Statistical Physics: Project Overview and Detailed Guidance

Overview: During the second phase of the course, you are invited to participate in a 3-4 persons group research and presentation on a selected topic in statistical physics. You will give your presentation online during the werkcollege block on **Wed May 20th**, and these will be recorded and made available for the rest of the class to see. Each group member will individually present part of the project and will be graded on both topic understanding and presentation quality. The presentations should be structured as an introduction to your classmates and be created using Powerpoint, Keynote or similar software. A guide to giving a good talk is also given in the references. Your group members can be from any werkcollege section and you are to organize a group and topic by the end of **Wed, April 22nd.** Please send an email of your team membership and your first and second topic choices to Rosa Sinaaseappel: **rosa.sinaasappel@gmail.com**.

We have identified project ideas and related questions as outlined below and references are given in our class dropbox link. Each topic is limited to a maximum of 5 groups on a first-come basis. This is a chance to explore ideas in statistical physics that most interest you and that we cannot cover in lecture and we hope that you have fun! While any of the course staff can help you with basic project questions, we have designated the following particular experts: Ruben (Statistical physics in the early universe, Interacting particles and melting transitions), Greg (Renormalization group and Ising model), Ryan (The Ising model in 2D, Principal components, low-dimensionality and the Ising model), Dion (Brownian motion, Chaos ergodicity and fractals), Daan (Langevin in a cell, Polymers and random works), Rosa (Chaos, ergodicity and fractals, Zombie apocalypse).

Project: Statistical physics in the early universe

OBJECTIVE: To learn about the Boltzmann and Saha equations and how to numerically solve ordinary differential equations (ODE's). To simulate a random walk of photons and the diffusion equation in spherical coordinates. To study Fermi degenerate gas example.

Cosmology and astrophysics use many results of statistical physics. Discuss thermal evolution in the early universe and electron decoupling in particular. Define the time of first atom formation and the relic density of electrons in the universe using the Boltzmannn equation and the Saha equation. Simulate a random walk of photons passing through stellar matter and compute how long will it take for photon to reach the surface. Study a simple model of a white dwarf star based on a Fermi gas..

1. After the big bang and a short inflationary era, the evolution of the early universe can be described by local thermal equilibrium. Fortunately for us, because of particle decoupling the equilibrium was interrupted, which led to formation of our universe. One of the remarkable events that happened at that time was electron decoupling. At this time first atoms were formed. Define the time of first atom formation (time of decoupling) and the relic density of electrons in the universe after the first atoms formation. It is a good idea to start with a short discussion of thermal equilibrium in the early universe, as well as, of particle decoupling, it's conditions and why there is relic density left.

   In general, when thermal equilibrium is not satisfied, the number density evolves through the Boltzmann equation:

   $$\frac{1}{a^3}\frac{d(n_i a^3)}{dt} = C_i(n_j) \tag{1}$$

   where i labels the particle species, n_i is the particle number density, a is scale factor of the universe expansion and C_i is a collision term arising from interactions.

   Electrons are in the equilibrium with baryons via reactions such as:

   $$e^- + p^+ \rightarrow \gamma + H$$

   In this case, the Boltzmann equation for electron density can be written as:

   $$\frac{1}{a^3}\frac{d(n_e a^3)}{dt} = -\langle\sigma v\rangle \left(n_e^2 - (n_e^{eq})^2\right)$$

   where $\langle\sigma v\rangle$ is an average recombination cross section and n_e^{eq} us equilibrium electron number density. Using $n_e = X_e n_b$, where n_b is the baryon density; $n_b a^3 = const$; $x \equiv B_H/T$ one can rewrite the previous equation as:

   $$\frac{dX_e}{dx} = -\frac{\lambda}{x^2}[X_e^2 - (X_e^{eq})^2]$$

   where $\lambda \equiv \frac{n_b<\sigma v>}{xH}|_{x=1} = 3.9 \times 10^3(\frac{\Omega_b h}{0.03})$, $H \equiv \frac{\dot{a}}{a}$ is Hubble'a constant, h is the reduced Hubble constant, $\Omega_b = 0.05$ is the baryon density parameter and $B_H \equiv m_p + m_e - m_H$ is the binding energy of hydrogen.

Another way to describe electron density is to introduce the Saha equation, which is not suitable for defining the relic density, but does correctly predict the decoupling time.

Start with the definition of the number density of non-relativistic particles **in equilibrium**:

$$n_i^{eq} = g_i(\frac{m_i T}{2\pi})^{3/2} \exp{(\frac{\mu_i - m_i}{T})}$$

where g_i is the number of internal degree of freedom (find yourself how to calculate them). Now derive the Saha equation:

$$\left(\frac{1-X_e}{X_e^2}\right)_{eq} = \eta_b \frac{2.4}{\pi^2}\left(\frac{2\pi T}{m_e}\right)^{3/2} e^{B_H/T} \tag{2}$$

Hint: $n_b = \eta_b n_\gamma = \eta_b \times \frac{2.4}{\pi^2} T^3$, where $\eta_b \approx 10^{-9}$ is the baryon-to-photon ratio.

Another hint: $\mu_e + \mu_p = \mu_H$ (recall that $\mu_\gamma = 0$ since a photon is it's own antiparticle). To get rid of the μ dependence consider next ratio:

$$(\frac{n_H}{n_e n_p})_{eq}$$

Note also that the universe is electrically neutral.

2. Plot both the Boltzmann and Saha equation solutions with respect to inverse temperature in the range $10\ eV\ -\ 0.01\ eV$ on a log scale ($X_e = f(1/T)$). Compute the temperature of first atom formation. Translate this temperature to a time. What is the relic density of electrons?

   As reference values use $T_f = \mathcal{O}(10^{-1})eV$, $X_{e,relic} = \mathcal{O}(10^{-4})$.

   Note: you can use the Python method scipy.odeint to solve ODE's.

3. Random walks of photons

   Now let's move to another application of statistical physics in cosmology and astrophysics and talk about behavior of photons inside the Sun. As an approximation a star can be described as a huge volume of gas. Photons inside the star have to diffuse to escape.

   (a) The diffusion equation for photon density u_γ is:

   $$\frac{\partial u_\gamma}{\partial t} - \frac{c}{3\rho\kappa}\nabla^2 u_\gamma = 0 \tag{3}$$

   where c is the speed of light in vacuum, ρ is average medium density and $\kappa = \frac{\sigma_{Th}}{m_p} = 4 \times 10^{-2} m^2 kg^{-1}$), ($\sigma_{Th}$ is cross section of Thompson scattering). Assuming that $u_\gamma(x, 0) = \delta(x)$ where $x \in R^3$, find fundamental solution of diffusion equation. Compute $\langle r^2 \rangle(t) = \int_0^\infty r^2 u_\gamma(r, t) dV$. Calculate using your estimated $< r^2 >$ how long it will take to reach the surface of the Sun, if the photon was initially exactly in the middle.

(b) One can also describe photons in the Sun as a random walk. Assuming that the photon undergoes on average 8×10^{20} collisions with stellar matter and that it's mean free path is 1.8 cm, simulate it's path to the surface as a random walk. For the simulation build a square lattice and start the photon in the middle. There is no need to build an extremely large lattice. You can take a much smaller lattice (size depending on your computational abilities) and interpolate your averaged result onto real number of collisions that photon undergoes. How long will it take to reach surface in this case? Is your result comparable with previous answer ? Note: $\mathcal{O} = 10^3$ seconds off is okay.

4. White Dwarves (adapted from "Statistical mechanics: entropy, order parameters and complexity" by James P. Sethna)

   Stellar matter can be modelled as a Fermi sea of non-interacting electrons, with enough nuclei to balance the charge. Model a white dwarf as a uniform density of He^4 nuclei and a compensating uniform density of electrons, assuming Newtonian gravity and that chemical energy is given solely by the energy of a gas of non-interacting electrons (filling the levels to the Fermi energy).

   (a) Calculate the energy of a sphere with N zero-temperature non-relativistic non-interacting electrons and radius R. Calculate the Newtonian gravitational energy of a sphere of He^4 nuclei of equal and opposite charge density. At what radius is the total energy minimized?

   (b) Calculate the Fermi energy of the electrons in a white dwarf star of the mass of the Sun, assuming that it is composed of helium. Compare it to temperature inside the star, mass of electron. Can we assume that the electron gas is degenerate? Can we say that electrons are non-relativistic?

   (c) Assuming extremely relativistic electrons with $E = pc$, calculate the energy of a sphere of non-interacting electrons. Calculate M_0 at which electron energy is balanced with gravitational energy. Compare M_0 to the mass of Sun.

Project: The Ising model in 2D

OBJECTIVE: To learn about the 2D Ising model of ferromagnetism and to build simple Metropolis Monte Carlo simulations. Also familiarity with the exact solution of 2D Ising lattice from Onsager. Explore critical exponents and how to calculate them. Correlation time of the system.

Using Monte Carlo or other computational methods, numerically simulate the Ising model in 2D. Compare your results with the exact solution. Calculate critical exponents. Calculate the correlation time of the system.

Start with discussing 2D Ising model and the Metropolis algorithm for computational sampling of spin configurations.

1. Simulate a (relatively small) 2D Ising lattice (20×20) at different temperatures T, both below and above the critical temperature. Estimate the size of the average cluster at each temperature. Use your simulations to estimate the critical temperature. Also compute the average energy and heat capacity as a function of T.

   Onsager's exact solution in the absence of an external magnetic field is:

   $$F = -kT \ln Z, \tag{1}$$

   where $Z = \lambda^N$ and

   $$\ln \lambda = \ln(2 \cosh 2\beta J) + \frac{1}{\pi} \int_0^{\frac{\pi}{2}} dw \ln[\frac{1}{2}\{1 + (1 - K^2 sin^2 w)^{1/2}\}]$$
   $$K = \frac{2 \sinh(2\beta J)}{(\cosh(2\beta J))^2}$$

   and N is the size of the square lattice.

2. Discus the different critical exponents (α, β, γ, δ, ν, η). Try to estimate these exponents from your simulations and compare against exact results (which you can find online). Note: not all critical exponents are relevant for the case we are considering, i.e. with zero external magnetic field.

3. How do your previous results change if you change the connectivity (number of neighbours) of the 2D lattice? I.e. how do your results change if you consider a hectagonal or triangular lattice instead of a square lattice?

4. Calculate the correlation time of the system by examining the magnetization autocorrelation function, at different temperatures. What happens as you approach the critical temperature? The autocorrelation function is defined as:

   $$c(t) = \frac{\sum_{i=1}^{N-t} (\langle M(t+i)M(i) \rangle - \langle M \rangle^2)}{(N-t)(\langle M^2 \rangle - \langle M \rangle^2)} \tag{2}$$

where the average is over both lattice points and the time index $\{i = 1 : N - t\}$. (A possibly nice reference for this is http://itf.fys.kuleuven.be/~fpspXIII/material/Barkema_FPSPXIII.pdf).

5. Change the lattice size (for example 10×10, 50×50, 100×100) and plot the magnetization with respect to temperature. Compare with theoretical prediction. How does your result depend on the lattice size?

Project: Renormalization group and Ising model
(adapted from Schroeder "Introduction to Thermal Physics")

OBJECTIVE: To learn the basics of renormalization group transformations. Explore the 1D and 2D Ising model and investigate its behavior at different temperatures. Use renormalization group technique and investigates differences in behavior compared to the original Ising lattice.

The renormalization group transformation is an extremely useful tool and powerful concept in physics, which can teach us why we see such universal behavior in models: under the renormalization group, they can be seen to transform into the same effective model. Here, we will only illustrate transforming one version of the Ising model into another.

The basic idea of renormalization group technique is to perform partial evaluation of partition functions, by 'scaling up' and forgetting part of the microscopic degrees of freedom. Renormalization group transformation for a 1D Ising model is described below. 1D Ising model is described by next Hamiltonian:

$$\mathcal{H} = -J \sum_i S_i S_{i+1} \tag{1}$$

where $J > 0$. The canonical partition function is described:

$$\begin{aligned} Z &= \sum_{\{S_i=\pm 1\}} e^{-\mathcal{H}/kT} \\ &= \sum_{\{S_i=\pm 1\}} \prod_i e^{JS_iS_{i+1}/kT} \end{aligned} \tag{2}$$

Let's rescale our variable $J/kT \equiv K$.
One can sum partition function over to perform partial evaluation, for example, odd spins. This is called decimation.

$$Z = \sum_{\{S_{2i}=\pm 1\}} \prod_i \Big(\sum_{S_a=\pm 1} e^{K(S_{2i}S_a + S_aS_{2i+2})} \Big) \tag{3}$$

If this seems complicated, convince yourself with an example system of 5 or 6 spins.
Interaction is possible only between contiguous spins, so sums can be evaluated separately. After summation only even spins are left:

$$\begin{aligned} \sum_{S_a=\pm 1} e^{K(S_{2i}S_a + S_aS_{2i+2})} &= e^{K(S_{2i}+S_{2i+2})} + e^{-K(S_{2i}+S_{2i+2})} \\ &= 2cosh(-K(S_{2i} + S_{2i+2})) \end{aligned} \tag{4}$$

Let's now prove that summation over odd spins leads to interaction of the same form as (1) but with new constant K'.

$$Z = \sum_{\{S_{2i}=\pm 1\}} \prod_i 2cosh(-K(S_{2i} + S_{2i+2})) \equiv \sum_{\{S_{2i}=\pm 1\}} \prod_i z(K) e^{K' S_{2i}S_{2i+2}} \tag{5}$$

We want $2cosh(-K(S_{2i} + S_{2i+2})) = z(K)e^{K'S_{2i}S_{2i+2}}$ for every S_{2i} and S_{2i+1}. That way our new partition function again describes an Ising model.
Let's look at all possible configurations for S_{2i} and S_{2i+1}:

$$S_{2i} = +1, S_{2i+2} = +1 \Leftrightarrow z(K)e^{K'n} = 2cosh(2K) \tag{6}$$

$$S_{2i} = -1, S_{2i+2} = -1 \Leftrightarrow z(K)e^{K'} = 2cosh(2K) \tag{7}$$

$$S_{2i} = -1, S_{2i+2} = +1 \Leftrightarrow z(K)e^{-K'} = 2 \tag{8}$$

$$S_{2i} = +1, S_{2i+2} = -1 \Leftrightarrow z(K)e^{-K'} = 2 \tag{9}$$

You can solve these equations to find $K' = \frac{1}{2}\log(\cosh(2K))$.
This equation is called recursion relation for the coupling constant.

1. Derive recursion relations for 1D Ising model. Plot this relation, similar to the way you have plotted the mean-field consistency condition.

2. Start from a K of 0.9, and repeatedly carry out the recursion relation. Where does the coupling constant end up? How many iterations before it changes by a factor 10? This map has two fixed points, describe them. Which one is 'attractive'?

3. Argue what it means to repeatedly perform decimation, both physically, and in this equation. What do you expect the behavior of the 1D Ising model to be on very large length scales, in terms of temperature?

4. We move to the 2D Ising model. As you know, the 2D model exhibits a phase transition, where the 1D case does not. This can be seen from the renormalization group. Describe the procedure of the Migdal-Kadanoff approximation, and give its recursion relation. It will be similar to the 1D case, but there is a difference. Using the language of attractive and repulsive fixed points, explain why the 2D case has a phase transition. At what value of K does this occur? What is the relation between J and T_c, the temperature at the critical point? Remember this is only an approximation.

5. Simulate a 2D Ising lattice (90×90), for instance using the metropolis algorithm. Then split the initial lattice into blocks of 3×3. Replace each set of 9 spins with 1 renormalized spin using "majority rule", i.e. when more then half spins are down, the new spin is down. This will reduce lattice to 1/3 of it's size and the transformation itself is a version of a renormalization group transformation. Generate states of the large lattice at temperatures below and above T_c. Check the distribution of energies after scaling and try to infer what the temperature is of this new system, pretending J is the same for both. What happens to the temperature? When does it increase, when does it decrease with the transformation? What is the relation?

Project: Interacting particles and melting transitions

(based on Chapter 9: Molecular dynamics,
"Computational Physics" by NJ Giordano)

OBJECTIVE: To learn about the Lennard-Jones interaction and molecular dynamics simulations. Familiarity with the Verlet algorithm for solving equations of motion. Explore equilibrium properties of a dilute gas and through distributions of velocity and speed. Simulations of phase transitions: condensing and melting.

In theoretical physics, we always prefer to simplify systems, to make them non-interacting, i.e. ideal. However, in real life one faces interactions between system components and these can have profound consequences. Intermolecular interactions, for example, can be described by a Lennard-Jones potential. Simulate particles motion in dilute gas using the Verlet algorithm and calculate the velocity and speed distributions. Simulate condensing and melting transitions. Investigate total energy and temperature changes, as well as, mean square distance change between particles during melting transition.

Start with short overviews of interparticle interactions, specifically, talk about Lennard-Jones potential.

1. Interactions between molecules can be modeled by the Lennard-Jones potential:

$$V(r) = V_0\big[\big(\frac{r_0}{r}\big)^{12} - 2\big(\frac{r_0}{r}\big)^{6}\big], \tag{1}$$

where the associated force is $F = -\nabla V(r)$. Thus, each i^{th} particle in the system moves according to Newton's equation of motion which in two dimensions are:

$$\frac{dv_{i,x}}{dt} = a_{i,x}\,;\ \frac{dx_i}{dt} = v_{i,x}$$

$$\frac{dv_{i,y}}{dt} = a_{i,y}\,;\ \frac{dy_i}{dt} = v_{i,y}$$

$$a_{i,x} = \frac{1}{m}\sum_{k\neq i} f_{k,i} cos\theta_{k,i}$$

$$a_{i,y} = \frac{1}{m}\sum_{k\neq i} f_{k,i} sin\theta_{k,i}$$

where $f_{k,i} = -\nabla V(r_{ki})$ is a force of k^{th} particle on i^{th} particle and $\theta_{k,i}$ angle that line between i^{th} and k^{th} particles makes with x axis.

To solve for the motion of the system it is common to use either the Euler or Verlet algorithm. Here we will use Verlet, since it is characterized by good numerical stability and can be used for simulating systems with energy conservation.

Let's write the Taylor expansion of a position vector in time:

$$\vec{x}(t+\delta t) = \vec{x}(t) + \frac{d\vec{x}(t)}{dt}\delta t + \frac{d^2\vec{x}(t)}{dt^2}\frac{\delta t^2}{2} + \frac{d^3\vec{x}(t)}{dt^3}\frac{\delta t^3}{6} + \mathcal{O}(\delta t^4)$$

Analogously,

$$\vec{x}(t-\delta t) = \vec{x}(t) - \frac{d\vec{x}(t)}{dt}\delta t + \frac{d^2\vec{x}(t)}{dt^2}\frac{\delta t^2}{2} - \frac{d^3\vec{x}(t)}{dt^3}\frac{\delta t^3}{6} + \mathcal{O}(\delta t^4)$$

Then basics of Verlet algorithm can be written as:

$$\vec{x}(t+\delta t) = 2\vec{x}(t) - \vec{x}(t-\delta t) + \frac{F(t)}{m}\delta t^2 + \mathcal{O}(\delta t^4)$$

One can approximate the velocity as

$$\vec{v(t)} = \frac{\vec{x}(t+\delta t) - \vec{x}(t-\delta t)}{2\delta t} + \mathcal{O}(\delta t^3)$$

so that

$$\vec{x}(t+\delta t) = \vec{x}(t) + \vec{v}(t)\delta t + \frac{F(t)}{2m}\delta t^2 + \mathcal{O}(\delta t^4)$$

and

$$\vec{v}(t+\delta t) = \vec{v}(t) + \frac{F(t+\delta t) + F(t)}{2m}\delta t$$

(a) Define r_0 in (1).

(b) Make a 2D lattice of 16 atoms of Argon in a box with distances between atoms of more then $2r_0$ (dilute gas) in a box with **special periodic conditions**. Use reduced units ($u_0 = 1, r_0 = 1, m_{Ar} = 1$) to measure distances etc. Simulate the motion of particles under a Lennard-Jones potential using the Verlet integration algorithm.

Special periodic conditions imply that when particle reaches a wall it automatically appears from the other side with same direction of motion and speed (see Fig. 1).

(c) Estimate the probability distributions of speed and velocities of particles. Show that system reaches thermal equilibrium. What is the temperature here? Plot the temperature as a function of time.

2. Now let's investigate condensation. Make a lattice of 10×10 particles with lattice separation r_0. Initially the particles are static, but they move according to Newton's laws, once you start the simulation.

(a) Make pictures of particles configuration at different times. What change do you observe? What is the final structure of your lattice? Discuss the physical meaning of your result.

(b) Plot the averaged total energy and temperature changes of your system with respect to time. What does the energy distribution tell you about the properties of the Verlet algorithm? Can you estimate the approximate uncertainty of the Verlet method from your result?

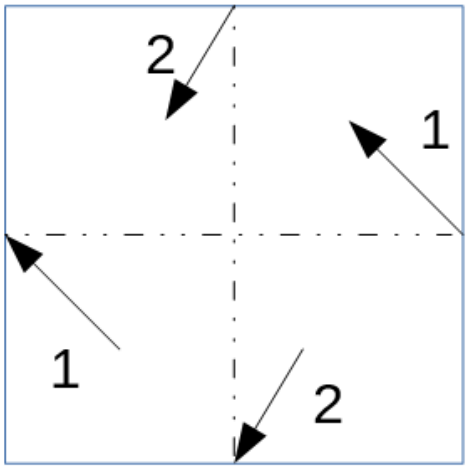

Figure 1: Periodic condition for Argon atoms in the box. When atom of Argon reaches walls of the box it automatically appears from the other side with same direction of motion and the same speed.

3. Next we'll investigate the opposite situation - the melting transition. To simulate melting one has to increase the kinetic energies of the particles manually.

   To rescale velocities one has to carefully rescale the positions of the particles in the Verlet algorithm. If $\vec{x_p}$ is the previous position and $\vec{x_c}$ is the current position, then we can manually rescale position like:

$$\vec{x}_c \to \vec{x}_c - R(\vec{x}_c - \vec{x}_p) \tag{2}$$

   where R is a velocity rescale factor.

   (a) Simulate the lattice for R=2 and Show how the particle configuration changes with time.

   (b) Estimate the averaged total energy and the time dependence of the temperature. Discuss your results.

   (c) Pick 2 random atoms and calculate their mean square displacement with time. Can you explain the fluctuations on a long-time scale?

   (d) Discuss the order of the melting phase transition.

Project: Principal Components, Low-dimensionality and the Ising Model

OBJECTIVE: Understand Ising model and be able to build a simple Monte Carlo generator to computationally sample spin configures. Introduction to Principal Components Analysis (PCA) and the covariance matrix. Explain order parameters.

At a critical temperature T_c, the Ising system undergoes a phase transition from order to disorder. The magnetization of a ferromagnetic state at $T < T_c$ falls to 0 at $T > T_c$ (paramagnetic state). Simulate an Ising 2D lattice using the Metropolis algorithm at different T near T_c. Using these spin configurations across all temperatures calculate the covariance matrix. Perform Principal Components Analysis by computing the eigenvalues and eigenvectors of the sampled covariance matrix. Calculate the mean magnetization per site and discuss why it can be used as an order parameter of phase transition.

1. Read the notes on Gaussian distributions and PCA and complete the simple covariance matrix exercise. Note also the attached reference on PCA.

2. To gain some practical experience with PCA in an interesting physical system, consider the prototypical classical Ising model with Hamiltonian

$$H = -J \sum_{(i,j)} \sigma_i \sigma_j,$$

where the spins take two values $\sigma_i = \{-1, +1\}$. Consider the model on a square lattice with periodic boundary conditions and set $J = 1$ as the energy unit. The system undergoes a phase transition at a temperature $T/J = 2/ln(1 + \sqrt{2})) \approx 2.269$ where a discrete Z_2 spin inversion symmetry is broken in the ferromagnetic phase below T_c and is restored in the disordered phase at temperatures above T_c. Write your own Monte Carlo simulation to generate 1000 uncorrelated spin configuration samples at 14 different temperatures $T/J = 1.6, 1.7, \ldots 2.9$ spanning the transition temperature. Collect the spin configurations into an $M \times N$ data matrix where $M = 14000$ is the total number of samples, and N is the number of lattice sites (N doesn't matter too much in this exercise, perhaps $N = 10^2$. How can you tell that your simulations are at least qualitatively correct?

3. Recall from the notes that covariance is a measure of strength of correlation of two sets of multi-dimensional random variables (link). When the mean of each random variable is zero, the covariance matrix can be constructed as:

$$C_X = \frac{1}{M} \boldsymbol{X} \boldsymbol{X}^{\boldsymbol{T}} \tag{1}$$

where N=100, $\boldsymbol{X}$ - data matrix $M \times N$

   (a) Describe the properties of covariance matrix.

   (b) Calculate the covariance matrix of your sampled data sets.

4. Let's try to find the biggest variation line using Principal Component Analysis (PCA) or in other words diagonalize covariance matrix and find biggest eigenvalue using PCA.

Our aim is to find a transformation $\boldsymbol{P}$ such that $Y = \boldsymbol{P}X$, and in the new coordinates,

$$\boldsymbol{C_Y} = \frac{1}{n}\boldsymbol{Y}\boldsymbol{Y^T} \tag{2}$$

is diagonal (we again assume that the mean of each random variable is either zero or subtracted away and n is the total number of samples).

The rows of $\boldsymbol{P}$ are called "principle components" of $\boldsymbol{X}$ and are eigenvectors of $\boldsymbol{C_X}$. Diagonal values of $\boldsymbol{C_Y}$ correspond to variance of C_X along i^{th} $\boldsymbol{P}$ row.

5. Apply PCA to the Ising data and examine the resulting eigenvalue spectrum of the covariance matrix. Is the data low-dimensional? Describe the eigenvector with the largest eigenvalue. Does it make sense?

6. Now calculate average magnetization per site using sampled data and plot it's temperature dependence:

$$m = \frac{1}{N}\sum_i \langle s_i \rangle \tag{3}$$

   (a) Why is average magnetization per site a useful order parameter?

   (b) Explain why equilibration time (time to reach thermal equilibrium) rises close to T_c (critical slow down phenomena). Plot magnetization time dependence.

7. Extra: Prove that eigenvalues of covariance matrix are equal to variance of eigenvectors.

Project: Brownian motion

OBJECTIVE To get acquainted with Brownian motion through the Langevin equation and numerics. Compare analytic and numeric solutions. Find spectral density of rapid random force. To check short- and long-time behavior.

1. Start by reading the Brownian&Langevin review. What was Einstein's contribution to the theory of Brownian dynamics?

2. Brownian motion in a medium is a well-known example of a stochastic process, and can be described by a particle experiencing both a frictional and random force

$$\frac{dx(t)}{dt} = v(t) \tag{1}$$
$$m\frac{dv(t)}{dt} = -\gamma v(t) + \xi(t), \tag{2}$$

   where $x(t)$, $v(t)$ and m are the Brownian particle position, velocity and mass, and γ is a friction coefficient. The density fluctuations in the medium are represented through $\xi(t)$, a random force. Solve the above equation of motion for the case of no random force. Does the particle behave as if it's in thermal equilibrium?

3. Assume that $\xi(t)$ is a rapid fluctuating and random driving force described by its first and second moments:

$$\langle \xi(t) \rangle_\xi = 0 \tag{3}$$
$$\langle \xi(t_1)\xi(t_2) \rangle_\xi = g\delta(t_2 - t_1), \tag{4}$$

   where the average is given with respect to Gaussian distribution and g is the strength of the force. Find the power spectral density of the random driving force by performing a Fourier transform of the correlation function $\langle \xi(t)\xi(0) \rangle$. What do we call a force with such a spectrum?

4. Now, we are going to simulate a Brownian particle numerically. We will work in the approximation of *overdamped* motion, meaning that $m\frac{dv(t)}{dt} = 0$. This corresponds to a particle in an infinitely viscous (thick, syrupy) fluid. Equation 2 becomes

$$\frac{dx(t)}{dt} = \frac{1}{\gamma}\xi(t). \tag{5}$$

   Numerically integrating functions including stochastic (random) elements such as $\xi(t)$ is a whole topic unto itself. In this case, the correct numerical integration scheme for $x(t)$ is

$$x[t_{i+1}] = x[t_i] + \frac{\chi[t_i]}{\gamma}\sqrt{g\Delta t},$$

   where $\chi[t_i]$ is a **normally distributed** random number (i.e. drawn from a Gaussian with mean 0 and variance 1) generated at each step i. Show numerically that the mean

square displacement of the Brownian particle is:

$$\langle (x(t) - x(0))^2 \rangle = \frac{2kT}{\gamma} t. \tag{6}$$

To get the prefactor, you have to use the expression for g that can be found in the Brownian & Langevin review. Make sure your timestep Δt is small enough so that it doesn't affect your results.

5. A possible extension is to redo the numerical experiment, but in a potential

$$V(x) = x^2. \tag{7}$$

First, update Equation 5 and the integration scheme, keeping in mind that $f(x) = -\frac{dV(x)}{dx}$. Plot the distribution (histogram) of the particle's position, $p(x)$. Is it what you expect?

Project: Langevin motion and ion crossing a cell

Based on LS Liebovitch and FP Czegledy, Ann. Biomed. Eng., Vol.20, pp 517-531 (1992).

OBJECTIVE: Student should get acquainted with Langevin equation and integration techniques to solve equation of motion (Verlet algorithm) with white noise as a random external force. Student investigates model of ion crossing a cell wall, draws phase-space portrait of ion. Student calculates average kinetic energy, finds ion velocities distribution.

The Langevin equation of motion describes Brownian particle kinetics. It can be also used to describe ions that enter or exit a cell. Using information given in a guidance to the project solve the Langevin equation for an ion numerically. Draw phase-space portrait of the motion, calculate it's average kinetic energy and the velocity distribution function.

Start with discussion about Brownian motion and Langevin equation.
To correctly depict Brownian motion in a medium one can use a classical Newtonian mechanics and write down so called Langevin equation of motion:

$$m\frac{d^2\vec{x}}{dt^2} + \gamma\frac{d\vec{x}}{dt} = \vec{F} \tag{1}$$

Langevin equation depicts motion of particle in a medium with friction γ under applied random force F.
Force can be written down as: $\vec{F}(x) = -\nabla V(x) + \vec{f}(x,t)$, where V is a background potential, $\vec{f}(x,t)$ is a random force with $\langle\vec{f}(x,t)\rangle = 0$

1. Langevin equation can be used to describe ion motion in/out cell in a protein channel. Two different ion states (channel is closed/ channel is open) correspond to two minimum in the potential. Assume next potential with two minimum:

$$V(x) = -\frac{x^2}{4} + \frac{x^4}{8} \tag{2}$$

   Forces that act on ion are listed below:

   1. frictional force $\gamma\frac{d\vec{x}}{dt}$;
   2. potential gradient force ∇V;
   3. environment influence $\vec{f}$.

   From now on, we are going to consider that the dimensionality of our space is one. For the environment influence force we will assume white noise that can be described as

$$\langle f(t_1)f(t_2)\rangle = 2D\gamma^2\delta(t_2 - t_1) \tag{3}$$

   where D - diffusion coefficient (see Einstein relation).

   Use $\gamma = 0.19$ and some adequate m.

   To find trajectory of a particle one has to integrate the equations of motion. We said that f is a random force, so it does not have a specific form. So, in every step we have to

sample it from a normal distribution. More specifically in order to numerically integrate (1) we have to employ the following solver:

$$\begin{aligned} x[i+1] &= x[i] + \Delta t\ v[i] + A[i] \\ v[i+1] &= v[i] + \frac{1}{2}\Delta t\ \left(\mathcal{F}_p(x[i+1]) + \mathcal{F}_p(x[i])\right) - \frac{\gamma}{m}\left(A[i] + \Delta t v[i]\right) + \sqrt{2D\gamma^2\Delta t}\ \chi[i] \end{aligned} \tag{4}$$

where $A[i]$ is

$$A[i] = \frac{1}{2}\Delta t^2\left(\mathcal{F}_p(x[i]) - \frac{\gamma}{m}v[i]\right) + \sqrt{2D\gamma^2}\Delta t^{3/2}\left(\frac{1}{2}\chi[i] + \frac{1}{2\sqrt{3}}\theta[i]\right) \tag{5}$$

and $\mathcal{F}_p$ is

$$\mathcal{F}_p = -\frac{dV}{dx} \tag{6}$$

The term $-\frac{dV}{dx}$ is the way $-\nabla V$ looks in one dimension. The variables χ and θ are the ones we draw from the normal distribution with zero mean and unit variance.

Simulate the motion of the ion with initial conditions $x(0) = v(0) = 0$ and take $t_{max} = 500s$. Plot the dependence of particle position on time. Repeat it 100 times and define the average period of an open channel.

2. Now, we want to visualize the movement of the ion in *phase space*, i.e. the (x, p)-plane ($p = mv$ is the momentum). Simulate the motion of the ion and plot a couple of trajectories in phase space for different values of T (the motion of the ion depends on T via the diffusion constant D, see above). Do the trajectories look like you expect?

3. Calculate the average kinetic energy of the ion and discuss the principle of equipartition of energy.

4. By performing your simulation, find the distribution (histogram) of the particle's velocity v. Is it consistent with Maxwell-Boltzmann statistics?

Project: Polymers and Random Walks

(adapted from "Statistical mechanics: entropy, order parameters and complexity" by James P. Sethna)

OBJECTIVE: To get acquainted with random walk Metropolis algorithm. Learn about self-avoiding random walks and some properties of random walks, such as radius of gyration. Also to learn about connectivity constant.

A polymer is a one-dimensional chain, that consists of smaller bonded monomer molecules. Polymer behavior in a solvent can be approximated by an uncorrelated random walk of straight segments several monomers in length. Simulate a normal random walk description of a gene and investigate it's end-to-end distance. Then simulate a self-avoiding random walk. Calculate radius of gyration, and the end-to-end distance statistics. Compare results for different random walks. Define the connectivity constant.

First of all, introduce polymers and their statistical behavior.

1. Let's first assume that polymers are standard random walks. Consider a gene with $N \cdot 150$ base pairs. DNA persistence length (length of polymer that can not bend, i.e. change course) is 50 nm, which corresponds to approximately 150 base pairs. Assume every 150 pairs, the DNA is able to turn at any angle.
   (a) Simulate the random walk of a gene using N=10, 50, 100, 500, 1000, 5000, 10000 base pairs in 2D. This can be done in multiple ways. Each time calculate end-to-end distance of your gene. Average your results for each N over 10^3 runs. How does end-to-end distance changes with the total length?
   (b) Investigate what number of base pairs on average is needed for a gene to first cross itself.
   (c) Calculate average radius of gyration for all simulated polymers and plot it with respect to N. Discuss the results.

   The radius of gyration can tell you more about size of your gene. It is proportional to the root mean square of distance between collection of segments and centre-of-mass. It can be calculated as:

$$R_g^2 = \frac{1}{N-1}\sum_{i=1}^{N} |\mathbf{r}_i - \mathbf{r}_{CM}|^2 \tag{1}$$

   where $\mathbf{r}_i$ are positions of ith segment and $\mathbf{r}_{CM} = \frac{1}{N}\sum_{i=1}^{N} \mathbf{r}_i$. N.B. the divisor $N-1$ comes from *Bessel's correction*.

2. A real polymer, however, is not a purely Markovian random walk, but a self-avoiding random walk (SAW) - polymers can't cross themselves. This changes their statistics. For the remainder of this document, we will consider only random walks on the lattice. This is because, on a lattice, an intersection is simply characterized by a lattice point already being occupied.
   (a) Repeat the steps of the previous half with simple lattice walks that do not self-avoid, and also with SAWs using the *pivot algorithm*. Try this for $N = 10, 50, 100, 500,$

again with a sample size of 10^3. How do your results change compared to the previous question?

The Pivot Algorithm consists of the following steps:

1. Draw an initial non-overlapping walk of length N. Conventionally, we use the straight line in one direction. Then repeat until enough samples have been found:
   (a) Choose a random lattice site of the walk (pivot site).
   (b) The pivot site divides the walk in two. Rotate the second half of the walk onto new lattice sites, by $\pi/2$, π or $3\pi/2$. These 3 suffice for 'ergodicity'.
   (c) Check if the resulting walk does not self-intersect (doubly occupy any sites). If not: accept the move and yield one sample. If yes, restore the previous walk.

   Because the pivot algorithm is a Metropolis algorithm, it will require a 'warm-up' period. Optimally, the number of warm-up steps is $c \cdot N$, for c some number of order 1-10. These first samples should not be used for statistics, because they're too similar to the starting path.

(b) Approximate the probability-density-function of end-to-end distance for SAWs of $N = 10$.

(c) Research the mean value of the (squared) end-to-end distance as a function of N, specifically its asymptotic. Compare with your simulation results.

3. Try to estimate the connective constant of a two-dimensional lattice. Perhaps you can think of your own way to do it, by counting paths of different lengths.[1]

[1] Otherwise, you may want to check out *"The Pivot Algorithm: A Highly Efficient Monte Carlo Method for the Self-Avoiding Walk"*, the 1987 work by Madras and Sokal, paragraph 5.2, and set $k = 1$.

Project: Chaos, ergodicity and fractals through the logistic map
(adapted from "Statistical mechanics: entropy, order parameters and complexity" by James P Sethna)

OBJECTIVE: Use a simple discrete map to study fixed points, bifurcations and chaos. Introduce the Feigenbaum number and Lyapunov exponents. Fractal nature of chaotic attractors.

In contrast to continuous-time systems, discrete maps can show remarkably complex behavior, even in 1D. Discuss the general properties of chaos. Investigate the behavior of the discrete logistic map, for both fixed point and and chaotic behavior. Discuss bifurcations and plot a bifurcation diagram. Explore the connection with fractals. Estimate Feigenbaum number and calculate the Lyapunov exponent in a chaotic regime.

First, it's worth reminding yourself about the types of behavior present in a 1D continuous dynamical system. Can there be oscillations (how do you know)? Can there be chaos (how do you know)? How do you describe the general behavior? Now, specifically consider the logistic map:

$$x_{t+1} = 4\mu x_t(1 - x_t) \tag{1}$$

1. An important advantage of discrete-time maps is that they are much easier to simulate then their continuous cousins, even in a chaotic regime. Investigate the behavior of the logistic map at different μ using a simulation. First of all, iterate initial points $0 < x_0 < 1$ for $\mu = 0.2$ and convince yourself that they are attracted to 0. Also show this analytically.

2. Plot a web diagram ($x_{t+1} = f(x_t)$) to determine if there any other fixed points, except for 0. A fixed point is defined as point for which $x' = f(x')$. Repeat the simulations for $\mu = 0.4$, 0.6. What changes do you see? Show that for $0.25 < \mu < 0.75$ a stable non-zero fixed point exists.

   Note: A Fixed point is called stable if small perturbations shrink after iteration.

   $$|f(x' + \varepsilon) - x'| \approx |df(x')/dx|\varepsilon < \varepsilon$$

   which is possible if $|df(x')/dx| < 1$.

3. Plot x_t with respect to t for $\mu = \{0.2, 0.4, 0.6, 0.8, 0.85, 0.88, 0.91\}$. What change of behavior do you see? Show that for $0.75 < \mu < (1 + \sqrt{6})/4$ there is a period-2 cycle. Using your script define the critical value of μ when one reaches chaotic behavior.

   If μ is slightly bigger 0.75, then period-2 bifurcation occurs. You can see it by looking at $\mu = 0.8, 0.85$ plot, where x_t jumps between two different values opposite to converging to one point as for $\mu = 0.2$, $\mu = 0.4$, $\mu = 0.6$. Bifurcations are qualitative changes in the asymptotic solution. If you increase to $\mu = 0.88$ period-2 cycle becomes unstable and converges to period-4 cycle. If we increase μ even more at some point we will reach infinite bifurcations regime or chaos. This chaotic behaviour can be seen for $\mu = 0.91$

4. At $\mu = 1$ an attractor fills the entire set of available states, however, not all states are weighted equally (i.e., Liouville's theorem does not hold). We quantify the weighting of the states on the attractor through the invariant density $\rho(x)$ which is unchanged by the equations of motion.

   Set $\mu = 1$ and use your simulation to sample $\rho(x)$ numerically by iterating a typical point x_0 many steps (say 5000) to find point x_a on the attractor. Continue to iterate, collecting enough data along the trajectory (say at least 10^4) points. Verify analytically that if $\mu = 1$:

$$\rho(x) = \frac{1}{\pi\sqrt{x(1-x)}} \tag{2}$$

   Note: you don't have to derive normalization factor $\frac{1}{\pi}$. Compare the analytic and numerical result. What $\rho(x)$ would we have in the case of an attracting fixed point?

5. Iterate N times starting from $x_0 = 0.5$ for a range of $0.8 < \mu < 1$ with $\delta\mu = 0.005$. To investigate asymptotic long-time solutions throw away M first results and save N-M iterations. Plot bifurcation diagram (x with respect to μ). Define dynamics regions on the bifurcation diagram you plotted.

6. Use the logistic map to estimate the Feigenbaum number:

$$\delta = \lim_{n\to\infty} \frac{r_n - r_{n-1}}{r_{n+1} - r_n}, \tag{3}$$

   where $r = 4\mu$ is the bifurcation parameter and n refers to the nth period-doubling bifurcation. In what sense is the Feigenbaum number universal?

7. Chaos is often associated with a fractal set which has non-integer dimension. For μ in the chaotic regime, measure the "dimension" of the logistic map and show it is fractal.

8. The system is chaotic if two trajectories that are initially close to each other deviate more and more with increasing time. Intuitively one know that separation between trajectories, δ grows as $e^{\lambda t}$, where λ is the Lyapunov exponent. For a 1D map, the Lyapunov exponent is defined as:

$$\lambda = \lim_{n\to\infty} \frac{1}{n} \sum_{i=1}^{n} \left.\frac{df}{dx}\right|_{x=x_i} \tag{4}$$

   where $f(x) = 4\mu x(1-x)$ and the $\{x_i\}$ are points sampled on the attractor.

   One can determine if system is chaotic by looking at sign of λ. If $\lambda > 0$ nearby trajectories deviate at large n - chaos. If $\lambda < 0$ nearby trajectories converge at large n.

   (a) Plot Lyapunov exponent for a range $0.5 < \mu < 1$. When the system becomes chaotic?

   (b) By comparison with bifurcation diagram define how the period doubling bifurcations look like at Lyapunov exponent plot?

Notice that even at very high μ there are points where $\lambda < 0$ - "islands of stability".

9. Investigate the two trajectories $\{x_0, f(x_0), f(f(x_0)), \dots f^n(x_0)\}$ and $\{y_0, f(y_0), \dots\}$, where $y_0 = x_0 + \delta(0)$, for $\mu = 0.6, 0.8, 0.99$.
   (a) How fast do the trajectories separate? Why do they stop separating?
   (b) Estimate the maximum Lyapunov exponent.

Project: Percolation theory and the zombie apocalypse

Based on "You can run, you can hide: The epidemiology and statistical mechanics of zombies"
A. Alemi et al, *Phys. Rev E* **92 052801 (2015)**

OBJECTIVE: Learn the basics of percolation theory. Simulate a toy problem in 2D space and investigate behavior at the percolation threshold. Learn about fractals.

Percolation theory is a powerful tool for the description of phase transitions. Imagine there was a terrible accident in one of the secret biology labs at the Academic Medical Center during which a zombie infection was spread. Discuss percolation theory. Simulate a toy model of the zombie apocalypses and investigate the dependence of zombie spread on the percolation probability. Investigate the behavior of percolation theory at the percolation threshold and it's connection to fractals.

Imagine a 2D lattice with sites of equal spacing. Sites are independent and the probability to occupy each site is p, with $1-p$ the probability of not being occupied. There will be an occupation probability p_c at which an infinite cluster can be achieved for the first time. Note: probability to get an infinite cluster with $p < p_c$ is 0, but is 1 when $p > p_c$. Discuss percolation theory and the definitions of the percolation threshold, probability of percolation, cluster number etc.

Let us introduce a "SZR" model of the Zombie Apocalypses (S - susceptible population, the uninfected humans; Z - zombies; R - destroyed zombies).
Rules of the game:

1. If a zombie bites a human, the human becomes a zombie - β determines rate of these events.

2. If human shots zombie in the head, zombie dies - κ determines this rate.

Note: we don't discuss usage of bomb on the infected regions.
The equations that describe population changes during the Zombie Apocalypse are:

$$\begin{aligned} \frac{dS}{dt} &= -\beta SZ \\ \frac{dZ}{dt} &= (\beta - \kappa)SZ \\ \frac{dR}{dt} &= \kappa SZ \end{aligned} \tag{1}$$

With $N = S + Z + R$ the total population and this number is fixed. Let $\tau = t\beta N$, $\alpha = \frac{\kappa}{\beta}$ and rewrite the above equations in terms of $\{S, Z, \tau, \alpha\}$. Interpret α. With initial conditions $\{R(0) = 0, Z(0), S(0)\}$, the solution of these equations can be written as:

$$\begin{aligned} Z(\tau) &= P - f(\tau), \\ S(\tau) &= \frac{f(\tau)}{1-\alpha} \end{aligned} \tag{2}$$

with

$$P \equiv Z(0) + (1-\alpha)S(0),$$
$$\mu \equiv \frac{S(0)}{Z(0)}(1-\alpha) = \frac{P}{Z(0)} - 1,$$
$$f(\tau) \equiv \frac{\mu P}{e^{\tau P/N} + \mu}$$

1. What will happen with (S,Z) as $\tau \to \infty$ if $\alpha < 1, P > 0$? In the case $\alpha > 1$ how many zombies are needed initially to destroy humanity? Plot $S(\tau), Z(\tau), R(\tau)$ for a variety of initial conditions with $\alpha = 0.2, 0.4, 0.6, 0.8, 1, 1.2, 1.4$. Does humanity survive in each case? What predictions can you make?

2. Let's look at the spread of zombies across across Earth. In our model, zombies also have superpowers to teleport through oceans, so there is no need to think about any possible delay in a spread of zombie disease. Start with a 2D square lattice of size $10^2 \times 10^2$, where each site is occupied initially by a human or zombie, for example with a random 10% of the sites as zombies. At latter times there are 3 possible conditions of each site:

   1. Human
   2. Zombie
   3. Destroyed zombie

   Now let's choose the following dynamics:

   1. Pick a neighboring zombie-human pair at random
   2. With probability $P_{\text{destroy}} = \frac{\kappa}{\beta+\kappa}$, destroy the zombie
   3. Pick another neighboring zombie-human pair at random
   4. Turn the human to zombie with probability $P_{\text{infect}} = \frac{\beta}{\beta+\kappa}$
   5. Repeat.

   Explore these dynamics for different values of α (you'll need to explore wider range of α then in the first part, say $0 \leq \alpha \leq 20$). Find the critical value of α the separates zombie domination from human survival.

3. Decreasing α from a value of when humans survive, find the value α_c when a cluster of zombies first spans the entire lattice.

4. Choose exactly α_c and do the simulation. Discuss your result. How is it connected with fractal theory? Define fractal structures and fractal dimension. Redo your simulations a few times for α_c. What are the average size of zombie and human clusters after some representative number of human-zombie interaction?

5. How would the percolation threshold depend on lattice connectivity?