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 αN 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 $N \to \infty$ with t,α 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 [**?**]:

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

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

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

To find the leading behavior as $N \to \infty$, 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

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

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 α 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 $t \lessapprox 0.2$ and $t \gtrapprox 0.8$, 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 $N \lessapprox 20$, a discrepancy near the peak is visible even for $t = 0.5$. The approximation visibly diverges as $\alpha \to 0$ for $t \lessapprox 0.2$ and as $\alpha \to 1$ for $t \gtrapprox 0.8$. This effect becomes more pronounced as N decreases. For $N \lessapprox 25$, this divergence overtakes the expected behavior of the discrete distribution, and so the approximation becomes poor.

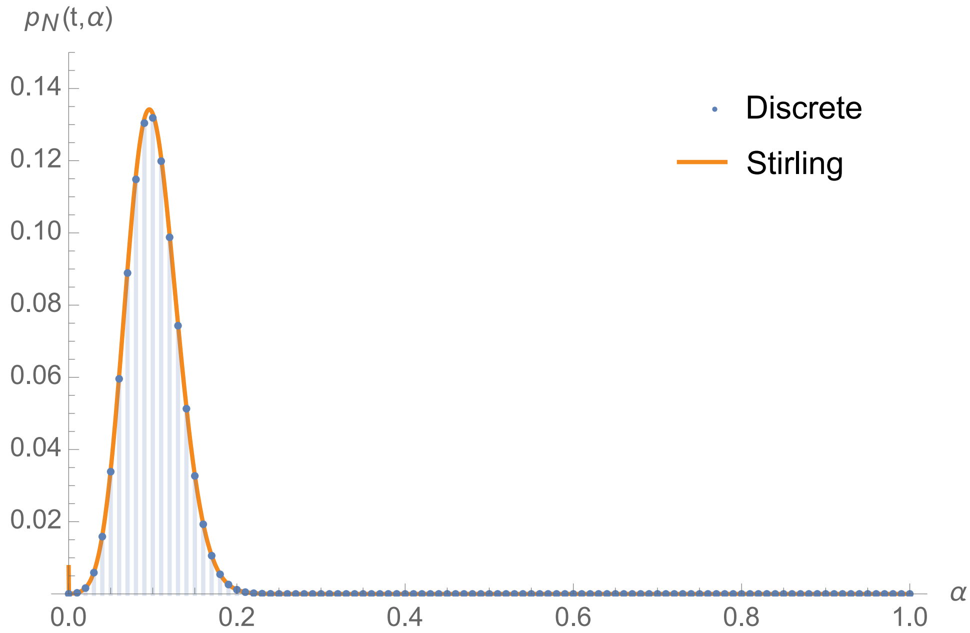

Figure 1: Comparison of the discrete expression ((2), blue) and Stirling's approximation to ((3), orange) $p_N(t,\alpha)$ as functions of $\alpha \in [0,1]$ for $N = 100$ and $t = 0.1$.

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 $\sigma^2 = Npq$ [**?**]. Thus, the mean and variance of (2) are,

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

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 [**?**]

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

with mean $\mu_G = \mu_B = Nt$ and standard deviation $\sigma_G = \sigma_B/\sqrt{N} = \sqrt{t(1-t)}$ [**?**]. (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

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

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 $t \to 0$ and $t \to 1$. 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 $\alpha, t \approx 1$.

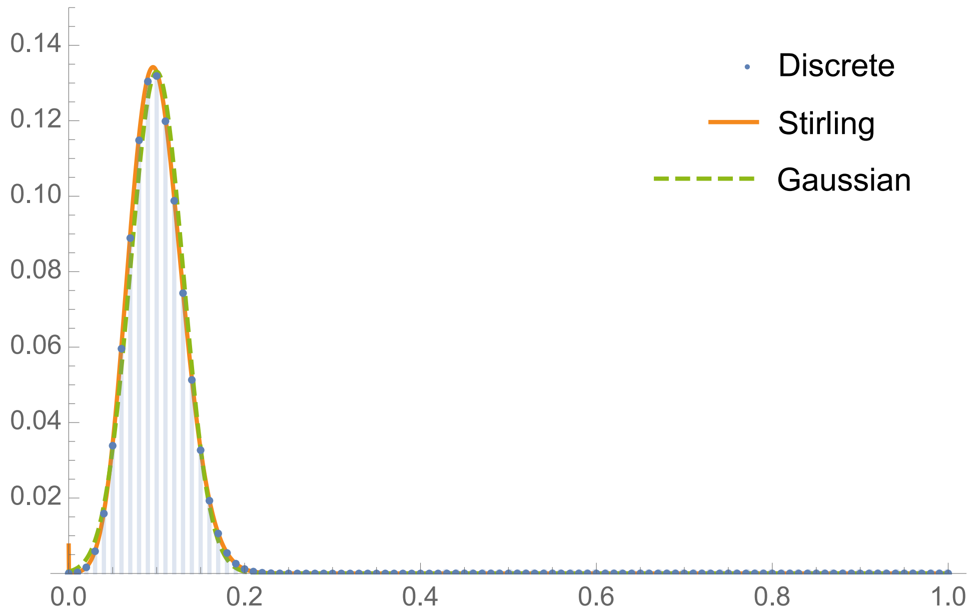

Figure 2: Comparison of the discrete expression ((2), blue), Stirling's approximation to ((3), orange), and CLT approximation to ((4), green) $p_N(t,\alpha)$ as functions of $\alpha \in [0,1]$ for $N = 100$ and $t = 0.1$.

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

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

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

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

This result suggests that the density does not fluctuate between two different samples of N independent random variables that are uniformly distributed on the circle.

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 σ_i, $i = 1, \ldots, N$. 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 $N \to \infty$.

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 $N \to \infty$ 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 ϵ, 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.

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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.