Kardar Ch. 2

Probability

To understand equilibrium properties of macroscopic systems, we can go a long way by studying the likelihood that the microscopic particles in the system are in a particular microscopic state. This is the essence of statistical mechanics.

The appropriate language for studying likelihoods is probability theory.

Consider a random variable x, with possible outcomes $S = \{x_1, x_2, \ldots\}$.

The outcomes may be continuous, e.g. velocities of gas particles.

An event is any subset of outcomes $E \subset S$, and is assigned a probability $p(E)$.

probabilities satisfy the following axioms:

i) Positivity $\quad p(E) \geq 0 \quad \forall E$

ii) Additivity $\quad p(A \text{ or } B) = p(A) + p(B)$ if A, B are disconnected events.

iii) Normalization $\quad p(S) = 1$, i.e. the random variable must have some outcome in S.

Probabilities can be assigned objectively or subjectively.

Objective probabilities — experimentally determined from the relative frequency of the occurence of an outcome in many tests of the random variable.

Subjective probability — related to lack of knowledge, and may be updated as more data becomes available.

Consider a die with 6 sides.

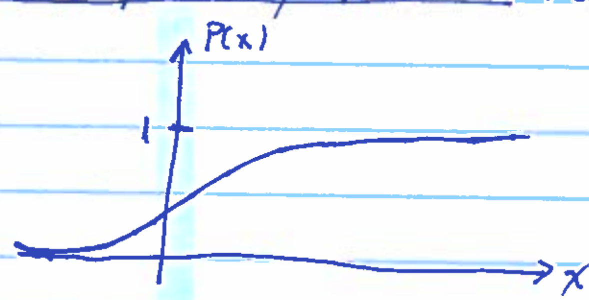
a) Roll the die 6,000 times. Around 1,000 times the roll is a 1. $\rightarrow p(\{1\}) \approx \frac{1}{6}$ objective

or

b) You have no reason to expect the die is unfair, so you assign a probability $p(\{1\}) = 1/6$. subjective

Definition: Real continuous random variable x, $S_x = \{-\infty < x < \infty\}$.

Cumulative probability function $P(x) = \text{prob (outcome} < x)$



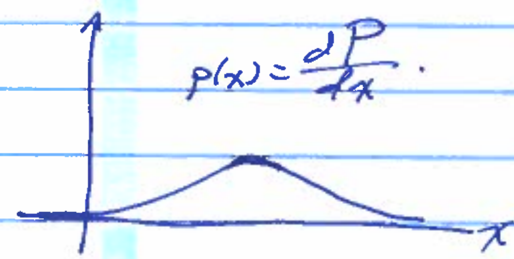
$P(-\infty) = 0$, $P(+\infty) = 1$

Probability density function (PDF) $p(x) = \frac{dP(x)}{dx}$

$p(x)\,dx = \text{prob}\left(E \in [x, x+dx]\right).$

$p(x) \geq 0$, $0 \leq p(x) < \infty.$

$\text{prob}(S) = \int_{-\infty}^{\infty} dx\, p(x) = 1.$



Expectation value of a function $F(x)$ of random var. x:

$$\langle F(x) \rangle = \int_{-\infty}^{\infty} dx\, p(x)\, F(x)$$

$F(x)$ is itself a random variable, with PDF
$p_F(f)\, df = \text{prob}\left(F(x) \in [f, f+df]\right).$

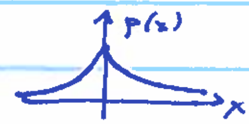
Suppose $F(x) = f$ has multiple solutions. Then

$$p_F(f)\, df = \sum_i p(x_i)\, dx_i \Rightarrow p_F(f) = \sum_i p(x_i) \left| \frac{dx}{dF} \right|_{x = x_i}$$

Jacobian of transform from x to F.

Example: $p(x) = \lambda/_2 e^{-\lambda|x|}$

$F(x) = x^2$

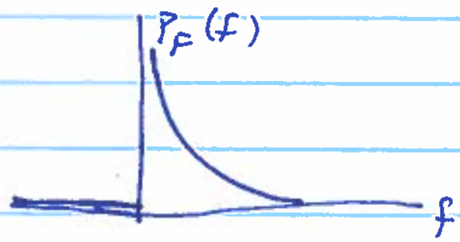


$F(x) = f$ has two solutions, real for $f > 0$: $x_\pm = \pm\sqrt{f}$

Jacobians: $\left|\frac{dx_\pm}{df}\right| = \left|\pm\frac{1}{2\sqrt{f}}\right|$

$f>0$: $\quad p_F(f) = \frac{\lambda}{2} e^{-\lambda\sqrt{f}}\left(\left|\frac{1}{2\sqrt{f}}\right| + \left|-\frac{1}{2\sqrt{f}}\right|\right) = \frac{\lambda e^{-\lambda\sqrt{f}}}{2\sqrt{f}}$

$f<0$: $\quad p_F(f) = 0$



Note: $p_F(f)$ diverges as $f \to 0^+$, but $\int_{-\infty}^{\infty} p_F(f)\, df = 1$.

Moments of the PDF:

$$m_n \equiv \langle x^n \rangle = \int dx\, p(x)\, x^n$$

Characteristic Function – generator of moments of the PDF

– Fourier transform of the PDF

$$\tilde{p}(k) = \langle e^{-ikx} \rangle = \int_{-\infty}^{\infty} dx\, p(x)\, e^{-ikx}$$

Inverse Fourier transform:

$$p(x) = \frac{1}{2\pi}\int_{-\infty}^{\infty} dk\, \tilde{p}(k)\, e^{+ikx}$$

Moments of the PDF are obtained by expanding $\tilde{p}(k)$ in a power series in k:

$$\tilde{p}(k) = \left\langle \sum_{n=0}^{\infty} \frac{(-ik)^n}{n!} x^n \right\rangle = \sum_{n=0}^{\infty} \frac{(-ik)^n}{n!} \langle x^n \rangle.$$

Moments about other points $\langle (x-x_0)^n \rangle$, obtained from

$$\langle e^{-ik(x-x_0)} \rangle = e^{ikx_0} \tilde{p}(k).$$

<u>Cumulant Generating Function</u> — Log of the characteristic fn.

$$\ln \tilde{p}(k) = \ln\left(\sum_{n=0}^{\infty} \frac{(-ik)^n}{n!} \langle x^n \rangle \right)$$

$$= \sum_{n=0}^{\infty} \frac{(-ik)^n}{n!} \langle x^n \rangle_c$$

Relation between moments and cumulants:

from expanding $\ln(1+\epsilon) = \sum_{n=1}^{\infty} (-1)^{n+1} \frac{\epsilon^n}{n}$

$\langle x_c \rangle = \langle x \rangle$ mean

$\langle x^2 \rangle_c = \langle x^2 \rangle - \langle x \rangle^2$ variance

$\langle x^3 \rangle_c = \langle x^3 \rangle - 3\langle x^2 \rangle \langle x \rangle + 2\langle x^3 \rangle$ skewness

$\langle x^4 \rangle_c = \langle x^4 \rangle - 4\langle x^3 \rangle \langle x \rangle - 3\langle x^2 \rangle^2 + 12 \langle x^2 \rangle \langle x \rangle^2 - 6\langle x \rangle^4$ curtosis

Cumulants describe the PDF and will be relevant in stat mech.

Graphical computation of the moments:

Represent the n^{th} cumulant as a connected cluster of n points:

 $\sim \langle x^3 \rangle_c$

The m^{th} moment is given by summing all partitions of m points into collections of cumulants:

$\langle x \rangle = \cdot = \langle x \rangle_c$

$\langle x^2 \rangle =$  $= \langle x^2 \rangle_c + \langle x \rangle_c^2$

$\langle x^3 \rangle =$ 

$$= \langle x^3 \rangle_c + 3 \langle x^2 \rangle_c \langle x \rangle_c + \langle x \rangle_c^3$$

Proof: $\displaystyle\sum_{m=0}^{\infty} \frac{(-ik)^m}{m!} \langle x^m \rangle = \exp\left[\sum_{n=1}^{\infty} \frac{(-ik)^n}{n!} \langle x^n \rangle_c\right]$

$$= \prod_n \underbrace{\sum_{p_n} \frac{(-ik)^{n p_n}}{p_n!} \left(\frac{\langle x^n \rangle_c}{n!}\right)^{p_n}}_{\exp\left[\frac{(-ik)^n}{n!} \langle x^n \rangle_c\right]}$$

Matching powers of $(-ik)^m$:

$$\langle x^m \rangle = \sum_{\{p_n\}}' m! \prod_n \underbrace{\frac{1}{p_n! (n!)^{p_n}}}_{} \langle x^n \rangle_c^{p_n}$$

where $\sum_n n p_n = m$

ways to partition m points into $\{p_n\}$ clusters of n pts

The normal (Gaussian) distribution

$$p(x) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left[-\frac{(x-\lambda)^2}{2\sigma^2}\right]$$

Characteristic function:

$$\tilde{p}(k) = \int_{-\infty}^{\infty} dx \, \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left[-\frac{(x-\lambda)^2}{2\sigma^2} - ikx\right]$$

$$\overset{z=x-\lambda}{=} \int_{-\infty}^{\infty} dz \, \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left[-\frac{z^2}{2\sigma^2} - ikz\right] e^{-ik\lambda}$$

complete the square:

$$\overset{w=z+ik\sigma^2}{=} \int_{-\infty}^{\infty} dw \, \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left[-\frac{w^2}{2\sigma^2}\right] \exp\left[-ik\lambda - \frac{k^2\sigma^2}{2}\right]$$

$$= \exp\left[-ik\lambda - \frac{k^2\sigma^2}{2}\right]$$

Cumulant generating function:

$$\ln \tilde{p}(k) = -ik\lambda - k^2\sigma^2/2 \qquad = \sum_{n=1}^{\infty} \frac{(-ik)^n}{n!} \langle x^n \rangle_c$$

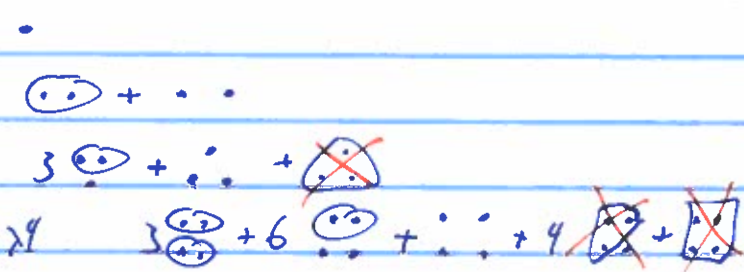
$$\Rightarrow \langle x \rangle_c = \lambda, \quad \langle x^2 \rangle_c = \sigma^2, \quad \langle x^n \rangle_c = 0 \text{ for } n > 2$$

$$\Rightarrow \langle x \rangle = \lambda$$

$$\langle x^2 \rangle = \sigma^2 + \lambda^2$$

$$\langle x^3 \rangle = 3\sigma^2\lambda + \lambda^3$$

$$\langle x^4 \rangle = 3\sigma^4 + 6\sigma^2\lambda^2 + \lambda^4$$



The Gaussian distribution will become especially important to us because of of its ubiquity due to the Central Limit Theorem, which we will encounter soon.

Binomial Distribution - describes a random variable with 2 outcomes: A with prob. p_A
B with prob. $p_B = 1 - p_A$

prob (in N trials event A occurs exactly N_A times) $= P_N(N_A)$

$$P_N(N_A) = \underbrace{\frac{N!}{N_A!(N-N_A)!}}_{\text{Number of arrangements of } N_A\ A\text{'s and } N_B\ B\text{'s.}} \underbrace{p_A^{N_A}\, p_B^{N-N_A}}_{\text{prob. of any particular ordered arrangement of } N_A\ A\text{'s and } N_B\ B\text{'s.}}$$

$(N_B = N - N_A)$

$$\binom{N}{N_A} \equiv {}_N C_{N_A} \equiv \frac{N!}{N_A!(N-N_A)!}$$

$=$ coefficient of $p_A^{N_A}\, p_B^{N-N_A}$ in the expansion of $(p_A + p_B)^N$.

Characteristic function:

$$\tilde{P}_N(k) = \langle e^{-ikN_A} \rangle = \sum_{N_A=0}^{N} \frac{N!}{N_A!(N-N_A)!} p_A^{N_A}\, p_B^{N-N_A}\, e^{-ikN_A}$$

$$= \left(p_A e^{-ik} + p_B\right)^N$$

Cumulant generating function:

$$\ln \tilde{P}_N(k) = N \ln\left(p_A e^{-ik} + p_B\right) = N \ln \tilde{P}_1(k)$$

$\rightarrow$ Cumulants for N trials $= N \times$ cumulant for 1 trial.

Note that for 1 trial, $N_A = 0$ or 1 $\Rightarrow \langle N_A^\ell \rangle = p_A \ \forall \ell$.

After N trials, $\langle N_A \rangle_c = N p_A$, $\langle N_A^2 \rangle_c = N(p_A - p_A^2) = N p_A p_B$

Standard deviation $\sigma = \sqrt{\langle N_A^2 \rangle_c} \sim \sqrt{N}$

$$\Rightarrow \frac{\sigma}{\langle N_A \rangle} \sim \frac{1}{\sqrt{N}}$$

Multinomial Distribution: More than 2 outcomes

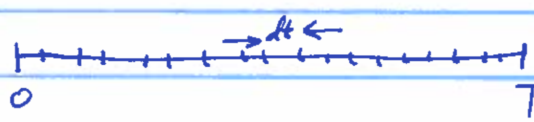
$$P_N(\{N_A, N_B, \ldots, N_M\}) = \frac{N!}{N_A!\, N_B! \cdots N_M!}\, p_A^{N_A}\, p_B^{N_B} \cdots p_M^{N_M}$$

where $N_M = N - N_A - N_B - \cdots - N_{M-1}$

Poisson Distribution: Describes probability of an event happening M times in an interval T, in terms of the prob. of the event happening once in a small interval dt, e.g. radioactive decay.

Assumes: a) prob (exactly 1 event in $[t, t+dt]$) $\propto dt$ as $dt \to 0$

b) prob(events in different intervals) are independent



$dt = \frac{T}{N}$ for some $N \gg 1$.

In each dt, prob(1 event) $= p = \alpha\, dt$ for some α.

prob(0 events) $= q = 1 - \alpha\, dt$.

prob(>1 event) ≈ 0.

c.f. binomial distribution (2 possible events w/ prob $p, q = 1-p$)

$$\tilde{p}(k) = (p e^{-ik} + q)^N = \lim_{dt \to 0} \left[1 + \alpha\, dt\,(e^{-ik} - 1)\right]^{T/dt}$$

$$= \exp\left[\alpha (e^{-ik} - 1) T\right]$$

using $\left(1 + \frac{x}{N}\right)^N \xrightarrow{N \to \infty} e^x$

Poisson PDF:

$$p(x) = \int_{-\infty}^{\infty} \frac{dk}{2\pi} \exp\left[\alpha(e^{-ik}-1)T + ikx\right]$$

$$= e^{-\alpha T} \int_{-\infty}^{\infty} \frac{dk}{2\pi} e^{ikx} \underbrace{\sum_{M=0}^{\infty} \frac{(\alpha T)^M}{M!} e^{-ikM}}_{\exp[\alpha T e^{-ik}]}$$

Use $\int_{-\infty}^{\infty} \frac{dk}{(2\pi)} e^{ik(x-M)} = \delta(x-M)$

$$\Rightarrow P_{\alpha T}(x) = \sum_{M=0}^{\infty} e^{-\alpha T} \frac{(\alpha T)^M}{M!} \delta(x-M)$$

Indicates discreteness $x \in \mathbb{Z}$ integers.

$$\Rightarrow \boxed{P_{\alpha T}(M) = e^{-\alpha T} \frac{(\alpha T)^M}{M!}}$$

Cumulants from $\ln \tilde{P}_{\alpha T}(k) = \alpha T (e^{-ik}-1)$

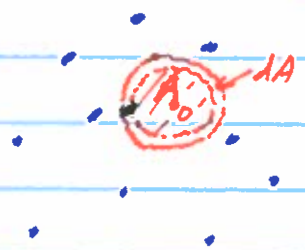
$$= \alpha T \sum_{n=1}^{\infty} \frac{(-ik)^n}{n!}$$

$$\Rightarrow \boxed{\langle M^n \rangle_c = \alpha T}$$

All cumulants are equal!

$\rightarrow \langle M \rangle = \alpha T$, $\langle M^2 \rangle = (\alpha T)^2 + \alpha T$, ...

Example: Consider a random Poisson sprinkling of dots on the page, with density $\sigma = \left\langle \frac{\#\text{ dots}}{\text{Area}} \right\rangle$.



Question: What is the probability that the nearest point is a distance between R and $R+dR$ from some point o?

- poisson distribution with $\alpha \to \sigma$
$T \to A$

prob $p(R)\,dR$ = prob (0 dots inside $r<R$) prob (1 dot in $r \in [R, R+dR]$)

$$= P_{\sigma A}(0)\, P_{\sigma dA}(1)$$

$$P_{\sigma A}(0) = e^{-\sigma A} = e^{-\sigma \overbrace{\pi R^2}^{A}}$$

$$P_{\sigma dA}(1) = e^{-\sigma dA}(\sigma dA)^1 = e^{-\sigma(\overbrace{2\pi R dR}^{dA})}\, \sigma \cdot \underbrace{2\pi R\, dR}_{dA}$$

$$\overset{\frac{dR}{R}\to 0}{=} \sigma \cdot 2\pi R\, dR$$

$$\Rightarrow \quad p(R)\,dR = e^{-\sigma A} \cdot \sigma \cdot 2\pi R\, dR$$

$$\boxed{p(R) = e^{-\sigma \pi R^2}\, \sigma \cdot 2\pi R}$$