After performing a sufficient number of loops, average the measurement results of the physical quantities.

One complete outer loop is referred to as one Monte Carlo step (1 MCS). As a practical note, after creating the program, test it with small N and a few MCS before performing large-scale computations.

Measuring M and χ in the Low-Temperature Phase $T < T_c$ In computer simulations, taking the limits $\lim_{h\to 0}\lim_{N\to\infty}$ is not practical. For sufficiently large systems (with system size $L \gg \xi$), by restricting the configurations to those with $s > 0$, these quantities can be effectively measured. Specifically,

$$M' = \langle |s| \rangle,$$
$$\chi' = \frac{N}{k_B T}(\langle s^2 \rangle - \langle |s| \rangle^2)$$

can be measured.

On the other hand, for $T > T_c$, one should measure $\chi = \frac{N}{k_B T}(\langle s^2 \rangle - \langle s \rangle^2)$, and χ' should not be measured because $M = \langle s \rangle = 0$ in this case.

2.5.2 Finite Size Scaling

Simulating near the critical temperature T_c is challenging. Regardless of how large the finite system size L is, as temperature T approaches T_c, eventually $L \gg \xi$, making it impossible to correctly account for the effects of interactions. Instead, one considers finite size scaling, which involves studying the behavior of finite-sized systems and extrapolating to the infinite system limit based on size dependencies.

Finite Size Scaling Hypothesis Let $p(s, L, T)$ be the probability of the spin configuration magnetization $s = \frac{1}{N}\sum S_i$ for a system of size L and temperature T. The finite size scaling hypothesis posits that

$$p(s, L, T) = \xi^{\beta/\nu} P\left(\frac{L}{\xi}, s\xi^{\beta/\nu}\right) \tag{85}$$

where P is a two-variable function independent of temperature T. In other words, the temperature dependence appears solely through the correlation length ξ. Here, the combination L/ξ and $s\xi^{\beta/\nu}$ are called the scaling variables. The function P is universal, meaning its form does not depend on temperature or system size, although it may depend on boundary conditions. The prefactor $\xi^{\beta/\nu}$ ensures that $P(x, y)$ behaves as a probability distribution in the second variable y ($\int dy P(x, y) = 1$).

Additionally,

$$\xi^{\beta/\nu} P\left(\frac{L}{\xi}, s\xi^{\beta/\nu}\right) = L^{\beta/\nu} \tilde{P}\left(\frac{L}{\xi}, sL^{\beta/\nu}\right) \tag{86}$$

defines another universal function $\tilde{P}$.

Using this form, we find that

$$\langle |s| \rangle_{L,T} = L^{-\beta/\nu} \tilde{M}\left(\frac{L}{\xi}\right),$$
$$\langle \chi \rangle_{L,T} = L^{\gamma/\nu} \tilde{\chi}\left(\frac{L}{\xi}\right),$$

where $\tilde{M}$ and $\tilde{\chi}$ are universal functions. These functions are the desired quantities.

From this, we see that an effective method to determine the critical exponents is available. At the critical temperature $T = T_c$, since $\xi = \infty$, both $M(0)$ and $\chi'(0)$ become constants independent of system size L. Therefore, by performing log-log plots of data for different system sizes L, the ratios β/ν and γ/ν can be determined. Once these are obtained, the functional forms of $\tilde{M}$ and $\tilde{\chi}$ can be determined. Specifically, by plotting $ML^{\beta/\nu}$ against $|T - T_c|\xi^{1/\nu}$, data from all system sizes L should collapse onto a single curve.

Exercise 2.5.1

3. For example, set $N = 4^2$, $k_B T = 0.5, 5$ (using $J = 1$ as the unit), and measure s and $|s|$ up to 200 Monte Carlo steps (MCS). Observe how they change as functions of MCS.

4. Measure magnetization, susceptibility, internal energy, specific heat, etc., as functions of temperature. Estimate the position of the critical temperature T_c (around $k_B T = 1.5 \sim 3$). For convenience in later analysis, record quantities such as $M = \langle s \rangle$, $M' = \langle |s| \rangle$, $\langle s^2 \rangle$, $\langle s^4 \rangle$, $\langle H \rangle$, $\langle H^2 \rangle$, etc.

5. Perform the same measurements for several lattice sizes and discuss the differences due to system size.

2.5.3 Binder Parameter

In the above discussion, the critical temperature T_c was assumed to be already determined exactly. A useful quantity for determining the critical temperature is the Binder parameter, defined as

$$U_L(T) := 1 - \frac{\langle s^4 \rangle_L}{3\langle s^2 \rangle_L^2} \tag{87}$$

For $T > T_c$, $U_L \to 0$ as $L \to \infty$. For $T < T_c$, $U_L \to \frac{2}{3}$ as $L \to \infty$. Under the finite size scaling hypothesis, assuming $U_L(T)$ behaves as

$$U_L(T) = 1 - \frac{\tilde{\chi}_4(L/\xi)}{3\tilde{\chi}_2(L/\xi)^2} \tag{88}$$

where $\tilde{\chi}_4$ and $\tilde{\chi}_2$ are universal functions, the Binder parameter $U_L(T)$ at the critical temperature $T = T_c$ becomes a size-independent constant U^*. Therefore, by plotting $U_L(T)$ for different system sizes L against temperature T, the curves will intersect at $T = T_c$, allowing an accurate determination of the critical temperature.

Exercise 2.5.3

1. Use the Binder parameter to accurately determine T_c.
2. Analyze the size dependence of data just above the transition point to determine the critical exponents β/ν and γ/ν.
3. Plot the magnetization M and susceptibility χ as functions of the scaling variables. Specifically:
   (a) Plot $ML^{\beta/\nu}$ versus $|T - T_c|L^{1/\nu}$.
   (b) Plot $\chi L^{-\gamma/\nu}$ versus $|T - T_c|L^{1/\nu}$.

   Adjust the value of ν such that data from all system sizes L collapse onto a single universal curve.
4. Investigate other boundary conditions (e.g., free boundaries) and analyze their effects on the results.
5. Under the finite size scaling hypothesis, demonstrate the relations

$$\frac{1}{\nu} = \frac{\log\left(\frac{dU_L}{dL} \Big/ \frac{dU_{bL}}{dL}\right)}{\log b},$$
$$\frac{\gamma}{\nu} = \frac{\log(\chi(bL)/\chi(L))}{\log b}.$$

   Use these relations to determine $1/\nu$ and γ/ν. Specifically, for a fixed L, plot $\log\left(\frac{dU_L}{dL} \Big/ \frac{dU_{bL}}{dL}\right)$ against $1/\log b$, which should yield a straight line. Ideally, all such lines for different L should intersect at $1/\log b = 0$.

Reference For the 2-dimensional Ising model on a square lattice, the exact solutions are known:

$$d = 2,\ \beta = \frac{1}{8},\ \nu = 1,\ \gamma = \frac{7}{4},\ \eta = \frac{1}{4}, \tag{89}$$

$$\frac{1}{k_B T_c} = \beta_c = \frac{1}{2}\ln(\sqrt{2}+1), \quad k_B T_c = 2.26919 \tag{90}$$

Additionally,

$$\text{Triangular lattice: } e^{2\beta_c} = \sqrt{3},$$
$$\text{Hexagonal lattice: } e^{2\beta_c} = 2 + \sqrt{3}.$$

3 Modeling (Free Research)

Based on what you have learned about nonlinear dynamical systems and Monte Carlo methods, conduct independent research on a natural phenomenon that interests you.