Some questions/problems you should be able to work out.

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1. Random numbers, distributions.

   (a) If X is uniformly distributed between 0 and 1 and f is a function, how is the random variable $Y = f(X)$ distributed?
   i.e., given $p_X(x) = 1$ for $x \in [0, 1]$ and $p_X(x) = 0$ for $x \notin [0, 1]$. What is $p_Y(y)$?
   Hint: the probability for finding X in the interval $[a, b]$ should equal the probability for finding Y in the interval $[f(a), f(b)]$. Also when a and b are infinitesimally close to each other.

   (b) The random variable X is uniformly distributed between 0 and 1. Consider the variable $Y = -\ln X$. What is the probability distribution for Y?

   (c) Consider a large number (N) of random variables $\{X_i\}$, each having the same distribution with mean μ and variance σ^2. What is the distribution of $\sum_i X_i$?
   In other words: know the central limit theorem.

2. Inverse transform sampling, a.k.a. inverse CDF sampling, a.k.a. 'transformation method'.

   Reminder: To use inverse transform sampling, one first finds the cummulative distribution function (CDF) of the desired distribution. After that, the CDF is inverted.

   $$\mathcal{C}(y) = \int_{-\infty}^{y} p(z)dz \qquad\qquad y = f(x) = \mathcal{C}^{-1}(x)$$

   If x is uniformly distributed, then the transformation $y = f(x)$ will give a variable that is distributed according to $p(y)$. The range of x has to be chosen such that the values of y appear in the desired range.

   (a) Prove the result above.

   (b) Given a uniform random number generator in the range $[0, 1]$, find a transformation that would yield a random number y with the distribution

   $$p(y) = \begin{cases} e^{-y} & y \geq 0, \\ 0 & y < 0. \end{cases}$$

(c) We want to draw random numbers having the distribution

$$p(y) = \begin{cases} \mathcal{N}/y^2 & y \geq a, \\ 0 & y < a. \end{cases}$$

Determine the normalization constant $\mathcal{N}$ in terms of a.
Given a uniform random number generator in the range $[0, 1]$, find a transformation that would yield a random number y with this distribution.

3. Rejection method:

   (a) Generators for pseudo-random numbers distributed according to the normal distribution (with arbitrart centre and standard deviation) are widely available, e.g., the numpy.random.normal() function.
   Given such a generator, explain how using the rejection method you can generate pseudo-random numbers with the distribution

   $$f(x) = \frac{e^{-x^2/2}}{M(1+x^2)}$$

   where M is a normalisation constant.

4. Generating random numbers using MCMC:
   We want to sample random numbers according to the distribution

   $$p(x) = \begin{cases} \frac{2}{3}(1+x) & y \in (0, 1], \\ 0 & x \notin (0, 1]. \end{cases}$$

   using the Metropolis-Hastings algorithm.

   (a) Explain the condition under which the Metropolis-Hastings algorithm reduces to the Metropolis algorithm.

   (b) You decide to propose new values at random within the interval, without regarding the current value. Explain whether your proposal probability is symmetric.
   Your proposal scheme did not consider the current value. Will your acceptance probability depend on the current value?
   Write out the acceptance probability of moving to value x' if the current value of the Markov chain is x_{now}

(c) You decide instead to propose new values uniform-randomly from within an interval $(x_0 - \delta, x_0 + \delta)$ around the current value, where $0 < \delta < 0.5$. What is the problem when x_0 is close to the interval edges, i.e., $x_0 < \delta$ or $1 - x_0 < \delta$? Is the proposal probability symmetric? Explain how you could avoid this problem by considering the interval to be *periodic*, , i.e., by identifying the point $x = 0$ with the point $x = 1$. Write out pseudocode or a python snippet using the mod operator (%) to demonstrate how the interval is treated as periodic.

(d) It is considered good practice not to take every value from the Markov chain, but allow some steps between samples. Why?

(e) Let's represent the n-th step of the Markov chain as x_n. Explain how you would calculate the auto-correlation function. If you are averaging over something, state very clearly what you are averaging over.

5. Monte Carlo integration.

(a) Describe the idea of approximating an integral, using N numbers from a uniform random number generator.

(b) Derive the expected uncertainty (error) as a function of N.

(c) If your integral is d-dimensional, explain how the error scales with d.

(d) Explain why Monte Carlo integration becomes superior to other methods for large d.

6. Consider the cardoid-shaped region described by the inequality

$$(x^2 + y^2)^2 + 4y(x^2 + y^2) < 4x^2.$$

The cardoid lies entirely within the rectangular region

$$x \in [-3, 3], \quad y \in [-4, 1].$$

(a) Explain how you could calculate the area of the cardioid using a uniform random number generator.
Write this procedure as a step-by-step algorithm or pseudocode.

(b) Explain how you would calculate the center of mass of the cardioid, assuming the mass density to be uniform, using Monte Carlo integration.

(c) The cardiod-shaped area is charged, and carries surface charge density

$$\sigma(x, y) = y^2 \, e^{y-x^2} \ .$$

Explain how you could calculate the total charge carried by the cardioid-shaped area.

(d) *Programming exercise:* Write code to do each of the above.

7. Detailed balance and Metropolis:

(a) Derive the **master equation** for a stochastic process.

(b) Show that detailed balance is a sufficient condition for a stationary distribution.

(c) Show that detailed balance is not **necessary** for a stationary distribution.

(d) Describe the Metropolis algorithm (or Metropolis update rule). Show that the Metropolis update rule satisfies detailed balance.

8. Transition matrix (row stochastic matrix) for a Markov chain

A system has only three states (call them A, B, C). The system follows a Markov process described by the transition matrix

$$T \ = \ \begin{pmatrix} 1/3 & 1/3 & 1/3 \\ 3/4 & 0 & x \\ 1/2 & 1/2 & y \end{pmatrix}$$

(a) Find the transition probabilities which are not given, $x = T_{B \to C}$ and $y = T_{C \to C}$.

(b) If you take a very large sample from the Markov chain, what will be the occupancy probabilities of the three states?

In other words, find the probabilities in the stationary state.

Hint: Left eigenvector corresponding to a certain eigenvalue.

9. Ising model

(a) Write down the Hamiltonian for the ferromagnetic Ising model on a 1D chain with L sites. (The magnetic field term is not necessary.) The limits of your summation should be clearly and correctly written. The spin on site i should be represented as σ_i. What are the possible values that each σ_i can take?

Define the magnetization in terms of the σ_i's.

(b) What is the magnetization as a function of temperature? (You should know the answer from a simulation of the 1D Ising model.)

(c) For the 2D square-lattice ferromagnetic Ising model, sketch a plot of the magnetization as a function of temperature. Point out the temperature at which there is a phase transition.

(d) Consider the magnetic susceptibility χ of the 2D square-lattice ferromagnetic Ising model. Sketch plots of χ against the temperature T, for three different system sizes, say $L = 50$, $L = 100$, $L = 200$. Also sketch on the same plot the $\chi(T)$ curve for the infinite-size system.

(e) Explain the formula used to calculate the susceptibility.

Explain how you can calculate the susceptibility using the data from a Markov chain Monte Carlo simulation.

Explain how this formula for the susceptibility is derived from the definition $\chi = \dfrac{\partial M}{\partial B}$, where B is the magnetic field.

10. Other update rules (Alternatives to Metropolis).

(a) Show that the Glauber update rule satisfies detailed balance. (The update rule is listed in the slides for lecture 5.)

(b) For an Ising ferromagnetic model on a one-dimensional chain, show that the heat bath algorithm provides the same update rule as the Glauber update rule.

(c) You are performing MCMC on a 2D square-lattice Ising model

$$H = -J \sum_{<ij>} \sigma_i \sigma_j - B \sum_i \sigma_i$$

using **heat bath** updates. For the current Monte Carlo step, you have decided to try updating the spin at site α. The four neighbors of this site have spins -1, -1, $+1$, and -1 (three downs and one up).

What are the probabilities of choosing up or down for the spin at site α?

(d) For the previous problem 10c, now imagine that you've decided to do **Metropolis** updates. If the site α currently has spin down, what is the acceptance probability for a flip? If the site α currently has spin up, what is the flip probability?

(Since you've already selected site α for Metropolis, you don't have to worry about the proposal probability, only the acceptance probability.)

11. Transition matrix for a Metropolis Markov chain:

Consider the 2-site Ising model

$$H \;=\; -J\sigma_1\sigma_2 - B(\sigma_1 + \sigma_2)$$

where the two classical spins, σ_1 and σ_2, can each take values ± 1. Let's use the notation $x = e^{-2\beta J}$ and $y = e^{-\beta B}$.

We are performing Markov chain Monte Carlo on this model for inverse temperature β, using the Metropolis algorithm. At every step, one proposes a flip of one of the two spins chosen at random. The state space consists of 4 configurations:

$$A = (+,+) \qquad B = (+,-) \qquad C = (-,+) \qquad D = (-,-)$$

where, e.g., $(+,-)$ means $\sigma_1 = +1$ and $\sigma_2 = -1$.

(a) Write down the 4×4 transition matrix, also known as the row stochastic matrix or the Markov matrix.

Hint 1: In the Metropolis process, a transition probability is the product of the proposal probability and the acceptance probability. Make sure to work out both, for each pair of states.

Hint 2: Each row should sum to 1.

(b) Based on the energies of the 4 configurations, what are the probabilities of these configurations in thermal equilibrium?

(c) Form a row vector combining the probabilities in the stationary (thermal) state.

Explain why you expect this to be the left eigenvector of your stochastic matrix, corresponding to eigenvalue 1.

Check whether this expectation is correct for the vector and the matrix that you have constructed.