TD 5: From Diffusion to Large Deviations

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1 Diffusion Equation. In this exercise we solve explicitly the diffusion equation

$$\partial_t u = D\partial_x^2 u \tag{1}$$

over $\mathbb{R}^+ \times \mathbb{R}$ with initial condition $u(t=0,x) = u_0(x)$.

1. Show that we have the following similarity principle: if $u(t,x)$ is solution for $t > 0$ then $v(t,x) = u(\lambda t, \sqrt{\lambda}x)$ is solution too.

2. Heuristically, why can we expect to be able to restrict the partial differential equation in an ordinary differential equation with variable $s = \frac{x}{\sqrt{Dt}}$?

3. We define $u(t,x) = v\left(\frac{x}{\sqrt{Dt}}\right)$. Find an equation for v.

4. Solve the equation in v by imposing $u_0(x=0)$.

5. The previous solution is only partial because we have imposed the invariance by the dilatation λ but u_0 may be not non constant. To get the complete solution, the idea is then to perform a convolution between the kernel
$$K(t,x) = \frac{1}{\sqrt{4\pi Dt}} e^{-x^2/4Dt} \tag{2}$$
and the initial condition u_0. Check that K is solution of the diffusion equation and give the general solution.

6. (Bonus) Solve the diffusion equation using a Fourier transform.

2 Central Limit Theorem. We consider a series (X_n) of random variables which are independent and of identical distribution. We assume X to have moments of order 2 (*i.e.* the variance is well defined). We denote μ the mean and σ is mean-squared value of the distribution. We finally denote $S_n = \sum_{i=1}^n X_i$.

1. Prove Markov identity: let A be a positive random variable and $\epsilon > 0$, then
$$\mathbb{P}(A \geq \epsilon) \leq \frac{\mathbb{E}(A)}{\epsilon}. \tag{3}$$

2. Deduce the law of Large Numbers:
$$\frac{1}{n}S_n \longrightarrow \mu \tag{4}$$
where the limit is defined by: $\forall \epsilon > 0$, for large enough n, $\mathbb{P}(|\frac{1}{n}S_n - \mu| \geq \epsilon) \leq \epsilon$. A stronger version (the almost sure convergence) of this theorem can also be proved.

3. We denote $\varphi_X(t) = \mathbb{E}\left(e^{itX}\right)$ the characteristic function of X. This is the Fourier transform of its distribution. Express $\varphi_{\sqrt{n}(\frac{1}{n}S_n - \mu)}$ as a function of φ_Y where $Y = X - \mu$.

4. Give an estimate at second order of φ_Y when $t \to 0$.

5. Deduce the limit of $\varphi_{\sqrt{n}(\frac{1}{n}S_n - \mu)}$ when $n \to +\infty$ for infinitesimal t.

6. We admit Levy's theorem which states if φ_{X_n} converges to the characteristic function of some distribution X_∞, then $X_n \to X_\infty$. Deduce an expansion of $\frac{1}{n}S_n$ at order $o\left(\frac{1}{\sqrt{n}}\right)$. This is the Central Limit Theorem (CLT).

2 Beyond the Central Limit Theorem: the Large Deviations. In practice some events do happen and can be physically crucial. The goal of Large Deviation theory is to estimate the probability of such rare events. We use the same notations than is the previous exercise and denote p the distribution of X. We also assume X not to be almost sure (*i.e.* its distribution is not a Dirac).

1. Let $a \geq \mu$. Prove that for any $\lambda \geq 0$, we have

$$\mathbb{P}\left(\frac{1}{n}S_n \geq a\right) \leq e^{n(m(\lambda)-\lambda a)} \tag{5}$$

   where $m(\lambda) = \ln\left(\mathbb{E}\left(e^{\lambda X}\right)\right) = \ln\left(\int e^{\lambda x}\mathrm{d}p(x)\right)$.

2. We now want to optimize our estimate. We denote $f(\lambda) = m(\lambda) - \lambda a$. Study the form of this function and deduce that it admits a unique minimum for some $\lambda \geq 0$.

3. We denote $\bar{\lambda}$ this minimum and $\Omega(a) = f(\bar{\lambda})$ the grand deviations function. Similarly, we define Ω for $a \leq \mu$. When is Ω maximum? What is its maximum value?

4. Calculate $m'(\bar{\lambda})$ and $\Omega'(a)$. Do these relations remind you something?

5. Study the function Ω.

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

The Wikipedia Moment. RUDOLF CLAUSIUS (1822-1888).

Clausius was born in Köslin (now Koszalin, Poland) in the Province of Pomerania in Prussia. His father was a Protestant pastor and school inspector, and Rudolf studied in the school of his father. Clausius graduated from the University of Berlin in 1844 where he had studied mathematics and physics since 1840 with, among others, Gustav Magnus, Peter Gustav Lejeune Dirichlet and Jakob Steiner. He also studied history with Leopold von Ranke.

During 1848, he got his doctorate from the University of Halle on optical effects in Earth's atmosphere. Clausius's PhD thesis concerning the refraction of light proposed that we see a blue sky during the day, and various shades of red at sunrise and sunset (among other phenomena) due to reflection and refraction of light. Later, Lord Rayleigh would show that it was in fact due to the scattering of light, but regardless, Clausius used a far more mathematical approach than some have used.

In 1850 he became professor of physics at the Royal Artillery and Engineering School in Berlin and Privatdozent at the Berlin University. His most famous paper, Ueber die bewegende Kraft der Wärme ("On the Moving Force of Heat and the Laws of Heat which may be Deduced Therefrom") was published in 1850, and dealt with the mechanical theory of heat. In this paper, he showed that there was a contradiction between Carnot's principle and the concept of conservation of energy defended by Joule. Clausius restated the two laws of thermodynamics to overcome this contradiction (the third law was developed by Walther Nernst, during the years 1906–1912). This paper made him famous among scientists. Clausius's most famous statement of thermodynamics second law was published in German in 1854, and in English in 1856: "Heat can never pass from a colder to a warmer body without some other change, connected therewith, occurring at the same time."

In 1855 he became professor at the ETH Zürich, where he stayed until 1867. During that year, he moved to Würzburg and two years later, in 1869 to Bonn. During that period, in 1857, Clausius contributed to the field of kinetic theory after refining August Krönig's very simple gas-kinetic model to include translational, rotational and vibrational molecular motions. In this same work he introduced the concept of 'Mean free path' of a particle. In 1865, Clausius gave the first mathematical version of the concept of entropy, and also gave it its name. Clausius chose the word from the Greek of "transformation". He used the now abandoned unit 'Clausius' (symbol: Cl) for entropy. Clausius also deduced the Clausius–Clapeyron relation from thermodynamics. This relation, which is a way of characterizing the phase transition between two states of matter such as solid and liquid, had originally been developed in 1834 by Émile Clapeyron.

In 1870 Clausius organized an ambulance corps in the Franco-Prussian War. He was wounded in battle, leaving him with a lasting disability. He was awarded the Iron Cross for his services. His wife, Adelheid Rimpau died in 1875, leaving him to raise their six children. In 1886, he married Sophie Sack, and then had another child. Two years later, on 24 August 1888, he died in Bonn, Germany.