Physics 727: Assignment 1

(to be submitted by Tuesday, February 13, 2024)

1. Given a square matrix A of dimension $n \times n$ with all nonnegative entries, prove that A is irreducible if $(I + A)^{n-1}$ has all positive entries.

2. Consider the permutation matrix

$$T = \begin{pmatrix} 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix}.$$

   (a) Draw a directed graph showing how the states $\{|1\rangle, |2\rangle, \ldots, |6\rangle\}$ are reconfigured in each time step. Note that there is no branching. Argue that the effect of T is simply to permute the entries of whatever 6-vector it acts on. You should be able to convince yourself that $T \simeq (1\,5\,3)(2\,4)(6)$, which is the permutation expressed in cycle notation.

   (b) Determine whether T is irreducible. Contrast this with the result for the matrix representation of the permutation $(1\,2\,3\,4\,5\,6)$.

   (c) Determine whether T describes a stochastic process that is periodic; if so, determine the period by finding the smallest interger $k > 1$ such that $T^k = I$.

   (d) Are there subspaces of smaller periodicity than what you reported in question 1(d)? If so, what are they?

   (e) Imagine that all the zero entries of T are replaced by a small postive value $0 < \epsilon \leq 1/5$ and that all the unit entries are reduced accordingly to maintain the stochastic property:

$$T \to T_\epsilon = \begin{pmatrix} \epsilon & \epsilon & \epsilon & \epsilon & 1-5\epsilon & \epsilon \\ \epsilon & \epsilon & \epsilon & 1-5\epsilon & \epsilon & \epsilon \\ 1-5\epsilon & \epsilon & \epsilon & \epsilon & \epsilon & \epsilon \\ \epsilon & 1-5\epsilon & \epsilon & \epsilon & \epsilon & \epsilon \\ \epsilon & \epsilon & 1-5\epsilon & \epsilon & \epsilon & \epsilon \\ \epsilon & \epsilon & \epsilon & \epsilon & \epsilon & 1-5\epsilon \end{pmatrix}.$$

   Show that T_ϵ is aperiodic and irreducible (and hence ergodic).

   (f) Report the long-time equilibrium distribution $\pi^\star = \lim_{k\to\infty} (T_\epsilon)^k \pi^{(0)}$.

   (g) Speculate as to why even an infinitesimal value of ϵ is enough to restore ergodicity to the stochastic matrix.

   (h) What can you say about the timescale for the system to equilibrate and how it depends on ϵ? For instance, if you have two such stochastic systems, one with $\epsilon = 0.01$ and one with $\epsilon = 0.02$, how would the equilibration times compare?

3. Consider the matrix

$$\begin{pmatrix} 1/2 & 1/3 & 1/6 \\ 1/3 & 1/6 & 1/2 \\ 1/6 & 1/2 & 1/3 \end{pmatrix}$$

   (a) List the properties that make T a doubly stochastic matrix.

   (b) Draw a directed graph showing how the states $\{|1\rangle, |2\rangle, |3\rangle\}$ are reconfigured in each time step. Label the branching probabilities.

   (c) Determine whether T is irreducible.

(d) Determine whether T describes a stochastic process that is periodic; if so, determine the period by finding the smallest interger $k > 1$ such that $T^k = I$.

(e) Report the long-time equilibrium distribution $\pi^\star = \lim_{k\to\infty} T^k \pi^{(0)}$.

(f) Show that it takes about 30 time steps for the system to equilibrate from an initial state $\pi_i^{(0)} = \delta_{i,2}$ to agreement with the final distribution $\pi^\star$ at the 1 in 10^{16} level (double-precision floating point accuracy on a computer).

4. Consider an n-state system in equilibrium. Each state $i = 1, 2, \ldots, n$ is distributed according to probability π_i and has associated with it an energy ε_i and a particle occupancy N_i

(a) Suppose that the system is isolated from its environment so that the total energy $U = \sum_i \varepsilon_i \pi_i$ and total particle number $N = \sum_i N_i \pi_i$ are both held fixed. Augment the entropy $S = -\sum_i \pi_i \ln \pi_i$ with Lagrange multiplier terms in order to enforce the conservation of energy and particle number. Show that maximizing the entropy results in $\pi_i = Z^{-1} \exp(-\beta\varepsilon_i + \alpha N_i)$, where the normalization is given by the partition function $Z = \sum_i \exp(-\beta\varepsilon_i + \alpha N_i)$. (More commonly, one sees the expressions $Z = \sum_i \exp[-\beta(\varepsilon_i - \mu N_i)]$, with the correspondence $\alpha = \beta\mu$.)

(b) Using the result of part (a), prove that the entopy can be expressed as $S = \ln Z + \beta U - \alpha N$ (or $S = \ln Z + \beta U - \beta\mu N$).

(c) Let's treat small variations $\pi_i \to \pi_i + \delta\pi_i$. Show that those variations obey $\sum_i \delta\pi_i = 0$ and lead to changes $\delta U = \sum_i \varepsilon_i \delta\pi_i$ and $\delta N = \sum_i N_i \delta\pi_i$ in the total energy and particle number.

(d) Demonstrate that such variations in the entropy are related to independent variations in the energy and particle number according to $\delta S = \beta\delta U - \alpha\delta N$. Hence, the entropy $S = S(U, N)$ has partial derivatives $\beta = \partial S/\partial U$ and $\alpha = -\partial S/\partial N$ (or $\mu = -\beta^{-1}\partial S/\partial N$)

5. Start from the partition function $Z(\beta, \alpha) = \sum_i \exp(-\beta\varepsilon_i - \alpha N_i)$ in question 4 and define an expectation value operation

$$\langle \cdot \rangle = \frac{1}{Z} \sum_i (\cdot) \exp(-\beta\varepsilon_i - \alpha N_i).$$

For a statistical ensemble in which β and α are the control parameters, the internal energy and total particle number fluctuate about their average values. Show that such fluctuations are given by

$$\langle (\Delta E)^2 \rangle = \langle E^2 \rangle - \langle E \rangle^2 = \frac{\partial^2 \ln Z}{\partial \beta^2}$$

and

$$\langle (\Delta N)^2 \rangle = \langle N^2 \rangle - \langle N \rangle^2 = \frac{\partial^2 \ln Z}{\partial \alpha^2}.$$

N.B.: $z = e^\alpha$ is often referred to as the fugacity; both α and z are dimensionless. The chemical potential $\mu = \alpha/\beta$ is a rescaled quantity having units of energy (the energy required to add or remove one particle from the equilibrated system). It is more common to express the Boltzmann factor as $\exp(-\beta\varepsilon_i + \alpha N_i) = \exp[-\beta(\varepsilon_i - \mu N_i)]$.