Annotated notes from the lectures
Tuesday, January 28, 13-15.

January 2019

Statistical Physics (math327)

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LECTURE NOTES

KURT's

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Module Information

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Contact hours:

Weeks 1-7:	We will have *three hours of lecture* and *one tutorial*. There will be question sheets for the tutorials. You will work through part of these questions in your time before the tutorial (non-assessed). Key elements will be the discussed in the tutorial.
Week 8-9:	will host *two hours of lecture* and *two hours Computer Lab*. In the Computer Lab sessions, we will study a statistical phenomena (see page 108) with a computer experiment using MATLAB. A basic introduction to MATLAB will be provided, but familiarising yourself with MATLAB (if needed) could be beneficial. Support material to get started with MATLAB is provided at the VITAL page for math327.
Week 11-12:	will *three hours of lecture* and *one tutorial*, both will include exam revision sessions.

Assessment:

12%	Two assessed homeworks due in week 3 and week 6 with equal weighting. A clear and neat presentation of all this contributes to your mark.
8%	for a computer based project due in week 11.
80%	Standard Examination.

Resources:

This portfolio covers the lecture material, the questions and tasks for the tutorial and the computer based project.

The VITAL page for the module math327 has more support material. You might find the small podcasts e.g. on getting started with the software useful.

A list for further readings can be found at the end of these notes.

Contents

1 What is Statistical Physics?

The physical sciences try to unlock the laws of nature and to understand the everyday-life or experimental observations. "Understand" frequently means to find the mathematical description that reproduces a cluster of physics observations and that allows to make predictions for other observables.

Physics over the last century has been a tremendous success story: in experiments, we can now create a vacuum that is better than in outer-space, and the coldest place in the universe is in our solid state physics labs. Amazingly, the Mathematics to describe those realms of physics has been developed, in some cases, centuries before. Physicist now embark to find the Mathematics of the theory of everything, which will combine the description of the sub atomar with that of the grande scales - gravity.

The brand of "Statistical Physics" summarises those observations and laws of nature the successful mathematical description of which is *Probability Theory*. The quality of the mathematical description is usually outstanding to an extent that 'randomness' from the probabilistic description is hardly observed in the observables. In fact, `Ludwig Eduard Boltzmann` (1844-1906), the founder of statistical mechanics, had a hard time to defend his theories. His mental health deteriorated over the years, and he committed suicide on September 5, 1906, while on vacation with his wife and daughter in Duino, near Trieste.

While at Boltzmann's times, phenomena such as temperature, pressure and diffusion were the objective, probability theory now is at the heart of modern physics. For instance, when in neutron stars gravity becomes soo large that it crushes atoms by forcing electrons to combine with protons to form neutrons, it is probability theory that explains while the neutron matter does not collapse under the immense gravity. We will later understand the mathematics behind this (see quantum gases).

2 Central Limit Theorem

The high quality of probability theory descriptions can be traced to the involvement of some very large numbers. If we for instance go back to the stochastic description of properties of (classical) gases, 22.71 litres of gas under 'normal conditions' (a pressure of 100.00 kPa and a temperature of

0^0 Celsius) contain $6.02214086 \times 10^{23}$ gas particles (Avogadro's constant). If pressure arise from air particles colliding with the walls and pushing the 'out', why is the pressure not wildly fluctuating, but can be perfectly and reproducible measured? The mathematical answer lies in the Law-of-Large-Numbers and the Central-Limit-Theorem.

2.1 Probability Essentials

Experiment E and state ω: Each time an 'experiment' is performed, the world comes out in some state ω. The definition of the experiment includes the objects of interest.

Set of all states Ω: The set of all possible outcomes ω is denoted Ω and is called the universe of possible states. Note that it is obviously intricately tied to the experiment E.

Measurement $X(\omega)$: If we are interested in measuring some features of our states ω, we need to map each individual state ω to a one number X, in which we are interested. Hence, we can view X a function of ω and call it $X(\omega)$. In Mathematics, $X(\omega)$ is called *random variable.* After having performed the experiment E once, it is the result of the measurement of X on the state ω that E produced.

Set of outcomes A: If we input all possible states $\omega \in \Omega$ to the function $X(\omega)$ and collate the outcome in a set, we generate the set A of a possible outcomes. Mathematically, we can write:

$$X : \Omega \to A .$$

The set A can be finite, infinite and countable, or infinite and continuous.

Set of events F: An *event* is any subset of the set of all outcomes A. According to our interest, we can group these subsets together to form the `set of events` F.

<u>Examples:</u>

(A) Throwing a die:

E: "roll a die"; ω: "die is at rest"

Ω: "all possible positions"

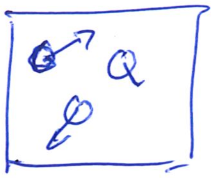
measurement: $X(\omega)$ = number comes out on top

A: outcome space: $A = \{1, 2, 3, 4, 5, 6\}$

(B) Toss of a coin four times:

$A = \{HHHH, HHHT, HHTH, HTHH, THHH,$
$HHTT, HTHT, HTTH, THHT, THTH, TTHH,$
$HTTT, THTT, TTHT, TTTH, TTTT\}$

(C) Argon (gas) atoms in a container:



ω: positions of the atoms and their velocity

In many cases, we want to characterise the states ω and introduce a unique number as a qualifier for the states. This means that we introduce a random variable $L(\omega)$ as a 'label'. Since the label is unique, this function is *isomorphic*:

$$\omega \leftrightarrow L(\omega)$$

and we can synonymously use the set of outcomes A for Ω. We need to be careful since not all textbooks make the distinction between A and Ω, which can be a source of confusion.

Probability P: Every *event* has a probability P of occurring. Mathematically, we define the *probability measure* function P as

$$P : \mathcal{F} \rightarrow [0, 1] .$$

The probability measure function must satisfy two requirements:

- The probability of a countable union of mutually exclusive events must be equal to the countable sum of the probabilities of each of these events.
- The probability of the outcome set A must be equal to 1. This simply means that the experiment E must produce an outcome. This makes sense than we would simply say that the experiment did not take place if no output was produced.

The triple $(A, \mathcal{F}, P)$ is called `probability space`.

Examples:
(A) Assume that an experiment can only produce N possible states as outcomes. In this case, the state space is given by

$$\Omega = \{\omega_1, \omega_2, \dots \omega_N\} .$$

Assume that we have a random variable $X(\omega)$ with the property

$$\text{if} \qquad X(\omega_i) \neq X(\omega_k), \Rightarrow \omega_i \neq \omega_k .$$

We do *not* exclude, that $X(\omega_i) = X(\omega_k)$ for some pair i, k $i \neq k$. We then define the set A of outcomes by all $X(\omega_i)$ that are different. The size of the set is $n \leq N$:

$$A = \{X_1 \dots X_n\} .$$

We could now choose as events the random variables X_i itself. The event space hence is given by

$$\mathcal{F} = \{X_1 \dots X_n\} .$$

We then can assign probabilities to each of these events:

$$P(X_i) =: p_i , \qquad i = 1 \dots n .$$

Since these events are all mutually exclusive by construction, we find e.g. for $i \neq k$:

$$\begin{aligned} P(X_i \text{ or } X_k) &= P(X_i) + P(X_k) \\ P(X_1 \text{ or } X_2 \text{ or } \dots \text{ or } X_n) &= \sum_{i=1}^{n} P(X_i) = 1 . \end{aligned}$$

Let us now consider some a specific examples:

Throwing a die:

$A = \{1, 2, 3, 4, 5, 6\}$

p_i : probability to get "i"

"fair": $p_1 = p_2 = p_3 = p_4 = p_5 = p_6 =: p$

$$P(1 \cup 2 \dots \cup 6) = \sum_{i=1}^{6} p_i \overset{!}{=} 1$$

$$p \cdot \sum_{i=1}^{6} 1 = 1 \Rightarrow 6p = 1 \quad p = 1/6$$

Roulette:

$A = \{0, 1, 2, \dots 36\}$

"fair": $p_0 = p_1 = p_2 = \dots = p_{36} = 1/37$

$F = \{$"red", "black", "green"$\}$

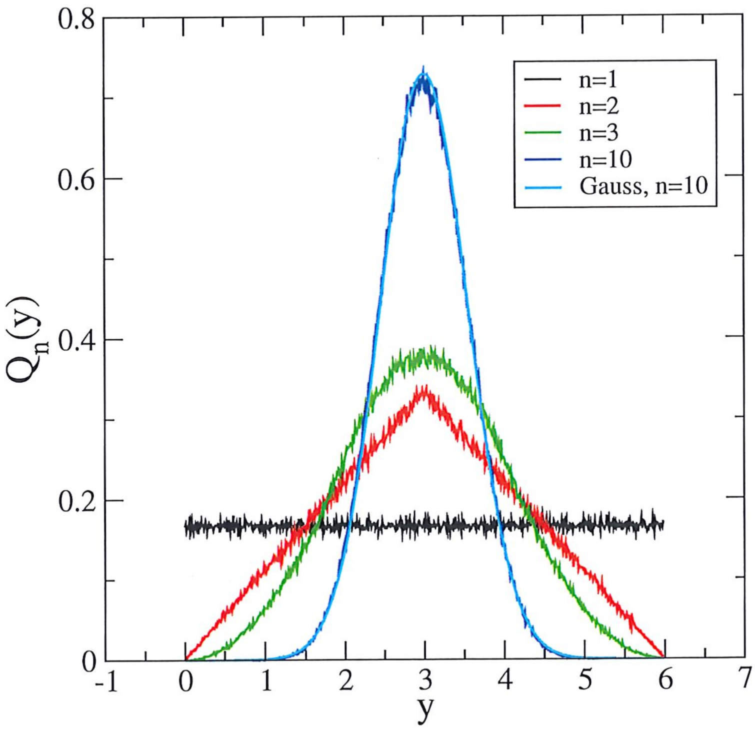
$$P_{red} = P(1 \cup 14 \cup 9 \dots) = \underbrace{P(1) + P(14) + \dots}_{18} = \frac{18}{37}$$

$P_{black} = 18/37$ $\quad P_{green} = 1/37$

Addendum page 10: Roulette – European Tables

The standard European table has 18 black, 18 red and one green pocket (numbered 0) making 37 pockets in all.

Addendum page 15: Central limit theorem



Toss a *fair* coin four times

fair

16 possib. ; $p_1 = \ldots = p_{16} = \frac{1}{16}$

$\mathcal{F} = \{$ equal # of H and T, not # $\}$

$p_{eq.} = \frac{6}{16}$ $\quad$ $p_{not.\,eq} = \frac{10}{16}$

Comments:

- Defining the probabilities is called *modelling*. Symmetries are a powerful way to inform this choice. E.g., for a so-called "fair" die, we expect that every side of the side shows up top with equal probability. This demand is actually enough to fix the probabilities p_i, $i = 1 \ldots 6$.

- Rather than modelling, we could try to infer the probabilities from the abundance of certain events. To this end, we could repeat an experiment n times and the Law-of-Large-Numbers can then help us to infer the probabilities.

2.2 The Law of Large Numbers

Suppose we carry out an experiment with a finite set of outcomes

$$A = \{X_1, X_2, \ldots, X_{N_s}\} .$$

We consider each of the possible outcomes as events implying that the event space $\mathcal{F}$ is equal to the set of outcomes, $\mathcal{F} = A$. As discussed before, we can assign probabilities

$$p_i = P(X_i) \qquad \text{with } p_i \in [0,1], \qquad \sum_{i=1}^{N_s} p_i = 1 .$$

We will use a slightly more elegant notation and write:

$$\sum_{X \in A} P(X) = 1 .$$

We then introduce the mean μ and the variance σ^2 in usual way by

$$\mu = \langle X \rangle = \sum_{X \in A} X\, P(X) , \tag{1}$$

$$\sigma^2 = \langle (X-\mu)^2 \rangle = \sum_{X \in A} (X-\mu)^2\, P(X) . \tag{2}$$

We now *repeat* the experiment n-times, and call this a new experiment with outcome space B. For $n = 4$, this space looks like:

e.g. $\{X_1 X_1 X_1 X_1, X_1 X_1 X_1 X_2, X_{N_s} X_4 X_1 X_3,$
... $\}$

We call the outcome of the ith repetition $X^{(i)} \in A$, $1 \leq i \leq n$. The individual experiments are carried out *independently.* If one particular element of the outcome space B is given by

$$\omega = \{X_i^{(1)} X_k^{(2)} X_l^{(3)} X_m^{(4)}\} ,$$

the probability of this element is given by:

$$P(\omega) = P\left(X_i^{(1)}\right) P\left(X_k^{(2)}\right) P\left(X_l^{(3)}\right) P\left(X_m^{(4)}\right) .$$

Let us now return to the general case of n independent repetition of the same experiment.The *arithmetic mean*

$$\frac{1}{n} \sum_{i=1}^{n} X^{(i)}$$

?

is itself a random variable (it e.g. depends on the outcome of the first experiment $X_i^{(1)} \in A$), but we would expect that this has something to do with the mean μ. To reveal this connection, we calculate

$$(*) \quad \sum_{i=1}^{n} a_i \sum_{k=1}^{n} b_k = \sum_{i,k=1}^{n} a_i b_k$$

$$\left\langle \left(\frac{1}{n} \sum_{i=1}^{n} X^{(i)} - \mu \right)^2 \right\rangle_B = \left\langle \left(\frac{1}{n} \sum_i (X^{(i)} - \mu) \right)^2 \right\rangle$$

$$= \frac{1}{n^2} \left\langle \sum_i (X^{(i)} - \mu) \sum_k (X^{(k)} - \mu) \right\rangle$$

$$\overset{(*)}{=} \frac{1}{n^2} \left\langle \sum_{i,k} (X^{(i)} - \mu)(X^{(k)} - \mu) \right\rangle$$

$$= \frac{1}{n^2} \sum_{i,k} \underbrace{\left\langle (X^{(i)} - \mu)(X^{(k)} - \mu) \right\rangle}$$

$$\left\langle (X^{(i)} - \mu)(X^{(k)} - \mu) \right\rangle = \sigma^2 \delta_{ik} \qquad \delta_{ik} = \begin{cases} 1 & \text{for } i=k \\ 0 & \text{else} \end{cases}$$

$$= \frac{\sigma^2}{n^2} \sum_{i,k} \delta_{ik} = \frac{\sigma^2}{n^2} \sum_{i=1}^{n} 1 = \frac{\sigma^2}{n^2} n$$

$$= \frac{\sigma^2}{n}.$$

This then implies:

$$\sigma^2 = \left\langle (X^{(i)} - \mu)^2 \right\rangle$$

$X^{(i)}$ is a sequence of random numbers with exitsting mean and standard deviation:

$$\langle X^{(i)} \rangle = \mu \, , \qquad \langle (X^{(i)} - \mu)^2 \rangle = \sigma^2 \, ,$$

we then find:

$$\lim_{n\to\infty} \frac{1}{n} \sum_{i=1}^{n} X^{(i)} = \mu \, . \qquad \text{(Law of Large Numbers)} \, .$$

2.3 Central Limit Theorem

A quick word in case we are dealing with a *continuous random variable* X. We specialise to the important case that X is a real number. Such as distribution has a probability density function $p(x)$, and therefore its probability of falling into a given interval, say $[a, b]$, is given by the integral

$$P\big(a \le X \le b\big) = \int_a^b p(x) \, dx \, .$$

We are now prepared to look at the Central Limits Theorem (CLT):

Let $X_1, X_2, ..., X_N$ be a sequence of N independent and identically distributed random variables. The probability distribution function $p(x)$ can be arbitrary, but we assume that mean and variance exist:

$$\langle x^\ell \rangle = \int x^\ell \, p(x) \, dx \quad \ell = \{1, 2\}, \qquad \mu := \langle x \rangle \, , \qquad \sigma^2 = \langle x^2 \rangle - \langle x \rangle^2 \, .$$

Define a new random variable S by

$$S = \sum_{i=1}^{N} X_i \, .$$

For sufficiently large N, the probability distribution of S is given by a normal distribution:

$$p(s) \to \frac{1}{\sqrt{2\pi \, N\sigma^2}} \exp\left\{ - \frac{(s - N\mu)^2}{2N\sigma^2} \right\} .$$

There are many versions of the CLT. This version is the one we are using throughout this lecture. Proofs can be found in many textbooks. Here, we focus on a first application: (normal) diffusion.

page 15: alternative present. of CLT

$$A = \frac{1}{N}\Big(\underbrace{\sum_{i=1}^{N} X_i}_{}\Big)^{S} \quad \text{compare:} \quad \underline{A} = \frac{1}{N}\underline{\underline{S}} \rightarrow S = NA$$

$$p(a) = \text{const.} \exp\left\{-\frac{(\hat{N}a - N\mu)^2}{2N\sigma^2}\right\} = \text{const.} \exp\left\{-N\frac{(a-\mu)^2}{2\sigma^2}\right\}$$

$$\int p(a)\,da = 1 \quad \Rightarrow \quad p(a) = \sqrt{\frac{N}{2\pi\sigma^2}} \exp\left\{-N\frac{(a-\mu)^2}{2\sigma^2}\right\}$$

2.4 Diffusion on a line

Assume that we walk on a line with a given step length. At each step, we independently decide whether we step to the right (probability p) or to the left (probability $q = 1 - p$). Also assume that we perform N steps. We will vary N later. If each step does take time Δt, the time t after N steps is simply given by

$$t = \Delta t \, N \,. \tag{3}$$

If L/R denotes a as step to the left / right, a typical event looks like:

LRRLLLRLRRLRL $\quad N=13$ $\underbrace{\qquad\qquad}_{N}$ Prob = $q\,p\,p\,q\,q\,q\,p\,\ldots$

The probability that *exactly* this event occurs is given by:

2^N possibilities; $\quad p^n \times q^{N-n} \quad (q = 1-p)$ n: steps to the right $\quad n=6$

The interesting question is: where are we after time t (or N steps)? Since stepping is a radom process, we need to refine this question: Where are we most likely or more precise, if we do this experiment many times, what is the average position $\langle x \rangle$? We then would want to know: how precisely do we know this average or what is the variance $\langle x^2 \rangle - \langle x \rangle^2$?

If k is the total number of steps to the right, we have $N - k$ steps to the left, and our position would be:

$$x = k - (N - k) = 2k - N \,.$$

The order with which we step to the left or right does not the postion x with which we ~~wend~~ end up. For example, take $N = 5$ and let us write down all events for which end up at $x = 3$:

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page 16:

Box 1: LRRLLLRLRLL...RL
$\underbrace{\hspace{6cm}}_{N}$

Box 2: we have N slots; each slot has 2 possibilities: L or R
$\Rightarrow 2^N$ possibilities

"fair": each event has the same probability
$p_i = p \quad \forall\, i = 1 \dots 2^N$

demand: $\sum_{i=1}^{2^N} p_i = 1 \qquad p \cdot \sum_{i=1}^{2^N} 1 = 1 \qquad p = 2^{-N}$

page 17: 5 steps; need $x=3$:

Box 1: RRRRL, RRRLR, RRLRR, RLRRR, LRRRR

Box 2: 2^5 possibilities in total; 5 events give us $x=3$:

$P(x=3) = 5/2^5$ ("fair": $p_L = p_R$)