TD 8: Markov Processes

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A random process X_t can be viewed as a family of random numbers, indexed by the label t. For each time t, X_t may obey a different probability distribution $p(x,t)$. The values of the random process at different times t, t' may or may not depend on each other. The conditional probability $p(x_n, t_n|x_{n-1}, t_{n-1}, ...x_1, t_1)$ is defined as the probability of X_{t_n} taking the value x_n, given that X_{t_i} takes the value x_i for each $i \in \{1, ..., n-1\}$. If

$$p(x_n, t_n|x_{n-1}, t_{n-1}; ...; x_1, t_1) = p(x_n, t_n), \tag{1}$$

X_t is a *purely random process*, where the values of X_t at different times are independent, which cannot describe a physical continuous dependence on time. The second simplest case,

$$p(x_n, t_n|x_{n-1}, t_{n-1}; ...; x_1, t_1) = p(x_n, t_n|x_{n-1}, t_{n-1}), \tag{2}$$

defines a *Markov process*. One also calls $p(x, t|x', t')$ *transition probability*.

Basics of Markov Chains.

1. Show that for Markov process, the n-point joint probability density reduces to

$$p(x_n, t_n; ...; x_1, t_1) = p(x_n, t_n|x_{n-1}, t_{n-1})p(x_{n-1}, t_{n-1}|x_{n-2}, t_{n-2})...p(x_2, t_2|x_1, t_1)p(x_1, t_1). \tag{3}$$

2. Show further that this implies

$$p(x_3, t_3|x_1, t_1) = \int p(x_3, t_3|x_2, t_2)p(x_2, t_2|x_1, t_1)\mathrm{d}x_2. \tag{4}$$

   This relation is known as Chapman-Kolmogorov equation.

3. *(Bonus)* For pure Brownian motion, the transition probability is:

$$p(x_2, t_2|x_1, t_1) = \frac{1}{\sqrt{4\pi(t_2 - t_1)}} e^{\frac{-(x_2-x_1)^2}{4(t_2-t_1)}},$$

   meaning that they depend only on the difference in positions and times. Show that such transition probability satisfies the Chapman-Kolmogorov equation.

The Master Equation. Consider the transition probability from some state x'' at time t to another state x at time $t + \Delta t$ for Δt small,

$$p(x, t + \Delta t|x'', t) = (1 - a(x, t)\Delta t)\delta(x - x'') + W(x, x'', t)\Delta t + O(\Delta t^2). \tag{5}$$

Here the term involving $\delta(x - x'')$ is the probability to be at the same point after Δt, while $W(x, x'', t)$ (*the rate function*) is the probability to transition from x'' to x within the time interval Δt.

4. Determine $a(x, t)$ from the constraint of normalisation.

5. Use the Chapman-Kolmogorov equation to show that

$$\partial_t p(x, t|x', t') = \int \left[W(x, x'', t)p(x'', t|x', t') - W(x'', x, t)p(x, t|x', t')\right] \mathrm{d}x''. \tag{6}$$

   This is the so-called *continuous-time master equation*, which implies,

$$\partial_t p(x, t) = \int \left[W(x, x', t)p(x', t) - W(x', x, t)p(x, t)\right] \mathrm{d}x'. \tag{7}$$

The Fokker-Planck Equation. We now want to perform an expansion to find a partial differential equation describing our process.

6. Write $W(x,x',t) = w(x',r,t)$ with $r = x - x'$. Show that the Master equation implies
$$\partial_t p(x,t) = \int [w(x-r,r,t)p(x-r,t) - w(x,-r,t)p(x,t)]\,\mathrm{d}r. \tag{8}$$
Expand the first argument of $w(x-r,r,t)p(x-r,t)$ around x (*Kramers-Moyale expansion*) to show that
$$\partial_t p(x,t) = \sum_{n=1}^{\infty} (-\partial_x)^n \,[D_n(x,t)p(x,t)], \tag{9}$$
where $D_n = \frac{1}{n!}\int w(x,r,t)r^n \mathrm{d}r$. This series may terminate at order 2, in which case we obtain the Fokker-Planck equation:
$$\partial_t p(x,t) = -\partial_x[D_1(x,t)p(x,t)] + \partial_x^2[D_2(x,t)p(x,t)]. \tag{10}$$

7. Show that the Fokker-Planck equation can be written as a conservation law $\partial_t p = \partial_x J$, write down J.

8. Assume $x \in \mathbb{R}$ and $p(x,t) \overset{x\to\pm\infty}{\to} 0$ sufficiently fast. What equation does the mean $\langle x \rangle$ obey?

9. Given two solutions $p_1(x,t), p_2(x,t)$ of the Fokker-Planck equation starting from different initial conditions, consider $H(t) = \int p_1 \ln(p_1/p_2)\mathrm{d}x$, that we assume well defined. Show that $H(t) \geq 0$ and that $\frac{\mathrm{d}}{\mathrm{d}t}H(t) \leq 0$. What does this tell us about the long-time behaviour of the solutions? Discuss.

——— *Only when you have finished all the exercises* ———

The Wikipedia Moment. LUDWIG BOLTZMANN (1844-1906).

Boltzmann was born in Erdberg, a suburb of Vienna. He received his primary education at the home of his parents. Boltzmann attended high school in Linz, Upper Austria. When Boltzmann was 15, his father died.

Starting in 1863, Boltzmann studied mathematics and physics at the University of Vienna. He received his doctorate in 1866 and his venia legendi in 1869. Boltzmann worked closely with Josef Stefan, director of the institute of physics. It was Stefan who introduced Boltzmann to Maxwell's work.

In 1872, long before women were admitted to Austrian universities, he met Henriette von Aigentler, an aspiring teacher of mathematics and physics in Graz. She was refused permission to audit lectures unofficially. Boltzmann supported her decision to appeal, which was successful. On 17 July 1876 Ludwig Boltzmann married Henriette; they had three daughters and a son.

After Vienna, Boltzmann went back to Graz to take up the chair of Experimental Physics. Among his students in Graz were Svante Arrhenius and Walther Nernst. He spent 14 happy years in Graz and it was there that he developed his statistical concept of nature.

Boltzmann's most important scientific contributions were in kinetic theory, including for motivating the Maxwell–Boltzmann distribution as a description of molecular speeds in a gas. Maxwell–Boltzmann statistics and the Boltzmann distribution remain central in the foundations of classical statistical mechanics. They are also applicable to other phenomena that do not require quantum statistics and provide insight into the meaning of temperature.

Most chemists, since the discoveries of John Dalton in 1808 shared Boltzmann's belief in atoms and molecules, but much of the physics establishment did not share this belief until decades later. Only a couple of years after Boltzmann's death, Perrin's studies of colloidal suspensions (1908–1909), based on Einstein's theoretical studies of 1905, confirmed the values of Avogadro's number and Boltzmann's constant, convincing the world that the tiny particles really exist.

This is in this context that Boltzmann introduced his famous formula for entropy $S = k\log(W)$. W is Wahrscheinlichkeit, a German word meaning the probability of occurrence of a macrostate or, more precisely, the number of possible microstates corresponding to the macroscopic state of a system — the number of (unobservable) "ways" in the (observable) thermodynamic state of a system that can be realized by assigning different positions and momenta to the various molecules.

In 1894, Boltzmann succeeded his teacher Joseph Stefan as Professor of Theoretical Physics at the University of Vienna. Boltzmann spent a great deal of effort in his final years defending his theories. In 1895, Georg Helm and Wilhelm Ostwald presented their position on energetics at a meeting in Lübeck. They saw energy, and not matter, as the chief component of the universe. Boltzmann's position carried the day among other physicists who supported his atomic theories in the debate.

In 1906, Boltzmann's deteriorating mental condition forced him to resign his position, and his symptoms indicate he experienced what would today be diagnosed as bipolar disorder. Four months later he died by suicide on 5 September 1906, by hanging himself while on vacation with his wife and daughter. His tombstone bears the inscription of Boltzmann's entropy formula: $S = k\log(W)$.