Summer Term 2020

Heidelberg University - Faculty of Physics and Astronomy
Problem Set

1 Introductory Remarks

- Due to the circumstances, the problems to be solved will not be handed out in three sets as originally advertised. Rather, the entirety of the problems are listed. This holds true for the programming problems.
- The conditions are also changed due to limited interaction in the recital sections.
- The following rules apply:
  - There is no minimum points to reach. Hence, the exercises are not marked with points that can be reached.
  - The programming exercises are also not mandatory.
- You are strongly advised to takle the analytical as well as one of the suggested programming problems. We are offering help on tackling the exercises in online meetings as was announced in the LSF:
- **Recital Session**
  - Philosophenweg 12 / R 105 (Face-toFace: canceled)
    14:15 -15:45
  - changed to online at
    14:15 -15:45
  - Link will be provided on the course website.
- Helping me out will be Kunhe Li.

2 Problems

- **Random Walk**

  A particle moves on a $d = 1$, infinite lattice. The distance between two neighbouring nodes is a. In the interval τ the particle moves by $n \neq 0, n \in \mathbf{Z}$ nodes (the particle cannot stay on the same node), and the jumps to the left or to the right are equally probable. The probability of jumping by $|n|$

  i) is proportional to $|n|^{-1}$;
  ii) is proportional to $|n|^{-2}$;
  iii) is proportional to $|n|^{-4}$;
  iv) is proportional to $q^{-|n|}$, where $0 < q < 1$.

  Questions:

a) Are all the above processes well defined?

b) Normalize the probabilities if the processes are well defined.

c) Which processes approach the diffusion in the limit

1. $a \to 0$
2. $\tau \to 0$

- **Random Walk**

  Find all possible random walks without self-intersections on the square lattice for length N=1,2,3, . . . and compute their mean square displacement.

- **Diffusion with absorbing boundaries**

  Consider diffusion in the presence of two concentric 2-dimensional (d-dimensional) absorbing circles (spheres) A and B with radius $R_A = 1$ and $R_B = R > 1$. Find the conditional absorbing probabilities $P_A(r)$ and $P_B(r)$ when the diffusion is startet at time zero at a point r with distance $0 \leq r < \infty$ to the center. Find the mean times to absorbtion for $0 \leq r < R$.

- **Phase Transition**

  Consider a system with a one component order parameter $m(r)$. Consider the Ginzburg-Landau functional

$$F[m(r)] = \int dr(f(m) + \frac{1}{2}\alpha(\nabla m)^2)$$

  with

$$f(m) = \frac{b}{2}m^2 + \frac{c}{4}m^4 + \frac{v}{2}(\Delta m)^2 - hm$$

  where $\alpha > 0$. We will expand the function. Such Ginzburg-Landau expansions are used, e.g., to describe systems that exhibit patterned phases, stripe patterns as for example in polymer systems, and lipid-water mixtures.

  a) Minimize F. (The result should be $bm + cm^3 - \alpha\Delta m + v\Delta^2 m - h$)

  b) Neglect the term cm^3 and carry out the Fourier transformation $m(r) \to \tilde{m}(k)$. Show that this results in

$$b\tilde{m} + \alpha k^2\tilde{m} + v(k^2)^2\tilde{m} = \tilde{h} \ .$$

  – Use the above equation to compute $\frac{\delta\tilde{m}(k)}{\delta\tilde{h}}$. Show that the maximum is at $k = 0$.

- **Reaction System**

  A protein changes between the conformations x_1 and x_2. The kinetic parameters k_{ij} determine the rate of the conformational changes. The input signal, u, together with the constant, K, represent introduction of x_2 to the system. Assume that we can measure x_2. All reaction rates are assumed to be given by expressions proportional to the concentration of the states they emanate from. That is, for a state i the differential equation is

$$\dot{x_i} = \sum_p k_{ip}x_p - \sum_q k_{qi}x_i$$

where p is the number of incoming and q the number of outgoing flows from the state i. This corresponds to mass action kinetics for a regular biochemical reaction network.

a) Determine the state space equations that describe the system.

b) Is the system stable?

c) What are the conditions on the kinetic parameters k_{ij} are needed?

- **Flory-Huggins**

  Consider the Flory-Huggins free energy

$$\begin{aligned} \Delta F &= \Delta U - T\Delta S \\ \frac{\Delta F}{N k_B T} &= \chi \phi_1 \phi_2 + \frac{\phi_1}{x_1} \ln \phi_1 + \frac{\phi_2}{x_2} \ln \phi_2 \end{aligned}$$

  where for solvent-solvent: $x_1 = x_2 = 1$, solvent-polymer: $x_1 = 1, x_2 =$ large and polymer-polymer: $x_1 = large, x2 =$ large.

  a) Where is the second-order phase transition point located?

  b) Show that the Flory-Huggins free-energy is related to the one in the previous excercise.

- **Polyelectrolytes**

  The perhaps simplest model for charged flexible polymers or polyelectrolytes is obtained using the Flory ansatz for the free energy

$$\beta F = \frac{R^2}{Nb^2} + \frac{kN^2q^2}{eR}$$

  where the interaction term is basically giving an electrostatic potential energy k^2/R to each of the N^2 interactions between the charged monomers, and is up to a numerical constant the electrostatic energy of a sphere of radius R with charge Nq dispersed through it. How does the radius R scale with N for this case?

- **Basis Functions**

  Given a test vector x_i, the output of a neural network is defined as

$$f(x_i) = \sum_{j=0}^{M} w_j \phi_j(x_i, v_j) \; . \tag{1}$$

  The weights of the neurons can be learned by employing the back-propagation rule with sample-based gradient descent. In the lecture neural networks with sigmoid neurons have been introduced, but it is possible to employ different basis functions:

  a) Which properties do these basis functions have to fulfill?

  b) Is the number of parameters for $\phi(x_i, v_j)$ limited? Could several different basis functions be used for the same neural network?

3 Numerical Problems

General remarks:

- You are given pointers to the literature with interesting numerical problems.
- You are not to repeat what has been done in the paper!
- Rather, the papers are meant as a starting point to develop ideas of how to tackle the problem in a simplified way.
- How you are approaching the solution and how far you are going will be determined in individual consultation, depending on your interests and skills.

Pointers to possible problems to be tackled:

- **DNA Origami**
  - Active Self-Assembly of Algorithmic Shapes and Patterns in Polylogarithmic Time
    https://dna.hamilton.ie/woods/download/nubots.pdf
  - Or

    Abstract from https://dl.acm.org/doi/10.5555/1459290.1459317:

    Self-assembling DNA complexes have been intensively studied in recent years aiming to achieve bottom-up construction of nanoscale objects. Among them, a DNA complex called DNA tile is known for its high programmability. By using a set of DNA tiles, we are able to self-assemble two-dimensional crystals with programmable patterns. This is called algorithmic self-assembly. In order to create a wide range of complex objects by this self-assembly process, we need a methodology to predict its behavior. Especially, the relationship between the error rates and growth speed is of our interest. To estimate these properties, we use thermodynamic simulations based on the Monte Carlo method. However, conventional simulation models assume some much simplified conditions, therefore cannot explain the results of crystal growth experiments. Here, we propose Realistic Tile Assembly Model (R-TAM), in which we model the detailed conditions of the experimental protocol. We will show that the simulation can explain growth process of DNA tile crystals in experiment.
  - Or

    Abstract from https://www.pnas.org/content/112/20/6313:

    Recent experiments have demonstrated that complex, three- dimensional nanostructures can be self-assembled out of thousands of short strands of preprogrammed DNA. However, the mechanism by which robust self-assembly occurs is poorly understood, and the same feat has not yet been achieved using any other molecular building block
- **Population genetic inference with Convolutional Neural Networks**

  From github: https://github.com/flag0010/pop_gen_cnn/

  This directory contains code for training and testing the neural networks described in this paper: The Unreasonable Effectiveness of Convolutional Neural Networks in Population Genetic Inference by Lex Flagel, Yaniv Brandvain, and Daniel Schrider. https://doi.org/10.1101/336073