1 Problematic moments of a probability distribution

Consider the probability density function

$$f(x) = c\left[\frac{\gamma}{(x-x_0)^2+\gamma^2}\right] \tag{1}$$

with $\gamma > 0$ and $-\infty < x_0 < \infty$, which is known as the Cauchy distribution in mathematics and as the Lorentz distribution in physics.

a) Calculate the normalization constant $c > 0$ and the median of the distribution for $\gamma = 1$ and $x_0 = 0$.

Any probability density function $f(x)$ must fulfill the normalization condition

$$1 = \int_{-\infty}^{\infty} f(x) \cdot dx \tag{2}$$

$$= \int_{-\infty}^{\infty} c \cdot \left[\frac{\gamma}{(x-x_0)^2+\gamma^2}\right] \cdot dx \tag{3}$$

$$= \frac{c}{\gamma} \cdot \int_{-\infty}^{\infty} \left[\frac{1}{(\frac{x-x_0}{\gamma})^2+1}\right] \cdot dx \tag{4}$$

$$= \frac{c}{\gamma} \cdot \int_{-\infty}^{\infty} \left[\frac{1}{z^2+1}\right] \cdot dz \qquad \text{with } z := \frac{x-x_0}{\gamma} \tag{5}$$

$$= \frac{c}{\gamma} \cdot \left[\arctan(z)\right]_{-\infty}^{\infty} \tag{6}$$

$$= \frac{c}{\gamma} \cdot \left(\frac{\pi}{2} - \left(-\frac{\pi}{2}\right)\right) \tag{7}$$

$$= \frac{c}{\gamma} \cdot \pi \tag{8}$$

$$\Rightarrow c = \frac{\gamma}{\pi} \tag{9}$$

Addition: The integral

$$\int_{\infty}^{\infty} \frac{dx}{1+x^2} \tag{10}$$

can be solved beautifully with complex analysis. Notice that from the residue theorem follows

$$\int_{\infty}^{\infty} \frac{dx}{1+x^2} = \oint \frac{dx}{(x+i)(x-i)} = 2\pi i \mathrm{Res}\left(\frac{1}{1+x^2}, i\right) = \pi. \tag{11}$$

The residue is given by

$$\mathrm{Res}\left(\frac{1}{1+x^2}, i\right) = \lim_{x\to i} (x-i)\frac{1}{1+x^2} = \lim_{x\to i} \frac{1}{x+i} = \frac{1}{2i}. \tag{12}$$

For the median x_m, we have to solve

$$\frac{1}{2} = \int_{-\infty}^{x_m} f(x) \cdot dx \tag{13}$$
$$= \int_{-\infty}^{x_m} c \cdot \left[\frac{\gamma}{(x-x_0)^2 + \gamma^2} \right] \cdot dx \tag{14}$$
$$= \frac{c}{\gamma} \cdot \left[\arctan(z) \right]_{-\infty}^{x_m} \tag{15}$$
$$= \frac{c}{\gamma} \cdot \left(\arctan(x_m) + \frac{\pi}{2} \right) \tag{16}$$
$$\Rightarrow x_m = \tan\left(\frac{\gamma}{2c} - \frac{\pi}{2} \right) ??? \tag{17}$$

Addition: In general, every symmetric distribution has median 0 from symmetry reasons.

b) Try to evaluate the first two moments of the distribution. What problem arises? Compare the situation to the Gaussian distribution and comment on the implications for large derivations from the median.

First moment:

$$\int_{-\infty}^{\infty} x \cdot f(x) \cdot dx = \int_{-\infty}^{\infty} c \cdot \left[\frac{\gamma \cdot x}{(x-x_0)^2 + \gamma^2} \right] \cdot dx \tag{18}$$
$$= \frac{c}{\gamma} \cdot \int_{-\infty}^{\infty} \left[\frac{x}{(\frac{x-x_0}{\gamma})^2 + 1} \right] \cdot dx \tag{19}$$

Second moment:

$$\int_{-\infty}^{\infty} x^2 \cdot f(x) \cdot dx = \int_{-\infty}^{\infty} c \cdot \left[\frac{\gamma \cdot x^2}{(x-x_0)^2 + \gamma^2} \right] \cdot dx \tag{20}$$
$$= \frac{c}{\gamma} \cdot \int_{-\infty}^{\infty} \left[\frac{x^2}{(\frac{x-x_0}{\gamma})^2 + 1} \right] \cdot dx \tag{21}$$

The problem that arises is that both of these integrals do not converge.

Implications?

2 Stationary limit of the overdamped Fokker-Planck equation

In the lecture, the Fokker-Planck equation was derived for constant drift velocity v and constant diffusion constant D. In the case that they are not constant, the Fokker-Planck equation reads

$$\dot{p}(x,t) = -\partial_x\Big(v(x)p(x,t)\Big) + \partial_x^2\Big(D(x)p(x,t)\Big) \tag{22}$$

To find the stationary limit, the left hand side $\dot{p}(x,t)$ is set to zero.

a) Consider an overdamped particle in one dimension with a harmonic potential $U(x) = \frac{1}{2}kx^2$ (k is the spring constant). This could be e.g. a colloid in an optical trap. Use the balance between friction force ξv (ξ is the friction coefficient) and potential force $-\partial_x U(x)$ to replace $v(x)$ in this equation. D is assumed to be constant. Solve for the stationary distribution $p_s(x)$. Note that both $p_s(x)$ and its derivative should vanish at $x = \pm\infty$.

From the balance between friction force ξv and potential force $-\partial_x U(x)$ we can deduce

$$\begin{aligned}\xi v(x) &= -\partial_x U(x)\\ &= -kx\\ \Rightarrow v(x) &= -\frac{kx}{\xi}.\end{aligned} \tag{23}$$

Assuming D to be constant, we get

$$\begin{aligned}\dot{p}(x,t) &= -\partial_x\Big(v(x)p(x,t)\Big) + \partial_x^2\Big(D(x)p(x,t)\Big)\\ \dot{p}(x,t) &= \frac{k}{\xi}p(x,t) + \frac{kx}{\xi}\partial_x p(x,t) + D\partial_x^2 p(x,t).\end{aligned} \tag{24}$$

The stationary solution is given where $\dot{p}(x,t) = 0$. Thus

$$0 = \frac{k}{\xi D}p(x) + \frac{kx}{\xi D}p'(x) + p''(x). \tag{25}$$

Ansatz: Gauss function $p \propto e^{-\lambda x^2}$. Then solve for λ and find

$$\lambda = \frac{k}{2D\xi}. \tag{26}$$

b) Compare to the Boltzmann distribution $p_s(x) \sim \exp\left(-\frac{U(x)}{k_B T}\right)$ and from this derive a relation between diffusion constant D and friction coefficient ξ.

We see that we get $p(x) \sim \exp\left(-\frac{kx^2}{2D\xi}\right)$. In comparison to the Boltzmann distribution, one can see:

$$\frac{U(x)}{k_B T} = \frac{kx^2}{2D\xi}\,, \tag{27}$$

$$\frac{1}{2k_B T} = \frac{1}{2D\xi}\,, \tag{28}$$

$$k_B T = \xi D\,. \tag{29}$$

c) Calculate the first and second moments of the stationary distribution. Interpret your results in terms of physics.

First, you have to find the normalization c then calculate the integrals

$$< x > = c \int_{-\infty}^{\infty} dx\; x e^{-\lambda x^2}\,, \tag{30}$$

$$< x^2 > = c \int_{-\infty}^{\infty} dx\; x^2 e^{-\lambda x^2}\,. \tag{31}$$

From symmetry, one can see that the first moment is zero because we integrate an anti-symmetric function over a symmetric intervall.
Carrying out the other integral yields for the second moment: $< x^2 >= D\xi/k$.

3 Information entropy

a) Reservoirs for energy and particle number: Consider a system in a fixed volume that not only exchanges energy but also particles with the surrounding. To calculate the probability distribution p_i, maximize the information (Shannon) entropy $S = -\sum_i p_i \log p_i$ under the joint conditions of normalization, of $U = \sum_i p_i E_i$ (mean energy) and $N = \sum_i p_i N_i$ (mean particle number). What physical meaning has the new Lagrangian multiplier associated to the condition in N?

Consider the function

$$f(p_i) = -\sum_i p_i \ln p_i - \lambda_1 \left(\sum_i p_i - 1\right) - \lambda_2 \left(\sum_i p_i E_i - U\right) - \lambda_3 \left(\sum_i p_i N_i - N\right). \tag{32}$$

The Lagrangian multipliers are responsible for the respective constraints like normalization, mean energy and mean particle number. The variation with respect to the probability distribution yields

$$\delta f(p_i) = -\left(\ln p_i + 1 + \lambda_1 + \lambda_2 E_i + \lambda_3 N_i\right) \delta p_i \overset{!}{=} 0. \tag{33}$$

Which in fact yields the following for the probability distribution:

$$p_i = e^{-(1+\lambda_1+\lambda_2 E_i+\lambda_3 N_i)}. \tag{34}$$

Now, apply the first constraint (normalization) to find λ_1:

$$\sum_i p_i = e^{-(1+\lambda_1)} Z = 1. \tag{35}$$

Here, we defined the partition sum $Z = \sum_i e^{-(\lambda_2 E_i+\lambda_3 N_i)}$. From the other constraints we find λ_2 and λ_3. The Lagrangian multiplier for N plays the role of the chemical potential. One can find the analogies:

$$\lambda_2 = \beta\,, \qquad \lambda_3 = \beta\mu\,, \tag{36}$$

to recover the probability distribution

$$p_i = \frac{1}{Z} e^{-\beta(E_i+\mu N_i)}\,. \tag{37}$$

b) Rational probabilities: if one does not know the probabilities of events, one can define so-called rational probabilities $\bar{p}$ such that entropy is maximized subject to the constraints imposed by the available information. Assume that in a certain game, a player can score any integer $n = 0, 1...$ and it is known that the mean score is μ. Use again the entropy and the method of Lagrange multipliers to show that when imposing the relevant constraints the rational choice is $\bar{p}_n = \frac{\mu^n}{(1+\mu)^{n+1}}$

We follow the same procedure. Now, the function would look like this:

$$f(p_i) = -\sum_i p_i \ln p_i - \lambda_1 \left(\sum_i p_i - 1\right) - \lambda_2 \left(\sum_n p_n n - \mu\right)\,. \tag{38}$$

Variation with respect to p_n yields

$$p_n = e^{-(1+\lambda_1+\lambda_2 n)}\,. \tag{39}$$

From the normalization condition we get:

$$p_n = \frac{1}{Z} e^{-\lambda_2 n}\,, \tag{40}$$

where $Z = \sum_n e^{-\lambda_2 n} = \frac{1}{1-e^{-\lambda_2}}$ is the geometrical series. From the constraint for μ we find:

$$\mu = \sum_n n p_n = \frac{1}{Z} \sum_n n e^{-\lambda_2 n} = -\frac{1}{Z} \partial_{\lambda_2} \sum_n e^{-\lambda_2 n} = -\partial_{\lambda_2} \ln Z = \frac{e^{-\lambda_2}}{1-e^{-\lambda_2}}\,. \tag{41}$$

This can be inverted to give

$$\lambda_2 = \ln\left(\frac{1+\mu}{\mu}\right)\,. \tag{42}$$

Thus, we obtain

$$p_n = \frac{1}{Z} e^{-\lambda_2 n} = e^{-\lambda_2 n}\left(1 - e^{-\lambda_2}\right) = \left(\frac{\mu}{1+\mu}\right)^n \left(1 - \frac{\mu}{1+\mu}\right) = \frac{\mu^n}{(1+\mu)^{n+1}}\,. \tag{43}$$