Statistical Physics & Thermodynamics

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Exercise 3.1: Normal distribution (6P)

The probability density function of the normal distribution with zero mean and variance σ^2 is given by

$$p(x) \;=\; \frac{1}{\sigma\sqrt{2\pi}}\, e^{-\frac{x^2}{2\sigma^2}}\,.$$

(a) Derive a recursion relation for the moments which expresses m_n in terms of m_{n-2}. The relation can be derived by partial integration of the defining integral. (2P)

(b) Apply this recursion relation to compute the first six moments $m_1, \ldots, m_6$. (1P)

(c) Derive the moment-generating function of the normal distribution given above. Hint: Try quadratic completion (quadratische Ergänzung) in the integrand. (2P)

(d) Compute all cumulants κ_n of the normal distribution given above from the cumulant-generating function. (1P)

Sample Solution

(a) The definition of the n-th moment of a continuous pdf reads

$$\langle x^n \rangle = \frac{1}{\sigma\sqrt{2\pi}} \int_{-\infty}^{+\infty} x^n e^{-\frac{x^2}{2\sigma^2}}\,\mathrm{d}x$$

Integrating the right hand side (rhs) by parts we obtain

$$\langle x^n \rangle = \left[\frac{1}{\sigma\sqrt{2\pi}}\frac{1}{n+1}x^{n+1}e^{-\frac{x^2}{2\sigma^2}}\right]_{-\infty}^{+\infty} - \frac{1}{\sigma\sqrt{2\pi}}\int_{-\infty}^{+\infty}\frac{1}{n+1}x^{n+1}\frac{-x}{\sigma^2}e^{-\frac{x^2}{2\sigma^2}}\,\mathrm{d}x.$$

Since the exponential part vanishes faster than any polynomial, the boundary terms do not contribute. The remaining expression reads

$$\langle x^n \rangle = \frac{1}{\sigma^2(n+1)}\,\langle x^{n+2}\rangle$$

or equivalently (shifting $n \to n-2$):

$$\langle x^n \rangle \;=\; \sigma^2(n-1)\,\langle x^{n-2}\rangle \qquad \Rightarrow \qquad m_n = \sigma^2(n-1)m_{n-2}\,.$$

(b) By symmetry all odd moments vanish, hence we only have to compute the even moments. The zeroth moment is the norm $m_0 = 1$, which anchors the recursion. Applying the recursion relation step by step we obtain:

$$\begin{aligned} m_2 &= \sigma^2 \\ m_4 &= 3\sigma^4 \\ m_6 &= 5\cdot 3\cdot \sigma^6 = 15\sigma^6 \end{aligned}$$

From here we can guess and prove the following solution (not required):

$$m_n = (n-1)(n-3)\cdots 3\cdot 1\cdot \sigma^n = \frac{n!}{(n/2)!2^{n/2}}\sigma^n$$

(c) We start with the definition of the moment-generating function

$$M(t) = \langle e^{xt} \rangle \;=\; \frac{1}{\sigma\sqrt{2\pi}} \int_{-\infty}^{+\infty} e^{xt} e^{-\frac{x^2}{2\sigma^2}}\, \mathrm{d}x$$

The integral on the rhs can be calculated by completion of the square (quadratische Ergänzung). To this end we shift the integration variable by $x \to x + \mu$, getting

$$M(t) = \frac{1}{\sigma\sqrt{2\pi}} \int_{-\infty}^{+\infty} e^{xt+\mu t - \frac{x^2+2\mu x+\mu^2}{2\sigma^2}}\, \mathrm{d}x$$

The method of completing the square amounts to choosing μ in such a way that the two terms which are linear in x cancel. This can be achieved by setting $\mu = t\sigma^2$. In addition, the x-independent parts can be pulled out. The remaining expression reads

$$M(t) = e^{t^2\sigma^2 - \frac{t^2\sigma^4}{2\sigma^2}} = e^{\frac{1}{2}t^2\sigma^2}\,.$$

It is straightforward to verify that the moments computed in part (b) are correctly reproduced by this function (not required).

(d) The cumulant-generating function of the normal distribution is particularly simple:

$$K(t) = \ln M(t) = \frac{1}{2}\sigma^2 t^2$$

Therefore, the normal distribution (with zero mean) possesses only a single non-vanishing cumulant, namely, $\kappa_2 = \sigma^2$, which is just the variance. This is in fact the most salient feature of the normal distribution: It has no properties (such as skewness and curtosis) except for the variance.

Exercise 3.2: Stirling's formula **(6P)**

In statistical physics, the Stirling formula $n! \approx \sqrt{2\pi n}\left(\frac{n}{e}\right)^n$ is frequently used to approximate the factorial $n!$ in combinatorical factors.

(a) Compute $ln(n!)$. (1P)

(b) Prove the somewhat weaker inequality

$$n\ln(n) - n \;<\; \ln(n!) \;<\; n\ln(n)$$

by comparing the power series of e^n to its nth term. (2P)

(c) Consider $\ln(n!)$. Derive an approximation by naively replacing the sum by an integral from 1 to n. Does it over- or underestimate $\ln(n!)$? (1P)

(d) Shifting both bounds of the integral by 1 you can find another bound on the opposite side so which gives you a different inequality $\ldots < \ln(n!) < \ldots$. (1P)

(e) Plot the stirling approximation $\ln\left[\sqrt{2\pi n}\left(\frac{n}{e}\right)^n\right]$, as well as the bounds of part (b) and part (d), all of them divided by the correct value $\ln(n!)$, for $n = 1, 2, 3, 4, 5$, and compare the accuracy of the respective bounds. (1P)

Sample Solution

(a) Taking the logarithm on both sides of $n! \approx \sqrt{2\pi n}\left(\frac{n}{e}\right)^n$ we get

$$\ln(n!) \approx \frac{1}{2}\ln(2\pi) + (n + \frac{1}{2})\ln(n) - n.$$

(b) Re-exponentiating this double-inequality gives

$$\frac{n^n}{e^n} \quad < \quad n! \quad < \quad n^n$$

The right inequality is trivial since $1 \cdot 2 \cdot 3 \cdots n < n \cdot n \cdot n \cdots n$. To prove the left inequality we write down the power series of $e^n = \sum_{k=0}^{\infty} \frac{n^k}{k!}$. In this series all terms are positive, hence the total series is strictly larger than its own nth term, i.e., $e^n > n^n/n!$. Sorting the terms this is just the left inequality.

(c) Take the logarithm and replace the sum by an integration:

$$\ln(n!) = \sum_{k=1}^{n} \ln k = \sum_{k=2}^{n} \ln k \approx \int_1^n \ln(\tilde{x})\, \mathrm{d}\tilde{x} = 1 + n\ln(n) - n$$

The approximation underestimates $\ln(n!)$ because the summand $\ln k$ is replaced by $\int_{k-1}^{k} \ln(\tilde{x})\, \mathrm{d}\tilde{x}$ and $\ln \tilde{x}$ is monotonously increasing.

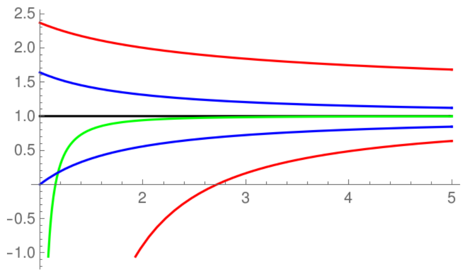
(d) Shifting the integration by one unit gives another approxmation:

$$\ln(n!) = \sum_{k=1}^{n} \ln k = \sum_{k=2}^{n} \ln k \approx \int_2^{n+1} \ln(\tilde{x})\, \mathrm{d}\tilde{x} = -n + (n+1)\log(n+1) + 1 - \log(4)$$

This approximation overestimates $\ln(n!)$ for analogous reasons as in (c). We therefore end up with

$$1 + n\ln(n) - n \quad < \quad \ln(n!) \quad < \quad -n + (n+1)\log(n+1) + 1 - \log(4)\,.$$

The figure shows the bounds divided by the exact value $\ln(n!)$: black=exact, green=Stirling, red=(b), blue=(d). Thus the inequality obtained in (d) is sharper than than the inequality (b) and Stirling (green) is much much better than both of them.




```
curves = {
    Log[Gamma[n + 1]],
    Log[Sqrt[2 Pi n] (n/E)^n],
    Log[n^n/E^n],
    Log[n^n],
    1 - n + n Log[n],
    1 - n - Log[4] + (1 + n) Log[1 + n]} / Log[Gamma[n + 1]] //Simplify;
  Plot[curves, {n, 1, L}, PlotStyle -> {Black, Green, Red, Red, Blue, Blue}]
```

(Σ = 12P)