

**Problem 1. Central limit theorem** Consider a one-dimensional system consisting of a large number of non-interacting particles on a circle of circumference  $L$ . Assume that the positions of the particles are independent random variables (i.r.v.) uniformly distributed on the circle.

**1.1** Find the probability  $p_N(t, \alpha)$  of observing exactly  $\alpha N$  of the  $N$  particles in a fixed arc of length  $tL$ , where  $t, \alpha \in [0, 1]$ . (For  $\alpha = 0$  this is called *gap* (or *void*) *formation probability*.)

Find the leading behavior of the result in the limit  $N \rightarrow \infty$  with  $t, \alpha$  fixed. (You may use the Stirling formula  $n! \approx n^n e^{-n} \sqrt{2\pi n}$ . A good sanity check for the answer is that  $\int_0^1 p_N(t, \alpha) d\alpha$  evaluated with a computer should be 1.)

Make a plot of this leading term as a function of  $\alpha \in [0, 1]$  for  $N = 100$  and  $t = 0.1$ , overlaid with the exact discrete distribution. Describe any qualitative changes in the plot as  $N$  and  $t$  change, and whether the asymptotic approximation breaks down anywhere.

**Solution.** Consider a single particle  $i$  on the circle. The probability of observing it in an arc of length  $tL$  is  $p = t$ . This is equivalent to a Bernoulli trial with failure probability  $q = 1 - p = 1 - t$ . The binomial distribution gives the probability of obtaining exactly  $n$  successes out of  $N$  such trials [1]:

$$P_p(n|N) = \binom{N}{n} p^n q^{N-n} = \frac{N!}{n! (N-n)!} p^n (1-p)^{N-n}. \quad (1)$$

Assuming  $n = \alpha N$  is an integer, the probability of observing  $\alpha N$  of the  $N$  particles in this arc is given by

$$p_N(t, \alpha) = \frac{N!}{(\alpha N)! (N - \alpha N)!} t^{\alpha N} (1-t)^{N-\alpha N}. \quad (2)$$

To find the leading behavior as  $N \rightarrow \infty$ , we use Stirling's approximation for  $N!$ ,  $(\alpha N)!$ , and  $(N - \alpha N)!$ . In doing so, we assume  $N, \alpha N, (1 - \alpha)N \gg 1$ . This yields

$$\begin{aligned} p_N(t, \alpha) &\approx \frac{N^N e^{-N} \sqrt{2\pi N}}{(\alpha N)^{\alpha N} e^{-\alpha N} \sqrt{2\pi \alpha N} (N - \alpha N)^{N-\alpha N} e^{-(N-\alpha N)} \sqrt{2\pi (N - \alpha N)}} t^{\alpha N} (1-t)^{N-\alpha N} \\ &= \frac{N^{N-\alpha N}}{\alpha^{\alpha N} N^{N-\alpha N} (1-\alpha)^{N-\alpha N} \sqrt{2\pi \alpha (N - \alpha N)}} t^{\alpha N} (1-t)^{N-\alpha N} \\ &= \frac{1}{\sqrt{2\pi \alpha (1-\alpha) N}} \left(\frac{t}{\alpha}\right)^{\alpha N} \left(\frac{1-t}{1-\alpha}\right)^{N-\alpha N}. \end{aligned} \quad (3)$$

A plot comparing this approximation to the exact, discrete distribution is shown in Fig. 1 as a function of  $\alpha \in [0, 1]$  for  $N = 100$  and  $t = 0.1$ . Both distributions becomes broader and shorter as  $t$  is increased to 0.5, and then narrower and taller as  $t$  is increased from there. The area under the curve becomes smaller as  $N$  increases, although its shape does not change. This makes sense because  $p_N(t, \alpha)$  as a function of  $\alpha$  is not a PDF; the PDF is  $P_t(k|N)$  as a function of  $k = \alpha N$ . The area under the curve of  $p_N(t, \alpha)$  is  $1/N$ .

For  $t \lesssim 0.2$  and  $t \gtrsim 0.8$ , the approximate distribution has a slightly sharper and higher peak than the discrete distribution. This is slightly visible in Fig. 1 This discrepancy becomes more pronounced as  $N$  decreases. For  $N \lesssim 20$ , a discrepancy near the peak is visible even for  $t = 0.5$ . The approximation visibly diverges as  $\alpha \rightarrow 0$  for  $t \lesssim 0.2$  and as  $\alpha \rightarrow 1$  for  $t \gtrsim 0.8$ . This effect becomes more pronounced as  $N$  decreases. For  $N \lesssim 25$ , this divergence overtakes the expected behavior of the discrete distribution, and so the approximation becomes poor.

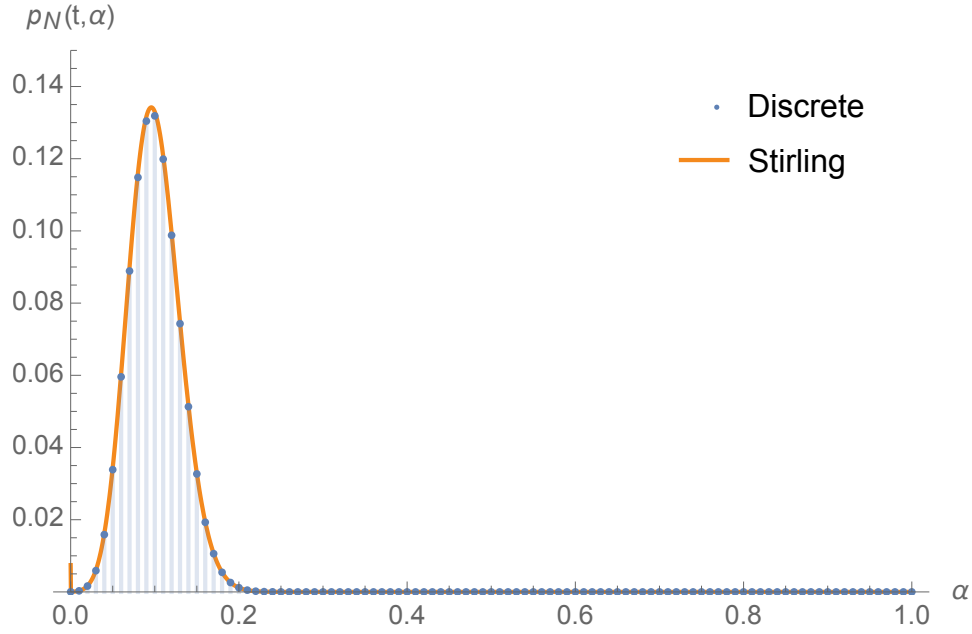


Figure 1: Comparison of the discrete expression ((2), blue) and Stirling's approximation to ((3), orange)  $p_N(t, \alpha)$  as functions of  $\alpha \in [0, 1]$  for  $N = 100$  and  $t = 0.1$ .

**1.2** In the large- $N$  limit, find the average number  $k$  (or the fraction  $\alpha = k/N$ ) of particles in the arc of length  $tL$  for a given  $t \in [0, 1]$ , and the fluctuation (variance) of this number, using the Central Limit Theorem. Plot the corresponding Gaussian distribution over  $\alpha \in [0, 1]$  and add it to the previous plot. How good is this approximation?

**Solution.** The mean of the binomial distribution is  $\mu = Np$ , and the variance is  $\sigma^2 = Npq$  [1]. Thus, the mean and variance of (2) are,

$$\mu_B = Nt, \quad \sigma_B^2 = Nt(1-t),$$

which correspond to the average number of particles in  $tL$  and the variance of that number, respectively.

By the Central Limit Theorem, we may approximate (2) by a Gaussian distribution [2]

$$P(x) = \frac{e^{-(x-\mu)^2/(2\sigma^2)}}{\sigma\sqrt{2\pi}},$$

with mean  $\mu_G = \mu_B = Nt$  and standard deviation  $\sigma_G = \sigma_B/\sqrt{N} = \sqrt{t(1-t)}$  [3]. (The factor of  $1/N$  in the variance is necessary because  $p_N(t, \alpha)$  is not normalized.) Since  $x$  is equivalent to  $k = \alpha N$ , this gives us the Gaussian distribution

$$p_N(t, \alpha) \approx \frac{e^{-N^2(\alpha-t)^2/2t(1-t)}}{\sqrt{2\pi t(1-t)}}. \quad (4)$$

This distribution is shown overlaid with the discrete distribution and Stirling's approximation in Fig. 2. The CLT approximation, being Gaussian, is perfectly symmetrical for all  $t$ , unlike the discrete function and Stirling's approximation, which both become more skew as  $t \rightarrow 0$  and  $t \rightarrow 1$ . This effect is visible in Fig. 2. The CLT is a worse approximation than Stirling in these cases, except when  $N$  is very large ( $\gtrsim 1000$ ). In this limit, the quality of both approximations is about the same. However, the CLT approximation has no singularities, making it a better approximation when  $\alpha, t \approx 0$  and  $\alpha, t \approx 1$ .

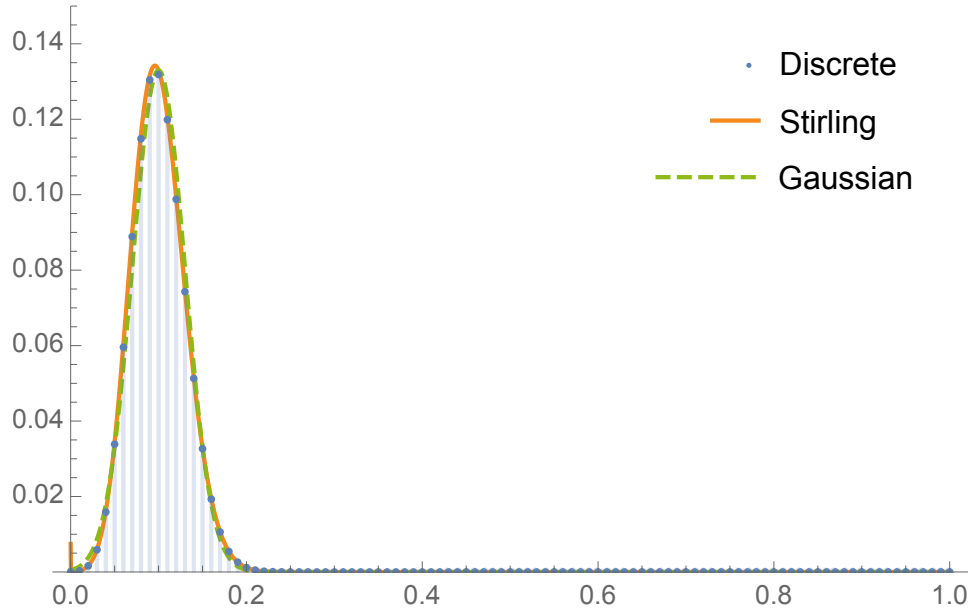


Figure 2: Comparison of the discrete expression ((2), blue), Stirling's approximation to ((3), orange), and CLT approximation to ((4), green)  $p_N(t, \alpha)$  as functions of  $\alpha \in [0, 1]$  for  $N = 100$  and  $t = 0.1$ .

**1.3** Defining the number density  $n(x) = \sum_{i=1}^N \delta(x - x_i)$ , compute the two-point correlation function

$$C(x, y) = \langle \delta n(x) \cdot \delta n(y) \rangle, \quad \delta n(x) = n(x) - \langle n \rangle,$$

which describes the fluctuations of the density.

**Solution.** Firstly, the mean  $\langle n \rangle$  is found by

$$\langle n \rangle = \frac{1}{L} \int_0^L n(x) dx = \frac{1}{L} \int_0^L \sum_{i=1}^N \delta(x - x_i) dx = \frac{1}{L} \sum_{i=1}^N \int_0^L \delta(x - x_i) dx = \frac{N}{L}.$$

Then

$$\begin{aligned} C(x, y) &= \frac{1}{L^2} \int_0^L \int_0^L \delta n(x) \delta n(y) dx dy = \frac{1}{L^2} \int_0^L \left( \sum_{i=1}^N \delta(x - x_i) - \frac{N}{L} \right) dx \int_0^L \left( \sum_{i=1}^N \delta(y - y_i) - \frac{N}{L} \right) dy \\ &= \frac{1}{L^2} \left( \sum_{i=1}^N \int_0^L \delta(x - x_i) dx - \frac{N}{L} \int_0^L dx \right) \left( \sum_{i=1}^N \int_0^L \delta(y - y_i) dy - \frac{N}{L} \int_0^L dy \right) \\ &= \frac{1}{L^2} \left( N - \frac{N}{L} \left[ x \right]_0^L \right) \left( N - \frac{N}{L} \left[ y \right]_0^L \right) \\ &= 0. \end{aligned}$$

This result suggests that the positions of different particles on the circles are not correlated [4]. This makes sense, because the locations of the particles are random and uniformly distributed, and the particles do not interact with one another.

## Problem 2. Entropy of simple systems

**2.1 Two-level systems** Consider a gas consisting of an even number  $N$  of non-interacting atoms with spins  $\sigma_i$ ,  $i = 1, \dots, N$ . The spin of each atom can take on the values  $\sigma_i = \pm 1$  with equal probability.

**2.1.1** What is the probability of a state with zero total magnetization? Determine the leading approximation for this probability in the limit  $N \rightarrow \infty$ .

**2.1.2** Let us place the atoms in a magnetic field  $h$ , so that the Hamiltonian becomes

$$H = -h \sum_{i=1}^N \sigma_i.$$

Find the total number of states at a fixed energy  $E$  and the entropy per atom in the limit  $N \rightarrow \infty$  assuming that the energy per atom  $\epsilon = E/N$  is kept fixed.

**2.1.3** Compute the temperature of this system using  $1/T = (\partial S / \partial E)_N$ . Show that this result determines  $\epsilon$ , the average energy per atom, as a function of temperature.

**2.1.4** Finally, compute the specific heat  $C(T, h)$ .

**2.2 Trapped atoms** Calculate the volume of the phase space for  $N$  classical non-interacting massive particles placed in a harmonic trap (i.e. a potential  $V(r) = m\omega^2 r^2/2$ ) with energies of at most  $E$ . Use it to calculate the entropy and the temperature.

**2.3 Three-level system** Consider a system of  $N$  independent atoms. Each atom may be in one of three states with energies  $-\epsilon, 0, \epsilon$ . Assume that the total energy of the gas is  $E = M\epsilon$ ,  $|M| \leq N$ . Calculate the entropy of the system and find the relation between the temperature and the energy. Also expand the results in the two special limits  $T \ll \epsilon$  and  $T \gg \epsilon$ .

**Problem 3. Quantum diatomic ideal gas** An ideal diatomic gas consists of non-interacting identical molecules  $H = \sum_{i=1}^N h_i$  which have three independent degrees of freedom  $h = h_K + h_V + h_R$ . The first one is the kinetic energy of translational motion  $h_K = \mathbf{p}^2/2m$ . The second is vibrational, i.e. each molecule is an oscillator with  $h_V = \pi^2/2 + \omega^2 q^2/2$ . The third is rotational  $h_R = \mathbf{L}^2/2I$ , where  $\mathbf{L}$  is the angular momentum. These three d.o.f. can be treated independently. Treat them as independent subsystems.

**3.1** Compute for each d.o.f. the equilibrium value of entropy as a function of energy.

**3.2** Compute for each d.o.f. the equilibrium value of energy as a function of entropy.

**3.3** Compute for each d.o.f. the equilibrium value of entropy as a function of temperature.

**3.4** Compute for each d.o.f. the equilibrium value of free energy as a function of temperature.

**3.5** Now consider all systems as quantum and repeat the calculations. This means that the momentum  $\mathbf{p}$  is quantized, each component of momentum taking the values  $p_k = (2\pi\hbar/L)k$ , where  $k$  is an arbitrary integer and  $L$  is the linear size of the box. Similarly, the energy of the vibrational modes is quantized as  $E_n = \hbar\omega(n + 1/2)$ , and the square of the angular momentum as  $L^2 = \hbar^2 l(l + 1)$ , where  $l$  is a non-negative integer. Discuss the quantum (low temperature) and the classical (high temperature) limits.

## References

- [1] E. W. Weisstein, “Binomial Distribution”. From MathWorld—A Wolfram Web Resource.  
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<https://mathworld.wolfram.com/CentralLimitTheorem.html>.
- [4] L. Landau and E. Lifshitz, “Statistical Physics”, volume 5, pp. 359–361. Pergamon Press, 2 edition, 1970.