

Lecture Notes for Advanced Math Techniques

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Chapter 1

Sequences, Series, and Convergence

1.1 Sequences

1.1.1 Convergence

$\{a_k\}_{k=1}^{\infty}$ is said to converge to L if given any $\epsilon > 0 \exists K ||a_k - L| < \epsilon \forall k > K$

1.1.2 Limit Point

Definition

L is a limit point if given any $\epsilon > 0$ there are infinitely many k such that:

$$|a_k - L| < \epsilon$$

Example 1

$$a_n = \frac{(-1)^n n}{n+1}$$

does not converge but has limit points ± 1 .

Alternative definition

L is a limit point if there exists a subsequence that converges to L

Completeness

The real numbers are the rational numbers + all limit points that the rational numbers can reach.

1.1.3 Bounded

Definition: $\{a_k\}_{k=1}^{\infty}$ is said to be bounded if $\exists m \forall k |a_k| < M$

Lemma: A sequence that is bounded implies that there exists at least one limit point. But, it does not imply convergence.

Example:

$$a_n = \cos(n^2)$$

is bounded and thus guaranteed to have a limit point. But, we do not know certainly where the limit point is. Note that just because \cos is periodic, that does not mean that all $L \in [-1, 1]$ is a limit point without invoking the transcendental nature of π . (imagine the period was 5)

1.1.4 Monotonicity

A sequence is monotonic if it changes in only one direction (includes staying the same - 3, 4, 4, 5 is valid). If a sequence is bounded + monotonic, it is said to converge.

1.1.5 Example

Sequence: $\{a_n\}_{n=1}^{\infty}, a_1 = 1, a_{n+1} = 7 - \frac{5}{a_n}$
 Suppose $1 < a_k < 7$,

$$\begin{aligned} a_k &< 7 \\ 7 - \frac{5}{a_{k+1}} &< 7 - \frac{5}{7} \\ a_{k+1} &< 7 - \frac{5}{7} < 7 \end{aligned}$$

The sequence is bounded by 7. Suppose $a_k < a_{k+1}$,

$$\begin{aligned} 7 - \frac{5}{a_k} &< 7 - \frac{5}{a_{k+1}} \\ a_{k+1} &< a_{k+2} \end{aligned}$$

The limit L satisfies the recurrence.

$$L = 7 - \frac{5}{L} \Rightarrow L^2 - 7L + 5 = 0$$

$$L = \frac{7 + \sqrt{29}}{2}$$

(eliminate negative case)

Note: This sequence of rational numbers converges to an irrational number. This technique is used for approximations of irrational numbers.

1.1.6 Basel's Problem

Sequence: $a_1, a_{n+1} = a_n + \frac{1}{(n+1)^2}$ This is clearly monotonic.

$$a_n = 1 + \frac{1}{2^2} + \frac{1}{3^2} \cdots$$

$\frac{1}{2^2} + \frac{1}{3^2} < 2 \cdot \frac{1}{2^2}$ $\frac{1}{4^2} + \frac{1}{5^2} + \frac{1}{6^2} + \frac{1}{7^2} < 2 \cdot \frac{1}{4^2}$ Continue this process to get,

$$a_n < 1 + \frac{1}{2} + \frac{1}{4} \cdots = 2$$

Euler proved this to converge to $\frac{\pi^2}{6}$.

1.1.7 Harmonic Series

Sequence: $a_1, a_{n+1} = a_n + \frac{1}{n+1}$ This is clearly monotonic.

$$a_n = 1 + \frac{1}{2} + \frac{1}{3} + \frac{1}{4} \cdots$$

$$\frac{1}{3} + \frac{1}{4} > 2 \cdot \frac{1}{4} \cdots$$

$$a_n > 1 + \frac{1}{2} + \frac{1}{2} \cdots$$

. Thus, the series is unbounded.

1.2 Series

1.2.1 Cauchy's Convergence Criterion

For Series: The series $\{S_k\}_{k=1}^{\infty}$ converges iff given any $\epsilon > 0$,

$$\exists N \mid |S_m - S_n| < \epsilon \text{ for } m, n > N.$$

For Partial Series: $S_n = \sum_{k=1}^n a_k \Rightarrow |\sum_{k=1}^{N+P} a_k| < \epsilon \forall P \in \mathbb{N}$

Note: Not only do the individual terms have to approach zero, but also, the sum of some number of terms approaches zero.

Example:

$$\frac{1}{2^n + 1} + \frac{1}{2^n + 2} \cdots + \frac{1}{2^n + 2^n} > 2^n \frac{1}{2^n + 2^n} = \frac{1}{2}$$

Thus, for $\epsilon = \frac{1}{2}$ this series breaks Cauchy's Convergence Criterion and does not converge.

1.2.2 An Interesting Result

Suppose $\{S_n\}_{n=1}^\infty$ diverges, where $S_n = \sum_{k=1}^n a_k$ with $a \geq 0 \forall k$. Note that this is monotonic. Consider $\sum_{k=1}^n \frac{a_k}{S_k}$,

$$\sum_{k=N+1}^{N+P} \frac{a_k}{S_k} = \frac{a_{N+1}}{S_{N+1}} + \frac{a_{N+2}}{S_{N+2}} + \cdots + \frac{a_{N+P}}{S_{N+P}} \geq \frac{a_{N+1}}{S_{N+P}} + \frac{a_{N+2}}{S_{N+P}} + \cdots + \frac{a_{N+P}}{S_{N+P}}$$

$$\sum_{k=N+1}^{N+P} \frac{a_k}{S_k} \geq \frac{S_{N+P} - S_N}{S_{N+P}} = 1 - \frac{S_N}{S_{N+P}} \rightarrow 1$$

So, $\sum_{k=1}^n \frac{a_k}{S_k}$ also diverges. Since each of its elements is smaller, it diverges slower than the initial one. Thus, there is **no slowest diverging series**.

1.2.3 Harmonic Series:

Suppose $a_k = 1 \forall k$. $\sum_{k=1}^\infty 1$ clearly diverges.

$$S_n = \sum_{k=1}^n 1 = n$$

$$\sum_{k=1}^\infty \frac{a_k}{S_k} = \sum_{k=1}^\infty \frac{1}{k}$$

or the harmonic series, diverges as well.

$$H_n = \sum_{k=1}^n \frac{1}{k} \approx \ln n$$

$$\sum_{k=1}^\infty \frac{\frac{1}{k}}{H_k} \approx \sum_{k=2}^\infty \frac{1}{k \ln k}$$

diverges as well.

1.2.4 Divergence Test

If $\lim_{k \rightarrow \infty} a_k \neq 0$, then $\sum_{k=1}^\infty a_k$ diverges. This is derived directly from Cauchy's Convergence Criterion.

1.2.5 Absolute Convergence

$\sum_{k=1}^\infty a_k$ is said to converge **absolutely** if $\sum_{k=1}^\infty |a_k|$ converges.

Statement: An absolutely convergent series is convergent.

Proof:

$$\left| \sum_{k=N+1}^{N+P} a_k \right| \leq \sum_{k=N+1}^{N+P} |a_k|$$

Lemma: If $\sum_{k=1}^{\infty} a_k$ converges absolutely, then given any $\epsilon > 0 \exists N :$
 $\sum_{k=N+1}^{N+P} |a_k| < \epsilon \forall P \in \mathbb{N}$

1.2.6 Direct Comparison Test

Given $\{a_k\}_{k=1}^{\infty}$ and $\{b_k\}_{k=1}^{\infty}$ are both sequences of positive numbers, if $a_k \geq b_k \forall k > K$, then

$$\sum_{k=1}^{\infty} b_k \text{ diverges then } \sum_{k=1}^{\infty} a_k \text{ diverges as well.}$$

$$\sum_{k=1}^{\infty} a_k \text{ converges then } \sum_{k=1}^{\infty} b_k \text{ converges as well.}$$

1.2.7 Limit Comparison Test

Given $\{a_k\}_{k=1}^{\infty}$ and $\{b_k\}_{k=1}^{\infty}$ are two sequences of positive terms, if

$$\lim_{k \rightarrow \infty} \frac{a_k}{b_k} = L \neq 0$$

then the sequences both converge or both diverge.

Proof

$$\lim_{k \rightarrow \infty} \frac{a_k}{b_k} = L \Rightarrow \text{given any } \epsilon > 0 \exists K |$$

$$|\frac{a_k}{b_k} - L| < \epsilon \forall k > K$$

$$L - \epsilon < \frac{a_k}{b_k} < L + \epsilon$$

$$b_k(L - \epsilon) < a_k < b_k(L + \epsilon)$$

Let $N > K$,

$$(L - \epsilon) \sum_{N+1}^{N+P} b_k < \sum_{N+1}^{N+P} a_k < (L + \epsilon) \sum_{N+1}^{N+P} b_k$$

As long as $L > 0$, then the LHS can be positive. Taking cases of convergence and divergence for $\sum_{N+1}^{N+P} b_k$, the Limit Comparison Test is proven.

1.2.8 Integral Comparison Test

Suppose $\{a_k\}_{k=1}^{\infty}$ is a sequence of positive, monotonic, decreasing terms and $f(x)$ is a continuous, monotonic, decreasing function satisfying $f(k) = a_k \forall k$.

$$\int_{n+1}^{m+1} f(k)dx < \sum_{n+1}^m a_k < \int_n^m f(k)dx$$

This not only shows both the integral and the sequence converging or diverging together, but it helps approximate the value.

Approximation of the Harmonic Series

Using Mathematica, $H_{100} = 5.1873775$. Estimate H_{10^6} .

$$\int_{101}^{10^6+1} \frac{1}{x} dx < \sum_{k=101}^{10^6} \frac{1}{k} < \int_{100}^{10^6} \frac{1}{x} dx$$

$$\ln \frac{10^6+1}{101} < \sum_{k=101}^{10^6} \frac{1}{k} < \ln(10^4)$$

$$H_{100} + \ln \frac{10^6+1}{101} < H_{10^6} < H_{100} + 4 \ln 10$$

For some n ,

$$H_{100} + \ln \frac{n+1}{101} < H_n < H_{100} + \ln \frac{n}{100}$$

The error of the bounds is,

$$\ln \frac{n}{100} - \ln \frac{n+1}{101} = \ln \left(\frac{101}{100} \cdot \frac{n}{n+1} \right)$$

This approaches $\ln 101 - \ln 100$ for large n . Note that the error doesn't change (that much) for significant changes in n .

Error of Harmonic Series

$$H_n - \ln(n+1)$$

is bounded and converges to the **Euler-Mascheroni constant**.

1.2.9 Geometric Series

$$S_n = 1 + r + r^2 + \cdots + r^n$$

$$rS_n = r + r^2 + \cdots + r^n + r^{n+1}$$

$$rS_n - S_N = r^{n+1} - 1$$

$$S_n = \frac{r^{n+1} - 1}{r - 1} \forall r \in \mathbb{C} \mid r \neq 1, S_n = n + 1 \text{ for } r = 1$$

Note that this works for complex numbers as well.

$$1 + r + r^2 + \cdots = \frac{1}{1 - r}; |r| < 1$$

1.2.10 Using the Taylor Series

Find a series for $\frac{1}{5-2x}$ centered at $x = 0$.

$$\frac{1}{5-2x} = \frac{1}{5} \cdot \frac{1}{1 - \frac{2x}{5}} = \frac{1}{5} \cdot \sum_{k=0}^{\infty} \left(\frac{2x}{5} \right)^k; |x| < \frac{5}{2}$$

Note that this is a disk in the complex plane. Find a series for $\frac{1}{5-2x}$ centered at $x = -4$. (powers of $x + 4$)

$$\frac{1}{5-2x} = \frac{1}{13-2(x+4)} = \frac{1}{13} \cdot \sum_{k=0}^{\infty} \left(\frac{2(x+4)}{13} \right)^k; |x+4| < \frac{13}{2}$$

Singularities

Singularities at which a series is undefined can pose a problem in convergence.

1.2.11 Root Test

Consider $\sum_{k=0}^{\infty} a_k$.

If $\lim_{k \rightarrow \infty} \sqrt[k]{|a_k|} = r$, then given any $\epsilon > 0, \exists K$:

$$r - \epsilon < \sqrt[k]{|a_k|} < r + \epsilon \Rightarrow (r - \epsilon)^k < |a_k| < (r + \epsilon)^k$$

$$\sum_{k=N+1}^{N+P} (r - \epsilon)^k < \sum_{k=N+1}^{N+P} |a_k| < \sum_{k=N+1}^{N+P} (r + \epsilon)^k \text{ for } N > K.$$

If $r < 1$, $\sum a_k$ converges absolutely.

If $r > 1$, $\sum a_k$ diverges absolutely.

If $r = 1$, the test is inconclusive.

1.2.12 Power Series

$$\sum_{k=0}^{\infty} c_k (z - z_0)^k \text{ converges on a disk, } |z - z_0| < \frac{1}{\lim_k \rightarrow \sqrt[k]{|c_k|}} = R$$

z_0 is the center of the series. R is the radius of convergence or the distance from the center to the nearest singular point.

Example

Find the Maclaurin series for $\frac{2}{3-2x+x^2}$.

$$\frac{2}{3-2x+x^2} = \frac{2}{3} \cdot \frac{1}{1-\frac{2x-x^2}{3}} = \frac{2}{3} \cdot \sum_{k=0}^{\infty} \left(\frac{2x-x^2}{3}\right)^k$$

Rearranging,

$$= \frac{2}{3} \left[1 + \left(\frac{2x-x^2}{3}\right) + \left(\frac{2x-x^2}{3}\right)^2 + \left(\frac{2x-x^2}{3}\right)^3 + \dots \right]$$

Expanding (can change region of convergence),

$$\begin{aligned} &= \frac{2}{3} \left[1 + \frac{2}{3}x + x^2 \left(-\frac{1}{3} + \frac{4}{9}\right) + x^3 \left(-\frac{2 \cdot 2}{9} + \frac{8}{27}\right) + \dots \right] \\ &= \frac{2}{3} \left[1 + \frac{2}{3}x + \frac{1}{9}x^2 - \frac{4}{27}x^3 + \dots \right] \end{aligned}$$

Note the power series in terms of x only converges in a disk while the original sum converges in a different region specifically $|2x-x^2| < 3$. Finding singularity points,

$$x^2 - 2x + 3 = 0 \Rightarrow \dots \Rightarrow x = 1 \pm i\sqrt{2}$$

Thus,

$$R = |1 \pm i\sqrt{2}| = \sqrt{3}$$

1.2.13 Ratio Test**1.2.14 Alternating Series Test**

The terms are monotonic decreasing in absolute value and the terms alternate signs. Then, the original sequence can be separated into 2 convergent subsequences. If the limit point of these 2 convergent subsequences is the same, $\lim_{n \rightarrow \infty} a_n = 0$, then the original sequence also converges.

1.2.15 Complication of Conditional Convergence

$$1 - \frac{1}{2} + \frac{1}{3} - \frac{1}{4} \dots$$

Argument 1:

The first term is 1, the next term has magnitude less than 1, so the sum is between $\frac{1}{2}$ and 1.

Argument 2:

Add the positive terms until it exceeds 3, then subtract $\frac{1}{2}$. Next add positive terms to 3, then subtract $\frac{1}{4}$, etc. So, the sequence converges to 3.

A Word of Caution

Rearranging terms in a conditionally convergent series can change the sum. The Alternating Series Test depends on the fact that the terms are added in order. Argument 2 destroys the meaning of the word converge.

1.2.16 Cauchy's Condensation Test

Suppose $\{a_n\}_{n=1}^{\infty}$ is decreasing and $a_n \geq 0$ for all $n \in \mathbb{N}$. Then, $\sum_{n=1}^{\infty} a_n$ and $\sum_{n=0}^{\infty} 2^n a_n$ converge or diverge together.

1.3 Taylor Series**1.3.1 Lagrange Error**

Let,

$$f(x) - f(x_0) = \int_{x_0}^x f'(t) dt$$

Doing repeated integration by parts tabularly,

$$\begin{aligned} &= \left[f'(t)(t-x) - \frac{1}{2}f''(t)(t-x)^2 + \frac{1}{3!}f^{(3)}(t)(t-x)^3 \right]_{x_0}^x - \int_{x_0}^x \frac{1}{3!}f^{(4)}(t-x)^3 dt \\ &= f'(t)(x-x_0) + \frac{1}{2}f''(t)(x-x_0)^2 + \frac{1}{3!}f^{(3)}(x-x_0)^3 - \int_{x_0}^x \frac{1}{3!}f^{(4)}(t-x)^3 dt \end{aligned}$$

So,

$$f(x) = \sum_{k=0}^n \frac{f^{(k)}(x_0)}{k!} (x-x_0)^k + \frac{1}{n!} \int_{x_0}^x f^{(n+1)}(x-t)^n dt$$

The integral part of this expression is the lagrange error when approximating a function with a set number of taylor series terms.

1.3.2 Building Block Series

$$\frac{1}{1-x} = 1 + x + x^2 + \cdots = \sum_{k=0}^{\infty} x^k, |x| < 1.$$

$$-\ln(1-x) = x + \frac{x^2}{2} + \frac{x^3}{3} + \cdots = \sum_{k=1}^{\infty} \frac{x^k}{k}, |x| < 1.$$

$$\arctan(x) = x - \frac{x^3}{3} + \frac{x^5}{5} \cdots = \sum_{k=0}^{\infty} \frac{(-1)^k x^{2k+1}}{2k+1}, |x| < 1.$$

Note the radius of convergence for this series is 1 as it is not defined for $x = \pm i$ even though it is defined for all reals.

$$(1+x)^n = 1 + nx + \frac{n(n-1)}{2}x^2 + \frac{n(n-1)(n-2)}{3}x^3 \cdots = \sum_{k=0}^{\infty} \frac{n!}{k!(n-k)!} x^k, |x| < 1.$$

$$e^x = 1 + x + \frac{x^2}{2!} + \frac{x^3}{3!} \cdots = \sum_{k=0}^{\infty} \frac{x^k}{k!}, |x| < \infty.$$

$$\sin(x) = x - \frac{x^3}{3!} + \frac{x^5}{5!} \cdots = \sum_{k=0}^{\infty} \frac{(-1)^k x^{2k+1}}{(2k+1)!}, |x| < \infty.$$

$$\cos(x) = 1 - \frac{x^2}{2!} + \frac{x^4}{4!} \cdots = \sum_{k=0}^{\infty} \frac{(-1)^k x^{2k}}{(2k)!}, |x| < \infty.$$

1.3.3 Derived Series

Example 1

Consider $f(x) = \frac{\sin(\sqrt{x})}{\sqrt{x}}$; $f(0) = 1$.

$$= \frac{1}{\sqrt{x}} \sum_{k=0}^{\infty} \frac{(-1)^k (\sqrt{x})^{2k+1}}{(2k+1)!} = \sum_{k=0}^{\infty} \frac{(-1)^k x^k}{(2k+1)!}$$

This can be used to find arbitrary derivatives.

$$\sum_{k=0}^{\infty} \frac{(-1)^k x^k}{(2k+1)!} = \sum_{y=0}^{\infty} \frac{f^{(y)}(0)}{y!} x^y$$

To compute, $f^{(10)}(0)$ look at the x^{10} term.

$$\frac{(-1)^{10} x^{10}}{21!} = \frac{f^{(10)}(0) x^{10}}{10!} \Rightarrow f^{(10)}(0) = \frac{10!}{21!}$$

Another Example

Consider $g(x) = \frac{\ln(3+2x^2) - \ln(3)}{x}$; $g(0) = 0$. Find $g^{(6)}(0)$.

$$\ln(3+2x^2) = \ln \left[3 \left(1 + \frac{2}{3} x^2 \right) \right] = \ln 3 + \ln \left(1 + \frac{2}{3} x^2 \right)$$

$$g(x) = \frac{\ln(1 + \frac{2}{3} x^2)}{x} = \frac{-\sum_{k=0}^{\infty} \frac{(-\frac{2}{3} x^2)^k}{k}}{x} = \sum_{k=1}^{\infty} \frac{(-1)^{k+1} (\frac{2}{3})^k x^{2k-1}}{k}, |x| < \sqrt{\frac{3}{2}}$$

$$= \sum_{y=0}^{\infty} \frac{g^{(y)}(0)}{y!} x^y$$

Since we are looking for x^6 but that makes $k = \frac{7}{2} \notin N$. This means that a x^6 term is absent.

$$g^{(6)}(0) = 0$$

An easier method is noticing $g(x)$ is odd which means all the even derivatives are 0. To find $g^{(7)}(0)$, observe $k = 4 \dots$

$$\frac{g^{(7)}(0)}{7!} x^7 = \frac{(-1)^5 \left(\frac{2}{3}\right)^4 x^7}{4} \Rightarrow g^{(7)}(0) = -\frac{2^2}{3^4} 7!$$

A Cooler One

Consider $h(x) = \int_0^x \frac{1 - \cos(2t^3)}{t^3} dt$. Find $h^{(13)}(0)$.

$$\begin{aligned} \frac{1 - \cos(2t^3)}{t^3} &= \frac{1 - \sum_{k=0}^{\infty} \frac{(-1)^k (2t^3)^{2k}}{(2k)!}}{t^3} = \frac{\sum_{k=1}^{\infty} \frac{(-1)^{k+1} (2t^3)^{2k}}{(2k)!}}{t^3} \\ &= \sum_{k=1}^{\infty} \frac{(-1)^{k+1} 2^{2k} t^{6k-3}}{(2k)!} \Rightarrow h(x) = \sum_{\infty} k = 1 \frac{(-1)^{k+1} 2^{2k} x^{6k-2}}{(2k)!(6k-3)} = \sum_{y=0}^{\infty} \frac{h^{(y)}(0)}{y!} x^y \end{aligned}$$

Since there is no natural k that makes this work, $h^{(13)}(0) = 0$.

Chapter 2

Products

2.1 Definition

Let $P_0 = 1$, $P_{k+1} = (1 + a_{k+1})P_k$. Given $\{a_k\}_{k=1}^{\infty}$, this defines a sequence of products $\{P_k\}_{k=1}^{\infty}$. Adding 1 in the definition, makes it easy to show convergence as the multiplicative term needs to tend to 1 or a_k needs to tend to 0. This sequence of infinite products is said to converge if $\lim_{k \rightarrow \infty} P_k$ exists and is **nonzero**. $\prod_{k=1}^{\infty} (1 + a_k)$ denotes this infinite product.

2.2 Convergence

The product can be turned into a sum using \ln . $\prod_{k=1}^{\infty} (1 + a_k)$ converges whenever $\sum_{k=1}^{\infty} a_k$ converges **absolutely**.

2.3 Representing a Polynomial

Suppose a polynomial $p(x)$ has roots $-1, 3, 5, \text{ and } 12$ each of multiplicity 1 with no other roots. And suppose $p(0) = 17$. Then,

$$p(x) = (x+1)(x-3)(x-5)(x-12) \cdot \frac{17}{(1)(-3)(-5)(-12)} = 17(1+x)\left(1-\frac{x}{3}\right)\left(1-\frac{x}{5}\right)\left(1-\frac{x}{12}\right)$$

This form is very important.

Chapter 3

Integration

3.1 Integration Techniques

3.1.1 Auxiliary Parameters

$$\text{Evaluate } \int_{-\infty}^{\infty} \frac{dx}{(x^2 + 1)^4}$$

Instead consider,

$$\int_{-\infty}^{\infty} \frac{dx}{ax^2 + b} = \frac{1}{a} \int_{-\infty}^{\infty} \frac{dx}{x^2 + \frac{b}{a}} = \frac{1}{a} \cdot \frac{1}{\sqrt{\frac{b}{a}}} \arctan\left(\frac{x}{\sqrt{\frac{b}{a}}}\right) \Big|_{-\infty}^{\infty} = \pi a^{-\frac{1}{2}} b^{-\frac{1}{2}}$$

Now, look at the derivatives with respect to the parameters.

$$\frac{\partial^3}{\partial b^3} \int_{-\infty}^{\infty} \frac{dx}{ax^2 + b} = -6 \int_{-\infty}^{\infty} \frac{dx}{(ax^2 + b)^4} = \pi \frac{-1}{2} \cdot \frac{3}{2} \cdot \frac{5}{2} a^{-\frac{1}{2}} b^{-\frac{7}{2}}$$

Now, plug in values for the parameters,

$$\int_{-\infty}^{\infty} \frac{dx}{(x^2 + 1)^4} = \pi \frac{-1}{6} \cdot \frac{-1}{2} \cdot \frac{3}{2} \cdot \frac{5}{2} \cdot 1 \cdot 1 = \frac{5\pi}{16}$$

3.1.2 Gaussian Integral

The gaussian integral is defined as follows:

$$\int_{-\infty}^{\infty} e^{-\alpha x^2} dx$$

Let,

$$I = \int_{-\infty}^{\infty} e^{-x^2} dx$$

Then,

$$\begin{aligned} I^2 &= \left(\int_{-\infty}^{\infty} e^{-x^2} dx \right) \left(\int_{-\infty}^{\infty} e^{-y^2} dy \right) \\ &= \int_{-\infty}^{\infty} dx \int_{-\infty}^{\infty} dy e^{-(x^2+y^2)} \end{aligned}$$

Switching to polar,

$$= \int_0^{\infty} r dr \int_0^{2\pi} \theta e^{-r^2} = 2\pi \int_0^{\infty} r e^{-r^2}$$

Using a u-substitution with $u = -r^2$,

$$= -\pi \int_0^{-\infty} e^u du = \pi$$

Returning to the first integral,

$$I = \int_{-\infty}^{\infty} e^{-x^2} dx = \sqrt{\pi}$$

For the original integral,

$$\int_{-\infty}^{\infty} e^{-\alpha x^2} dx = \frac{1}{\sqrt{\alpha}} \int_{-\infty}^{\infty} e^{-u^2} du = \sqrt{\frac{\pi}{\alpha}}$$

Now, taking derivatives,

$$\frac{\partial}{\partial \alpha} \Rightarrow - \int_{-\infty}^{\infty} x^2 e^{-\alpha x^2} = \frac{-1}{2} \sqrt{\pi} \alpha^{-\frac{3}{2}}$$

Chapter 4

The Zeta Function

4.1 The sin function, the Basel Problem, and more results

4.1.1 Beginning

$\sin(0) = 0$. So, let's divide by x to remove the factor of x in the expansion.

$$\frac{\sin(x)}{x} = (1 - \frac{x}{\pi})(1 + \frac{x}{\pi})(1 - \frac{x}{2\pi})(1 + \frac{x}{2\pi}) \cdots$$

Using difference of squares,

$$= (1 - \frac{x^2}{\pi^2})(1 - \frac{x^2}{4\pi^2})(1 - \frac{x^2}{9\pi^2}) \cdots$$

Note that we have not established these 2 functions are equivalent but that they have the same zeroes. This was used to say Euler's argument wasn't rigorous (the full thing took another 10 years). Without the proven rigour, let's suppose this statement. Expanding the product by powers of x ,

$$\begin{aligned} &= 1 - \frac{x^2}{\pi^2}(1 + \frac{1}{4} + \frac{1}{9} + \cdots) + \frac{x^4}{\pi^4}(\frac{1}{1 \cdot 4} + \frac{1}{1 \cdot 9} + \cdots + \frac{1}{4 \cdot 9} + \frac{1}{4 \cdot 16} + \cdots) - \cdots \\ &= 1 - \frac{x^2}{\pi^2} \sum_{n=1}^{\infty} \frac{1}{n^2} + \frac{x^4}{\pi^4} \sum_{n=1}^{\infty} \sum_{m=n+1}^{\infty} \frac{1}{n^2 m^2} + \cdots \end{aligned}$$

4.1.2 Deriving results

Using the Taylor series,

$$\frac{\sin(x)}{x} = 1 - \frac{x^2}{3!} + \frac{x^4}{5!} - \cdots$$

Note that these 2 expansions are equal. This **solves the Basel problem**.

$$\frac{-X^2}{3!} = \frac{-X^2}{\pi^2} \sum_{n=1}^{\infty} \frac{1}{n^2} \Rightarrow \sum_{n=1}^{\infty} \frac{1}{n^2} = \frac{\pi^2}{6}$$

We can use this for other series.

$$\left(\sum_{n=1}^{\infty} \frac{1}{n^2} \right) \left(\sum_{m=1}^{\infty} \frac{1}{m^2} \right) = \frac{\pi^4}{36}$$

Also,

$$\begin{aligned} &= \sum_{n=1}^{\infty} \frac{1}{n^4} + \sum_{n=1}^{\infty} \sum_{m=n+1}^{\infty} \frac{1}{m^2 n^2} + \sum_{n=1}^{\infty} \sum_{m=n+1}^{\infty} \frac{1}{m^2 n^2} \\ &\frac{\pi^4}{36} = \sum_{n=1}^{\infty} \frac{1}{n^4} + \frac{2\pi^4}{120} \Rightarrow \sum_{n=1}^{\infty} \frac{1}{n^4} = \frac{\pi^4}{90} \end{aligned}$$

Euler continued this all the way to $\sum_{n=1}^{\infty} \frac{1}{n^{26}}$.

4.1.3 Conversion

To write it in a closed form,

$$\frac{\sin(x)}{x} = \prod_{k=1}^{\infty} \left(1 - \frac{x^2}{k^2 \pi^2} \right)$$

Writing as a series,

$$\begin{aligned} \ln \frac{\sin(x)}{x} &= \sum_{k=1}^{\infty} \ln \left(1 - \frac{x^2}{k^2 \pi^2} \right) \\ &= - \sum_{k=1}^{\infty} \sum_{j=1}^{\infty} \frac{\frac{x^2}{k^2 \pi^2}}{j} \Rightarrow - \sum_{j=1}^{\infty} \frac{x^{2j}}{j} \frac{\zeta(2j)}{\pi^{2j}} \end{aligned}$$

Looking at cotangent,

$$\cot(x) - \frac{1}{x} = - \sum_{j=1}^{\infty} 2 \frac{\zeta(2j)}{\pi^{2j}} x^{2j-1}$$

4.2 Dirichlet Series

4.2.1 Zeta Series

This function is not really a dirichlet series but it's related.

$$\zeta(s) = \sum_{n=1}^{\infty} \frac{1}{n^s} = 1 + \frac{1}{2^s} + \frac{1}{3^s} + \dots$$

4.2.2 Eta Series

This series is an alternating Zeta Series.

$$\eta(s) = \sum_{n=1}^{\infty} \frac{(-1)^{n+1}}{n^2} = 1 - \frac{1}{2^s} + \frac{1}{3^s} - \dots$$

4.2.3 Lambda Series

This series is a Zeta Series with only odd terms.

$$\lambda(s) = \sum_{k=0}^{\infty} \frac{1}{(2k+1)^s} = 1 + \frac{1}{3^s} + \frac{1}{5^s} + \dots$$

4.2.4 Beta Series

This series is an alternating lambda series.

$$\lambda(s) = \sum_{k=0}^{\infty} \frac{(-1)^k}{(2k+1)^s} = 1 - \frac{1}{3^s} + \frac{1}{5^s} - \dots$$

4.2.5 Even Zeroes

Euler has given all the even zeroes of the zeta function.

$$\zeta(2) = \frac{\pi^2}{6}$$

$$\zeta(4) = \frac{\pi^4}{90}$$

$$\zeta(6) = \frac{\pi^6}{945}$$

4.2.6 Deriving Additional Values

$$\eta(2) = \frac{\pi^2}{12}$$

$$\lambda(2) = \frac{3\pi^2}{24}$$

4.2.7 Deriving Additional Results

$$\eta(s) = \zeta(s) - 2\left(\frac{1}{2^s}\zeta(s)\right) = (1 - 2^{1-s})\zeta(s)$$

$$\lambda(s) = \zeta(s) - \left(\frac{1}{2^s}\zeta(s)\right) = (1 - 2^{-s})\zeta(s)$$

$\beta(s)$ is not related to the other functions.

4.2.8 Apéry's Constant

Apéry's constant is $\zeta(3)$ because the French mathematician proved that it was irrational. For zeta, the odd's are hard and the even's are known exactly.

4.2.9 Catalan's Constant

Catalan's constant is $\beta(2)$. For β the even's are hard and the odd ones are known.

4.3 Weirstrass Approximation Theorem

You can approximate an arbitrarily continuous function by an arbitrary polynomial.

Chapter 5

The Gamma Function

5.1 Factorial and an Introduction to the Gamma Function

5.1.1 Introduction

Consider x as a positive integer and n as a large natural number.

$$(n+x)! = (n+x)(n+x-1)(n+x-2) \cdots n! \approx n^x n!$$

$$(x+n)! = (x+n)(x+n-1)(x+n-2) \cdots (x+1)x!$$

Dividing,

$$1 \approx \frac{n^x n!}{(x+n)(x+n-1)(x+n-2) \cdots (x+1)x!}$$

Rearranging,

$$x! \approx \frac{n^x n!}{(x+n)(x+n-1)(x+n-2) \cdots (x+1)}$$

Note that this is true for non-positive x .

$$(x-1)! \approx \frac{n^x n!}{(x+n)(x+n-1)(x+n-2) \cdots (x+1)(x)}$$

$$\lim_{n \rightarrow \infty} \frac{n^x n!}{(x+n)(x+n-1)(x+n-2) \cdots (x+1)} = \Gamma(x)$$

This is known as the gamma function.

5.2 Establishing a General Definition

5.2.1 Recurrence Relations and the Factorial Function

$$\Gamma(x+1) = \lim_{n \rightarrow \infty} \frac{n^x n!}{(x+1+n)(x+n) \cdots (x+1)}$$

$$= \lim_{n \rightarrow \infty} \frac{nx}{x+1+n} \cdots \frac{n^x n!}{(x+n)(x+n-1) \cdots (x+1)(x)}$$

Separating the product into two limits and simplifying,

$$\Gamma(x+1) = x\Gamma(x)$$

Let's look at $\Gamma(1)$.

$$\Gamma(1) = \lim_{n \rightarrow \infty} \frac{n \cdot n!}{(1+n)(n)(n-1) \cdots (2)(1)} = \lim_{n \rightarrow \infty} \frac{n \cdot n!}{(n+1)n!} = 1$$

$$\Gamma(2) = 2 \cdot \Gamma(1) = 2$$

$$\vdots$$

$$\Gamma(m) = (m-1)!$$

The gamma is also known as the shifted factorial function.

5.2.2 An Intuitive Derivation

$$\begin{aligned} \frac{1}{\Gamma(x)} &= \lim_{n \rightarrow \infty} \frac{(x+n)(x+n-1) \cdots (x+1)(x)}{n! \cdot n^x} \\ &= x \cdot \lim_{n \rightarrow \infty} \frac{x+n}{n} \cdot \frac{x+n-1}{n-1} \cdots \frac{x+2}{2} \cdot \frac{x+1}{1} \cdot n^{-x} \end{aligned}$$

Shifting,

$$\begin{aligned} \frac{1}{\Gamma(x+1)} &= \lim_{n \rightarrow \infty} \left[\left(1 + \frac{x}{n}\right) \left(1 + \frac{x}{n-1}\right) \cdots \left(1 + \frac{x}{2}\right) (1+x) n^{-x} \right] \\ &= \lim_{n \rightarrow \infty} \left[\prod_{k=1}^n \left(1 + \frac{x}{k}\right) \cdot n^{-x} \right] \end{aligned}$$

We want to move the n^{-x} term into the product. We know the following,

$$\lim_{n \rightarrow \infty} [H_n - \ln(n)] = \gamma$$

where γ is the Euler-Mascheroni constant. Using this, we can transform n^{-x} into a product.

$$n^{-x} = e^{-x \ln(n)} \approx e^{-x(H_n - \gamma)} = e^{\gamma x} e^{-x \sum_{k=1}^n \frac{1}{k}} = e^{\gamma x} \prod_{k=1}^n e^{-\frac{x}{k}}$$

Using this,

$$= \lim_{n \rightarrow \infty} \left[\prod_{k=1}^n \left(1 + \frac{x}{k}\right) \cdot n^{-x} \right] = \lim_{n \rightarrow \infty} e^{\gamma x} \prod_{k=1}^n \left[\left(1 + \frac{x}{k}\right) e^{-\frac{x}{k}} \right]$$

Note that for some fixed x , we can go out far enough until the exponent is very small. So for large k ,

$$(1 + \frac{x}{k})e^{-\frac{x}{k}} = (1 + \frac{x}{k})(1 - \frac{x}{k} + \frac{x^2}{2k^2} + \dots) = 1 - \frac{x^2}{k^2} + \frac{x^2}{2k^2} - \dots \approx 1 - \frac{x^2}{k^2}$$

Since $\frac{1}{k^2}$'s sum converges, this expression seems to converge. So,

$$\frac{1}{\Gamma(1+x)} \text{ is defined for all } x \in \mathbb{C}$$

5.2.3 A Rigorous Proof

This can be rigorously proved using the limit comparison test with $\frac{x^2}{k^2}$.

$$\begin{aligned} & \lim_{k \rightarrow \infty} \frac{(1 + \frac{x}{k})e^{-\frac{x}{k}} - 1}{\frac{x^2}{k^2}} \\ & \stackrel{LH}{=} \lim_{k \rightarrow \infty} \frac{\frac{-x}{k^2}e^{-\frac{x}{k}} + (1 + \frac{x}{k})(\frac{x}{k^2})e^{-\frac{x}{k}}}{-2\frac{x^2}{k^3}} \cdot \frac{k^2}{k^2} \\ & = \lim_{k \rightarrow \infty} \frac{x^2}{-2x^2} = \frac{-1}{2} \end{aligned}$$

5.3 The Reflection Identity

5.3.1 Continuing

$$[\Gamma(1+x)\Gamma(1-x)]^{-1} = e^{\gamma x} \prod_{k=1}^n e^{-\frac{x}{k}} \cdot e^{-\gamma x} \prod_{j=1}^n e^{\frac{x}{j}} = \prod_{k=1}^{\infty} \left(1 - \frac{x^2}{k^2}\right)$$

Using the sin function,

$$= \frac{\sin(\pi x)}{\pi x}$$

Taking the reciprocal,

$$\Gamma(1+x)\Gamma(1-x) = \frac{\pi x}{\sin(\pi x)}$$

$$x\Gamma(x)\Gamma(1-x) = \frac{\pi x}{\sin(\pi x)}$$

$$\Gamma(x)\Gamma(1-x) = \frac{\pi}{\sin(\pi x)}$$

This is known as the **Reflection Identity**.

5.3.2 Interesting Values

Using the reflection identity for $x = \frac{1}{2}$,

$$\Gamma^2\left(\frac{1}{2}\right) = \pi \Rightarrow \Gamma\left(\frac{1}{2}\right) = \sqrt{\pi}$$

$$\Gamma\left(\frac{3}{2}\right) = \frac{1}{2} \cdot \sqrt{\pi} = \left(\frac{1}{2}\right)!$$

Now, using the gamma function, we can get the values of all kinds of exotic factorials!

5.4 Finding a Maclaurin Expansion

$$\Gamma(1+z) = e^{-\gamma z} \prod_{k=1}^{\infty} \left[\left(1 + \frac{z}{k}\right)^{-1} e^{\frac{z}{k}} \right]$$

$$\ln \Gamma(1+z) = -\gamma z + \sum_{k=1}^{\infty} \left[\frac{z}{k} - \ln\left(1 + \frac{z}{k}\right) \right] = -\gamma z + \sum_{k=1}^{\infty} \left[\frac{z}{k} - \sum_{j=1}^{\infty} \frac{(-1)^{j+1} \left(\frac{z}{k}\right)^j}{j} \right]$$

Note that the first nested term is $\frac{z}{k}$ which cancels.

$$= -\gamma z + \sum_{k=1}^{\infty} \sum_{j=2}^{\infty} \frac{(-1)^j z^j}{k^j j} = -\gamma z + \sum_{j=2}^{\infty} \left(\frac{(-1)^j \zeta(j) z^j}{j} \right); |z| < 1$$

$$\ln \Gamma(1+z) = -\gamma z + \sum_{k=2}^{\infty} \frac{(-1)^k \zeta(k)}{k} z^k$$

5.5 Finding an Integral Representation

For large natural n , consider

$$\int_0^n t^{z-1} \left(1 - \frac{t}{n}\right)^n dt$$

Using repeated integration by parts,

$$= \left[\frac{t^z}{z} \left(1 - \frac{t}{n}\right)^n + \frac{t^{z+1}}{z(z+1)} n \left(1 - \frac{t}{n}\right)^{n-1} \frac{1}{n} + \frac{n(n-1)}{n^2} \left(1 - \frac{t}{n}\right)^{n-2} \frac{t^{z+2}}{z(z+1)(z+2)} + \dots \right]_0^n$$

Note that all terms are 0 except for the final one evaluated at n .

$$= \frac{n^{z+n}}{z(z+1)(z+2)\dots(z+n)} = \frac{n! n^z}{z(z+1)(z+2)\dots(z)}$$

This looks like the gamma function! We just need to add the limit.

$$\Gamma(z) = \int_0^{\infty} t^{z-1} e^{-t} dt; \Re(z) > 0$$

This gives us access to a number of integrals.

5.6 Integrating with the Gamma Function

Consider this example:

$$\int_0^\infty e^{-2x^3} dx$$

Setting $t = 2x^3$ and $x = (\frac{t}{2})^{\frac{1}{3}}$.

$$\begin{aligned} &= \int_0^\infty \frac{1}{2^{\frac{1}{3}}} \frac{1}{3} t^{-\frac{2}{3}} e^{-t} dt \\ &= \frac{1}{2^{\frac{1}{3}}} \cdot \frac{1}{3} \Gamma\left(\frac{1}{3}\right) = \frac{\Gamma\left(\frac{4}{3}\right)}{\sqrt[3]{2}} \end{aligned}$$

5.7 Generating Functions

5.7.1 $\Gamma(1 + \epsilon)$

Consider $\int_0^\infty \ln x \cdot e^{-x} dx$. First, let's consider $\int_0^\infty x^\epsilon e^{-x} dx$. We know this $= \Gamma(1 + \epsilon)$. So one option is differentiating the Gamma function. However, we can leverage series expansions instead.

$$\begin{aligned} \int_0^\infty e^{-x} x^\epsilon dx &= \int_0^\infty e^{-x} e^{\epsilon \ln x} dx = \int_0^\infty e^{-x} \sum_{k=0}^\infty \frac{(\epsilon \ln x)^k}{k!} dx \\ &= \sum_{k=0}^\infty \frac{\epsilon^k}{k!} \int_0^\infty e^{-x} \ln^k x dx = \Gamma(1 + \epsilon) \end{aligned}$$

We know that,

$$\Gamma(1 + \epsilon) = \exp(\ln \Gamma(1 + \epsilon)) = \exp\left(-\gamma\epsilon + \sum_{k=2}^\infty \frac{(-1)^k \zeta(k)}{k} \epsilon^k\right)$$

So,

$$\begin{aligned} \Gamma(1 + \epsilon) &= 1 + \left[-\gamma\epsilon + \sum_{k=2}^\infty \frac{(-1)^k \zeta(k)}{k} \epsilon^k\right] + \frac{1}{2!} \left[-\gamma\epsilon + \sum_{k=2}^\infty \frac{(-1)^k \zeta(k)}{k} \epsilon^k\right]^2 + \dots \\ &= 1 - \gamma\epsilon + \left(\frac{\zeta(2) - \gamma^2}{2}\right) \epsilon^2 + \dots \end{aligned}$$

So, we need to find the coefficient of ϵ^1 for the original integral.

$$\begin{aligned} k = 0 : \int_0^\infty e^{-x} dx &= 1 \\ k = 1 : \frac{\epsilon^1}{1!} \int_0^\infty \ln x \cdot e^{-x} dx &= -\gamma\epsilon \\ k = 2 : \frac{\epsilon^2}{2!} \int_0^\infty \ln^2 x \cdot e^{-x} dx &= \frac{\zeta(2) + \gamma^2}{2} \epsilon^2 \end{aligned}$$

So, we call $\Gamma(1 + \epsilon)$ the **generating function** for all these integrals.

5.7.2 Another Example

Consider $\int_0^\infty x^2 \ln x \cdot e^{-3x} dx$. Instead, let's consider $\int_0^\infty x^{2+\epsilon} e^{-3x} dx$. One method is to use a u-substitution for $u = 3x$,

$$\int_0^\infty x^{2+\epsilon} e^{-3x} dx = \left(\frac{1}{3}\right)^{3+\epsilon} \int_0^\infty u^{2+\epsilon} e^{-u} du = \frac{1}{27} \cdot e^{-\epsilon \ln 3} \cdot \Gamma(3 + \epsilon)$$

Interpreting this as a Maclaurin series like before,

$$\int_0^\infty x^{2+\epsilon} e^{-3x} dx = \sum_{k=0}^\infty \frac{\epsilon^k}{k!} \int_0^\infty x^2 \ln^k x \cdot e^{-3x} dx$$

Note we don't have an expansion for $\Gamma(3 + \epsilon)$ but we can use the recurrence relation. Then, we can expand as a series as before.

$$\begin{aligned} \frac{1}{27} e^{-\epsilon \ln 3} \Gamma(3 + \epsilon) &= \frac{1}{27} e^{-\epsilon \ln 3} (2 + \epsilon)(1 + \epsilon) \Gamma(1 + \epsilon) \\ &= \frac{2}{27} \left(1 + \frac{\epsilon}{2}\right) (1 + \epsilon) \exp\left(-(\gamma + \ln 3)\epsilon + \sum_{k=2}^\infty \frac{(-1)^k \zeta(k)}{k} \epsilon^k\right) \end{aligned}$$

Instead of doing all the work again we can use the result from before and replace γ for $\gamma + \ln 3$.

$$\begin{aligned} &= \frac{2}{27} \left(1 + \frac{3}{2}\epsilon + \frac{\epsilon^2}{2}\right) \left[1 - (\gamma + \ln 3)\epsilon + \left(\frac{\zeta(2) - (\gamma + \ln 3)^2}{2}\right) \epsilon^2\right] \\ &= \frac{2}{27} \left[1 + \left(\frac{3}{2} - \gamma - \ln 3\right) \epsilon + \dots\right] \end{aligned}$$

So, our original integral is when $k = 1$ and equals the coefficient of ϵ .

$$\int_0^\infty x^2 \ln x \cdot e^{-3x} dx = \frac{2}{27} \left(\frac{3}{2} - \gamma - \ln 3\right)$$

Chapter 6

The Beta Function

6.1 A Derivation

$$\begin{aligned}\Gamma(\alpha)\Gamma(\beta) &= \left(\int_0^\infty x^{\alpha-1}e^{-x}dx\right)\left(\int_0^\infty y^{\beta-1}e^{-y}dy\right) \\ &= \int_0^\infty dx \int_0^\infty dy x^{\alpha-1}y^{\beta-1}e^{-x-y}\end{aligned}$$

We can instead write this integral in terms of $x + y$ as it happens over the first quadrant. So, let $u = x + y$.

$$= \int_0^\infty du \int_0^u dx \cdot x^{\alpha-1}(u-x)^{\beta-1}e^{-u}$$

Now, let's use scaling substitutions. $t = \frac{x}{u}$.

$$\begin{aligned}&= \int_0^\infty du \int_0^1 u \cdot dt \cdot (ut)^{\alpha-1}(u-ut)^{\beta-1}e^{-u} \\ &= \int_0^\infty du \cdot uu^{\alpha-1}u^{\beta-1}e^{-u} \int_0^1 dt \cdot t^{\alpha-1}(1-t)^{\beta-1} = \Gamma(\alpha+\beta) \cdot \int_0^1 dt \cdot t^{\alpha-1}(1-t)^{\beta-1} \\ &\quad \int_0^1 dt \cdot t^{\alpha-1}(1-t)^{\beta-1} = \frac{\Gamma(\alpha)\Gamma(\beta)}{\Gamma(\alpha+\beta)} = B(\alpha, \beta)\end{aligned}$$

6.1.1 Alternate Form

Substituting $t = \frac{u}{u+1}$,

$$B(\alpha, \beta) = \int_0^\infty \frac{u^{\alpha-1}}{(u+1)^{\alpha+\beta}} du$$

6.2 Using Integral Forms

6.2.1 Nice Result

Using a substitution for x^n , we can eventually see that

$$\int_0^\infty \frac{x^{m-1} dx}{x^n + 1} = \frac{\pi}{n} \csc \frac{m\pi}{n} \quad \forall m, n \mid 0 < \frac{m}{n} < 1$$

6.2.2 Derivatives

Taking derivatives with respect to m ,

$$\int_0^\infty \frac{x^{m-1} \ln x}{x^n + 1} dx = -\frac{\pi^2}{n^2} \csc \frac{m\pi}{n} \cot \frac{m\pi}{n}$$

This gives us access to "natural logs" without worrying about expansions. Differentiating again,

$$\int_0^\infty \frac{x^{m-1} \ln^2 x}{x^n + 1} dx = \frac{\pi^3}{n^3} \csc \frac{m\pi}{n} \left(2 \csc^2 \frac{m\pi}{n} - 1 \right)$$

6.2.3 More Derivations

Expanding and rearranging $\Gamma(\alpha)\Gamma(\beta)$ results in

$$\int_0^{\frac{\pi}{2}} \cos^{2\alpha-1} \theta \sin^{2\beta-1} \theta d\theta = \frac{1}{2} B(\alpha, \beta)$$

Chapter 7

Probability Theory

7.1 Binomial Distribution

$$(x_1 + x_2)^n = \sum_{k=0}^n \binom{n}{k} x_1^k x_2^{n-k}$$

7.2 Basic Probability

A fair 6-sided die is rolled 5 times. What is the probability of exactly two 3's?

7.2.1 Outcomes

Divide favorable outcomes by possible outcomes.

$$= \frac{\binom{5}{2} \cdot 5^3}{6^5}$$

7.2.2 Raw Probability

Find the probability of getting a favorable outcome.

$$\binom{5}{2} \left(\frac{1}{6}\right)^2 \left(\frac{5}{6}\right)^3$$

7.3 Basics of Expected Value

$$expectedvalue = \sum_{results} (value)(probability)$$

For a die,

$$\begin{aligned}\langle k \rangle &= \frac{1}{6}(1 + 2 + 3 + 4 + 5 + 6) = \frac{6 \cdot 7}{6 \cdot 2} = 3.5 \\ \langle k^2 \rangle &= \frac{1}{6}(1^2 + 2^2 + \dots + 6^2) = \frac{6 \cdot 7 \cdot 13}{6} = \frac{91}{6} \neq \langle k \rangle^2\end{aligned}$$

7.3.1 Expectation of Square vs Square of the Expectation

Consider,

$$\begin{aligned}\langle (k - \langle k \rangle)^2 \rangle &= \langle k^2 - 2k\langle k \rangle + \langle k \rangle^2 \rangle = \langle k^2 \rangle - \langle 2k\langle k \rangle \rangle + \langle \langle k \rangle^2 \rangle \\ &= \langle k^2 \rangle - \langle k \rangle^2\end{aligned}$$

Since the LHS is ≥ 0 , this value is > 0 so $\langle k^2 \rangle > \langle k \rangle^2$. The variance is equal to this LHS value: $\sigma_k^2 = \langle (k - \langle k \rangle)^2 \rangle$. So, for the die, $\sigma_k = \sqrt{\frac{91}{6} - \frac{49}{4}}$. The probability of being in a standard deviation of a expected value is $P(2 \leq k \leq 5) = \frac{2}{3}$. If this distribution was normal, this value would be $\approx 68.2\%$.

7.3.2 Independence and Products

Given that k_1 and k_2 are two independent measurements, determine $k_1 + k_2$ and $\sigma_{k_1+k_2}^2$.

$$\begin{aligned}k_1 + k_2 &= k_1 + k_2 \\ \sigma_{k_1+k_2}^2 &= (k_1 + k_2)^2 - k_1 + k_2^2 \\ &= k_1^2 + 2k_1k_2 + k_2^2 - (k_1^2 + 2k_1k_2 + k_2^2) \\ &= k_1^2 - k_1^2 + 2k_1k_2 - 2k_1k_2 + k_2^2 - k_2^2\end{aligned}$$

Two outcomes are independent if and only if $k_1k_2 = k_1k_2$ always. So, given independence, we can simplify

$$\sigma_{k_1+k_2}^2 = \sigma_{k_1}^2 + \sigma_{k_2}^2$$

The value $k_1k_2 - k_1k_2$ measures the correlation between k_1 and k_2 .

7.4 Multinomial Distribution

This can be used to model distributions with more than 2 objects. Consider n objects being placed in m boxes. The number of ways to place r_1 in box 1, r_2 in box 2, \dots , and r_m in box m is

$$\binom{n}{r_1 r_2 \dots r_m} = \frac{n!}{r_1! r_2! \dots r_m!}; \sum_{i=1}^m r_i = n$$

Representing the distribution,

$$(x_1 + x_2 + \dots + x_m)^n = \sum_{r_1+r_2+\dots+r_m=n} \binom{n}{r_1 r_2 \dots r_m} x_1^{r_1} x_2^{r_2} \dots x_m^{r_m}$$

7.4.1 Application

A fair 6-sided die is rolled four times. k_1 is the number of 3's and k_2 is the number of 5's.

$$k_1 = \sum_{k=0}^4 \binom{4}{k} k \left(\frac{1}{6}\right)^k \left(\frac{5}{6}\right)^{4-k}$$

Taking a derivative of the binomial expansion and multiplying by x_1 ,

$$x_1 \frac{\partial}{\partial x_1} (x_1 + x_2)^n = nx_1(x_1 + x_2)^{n-1} = \sum_{k=0}^n \binom{n}{k} k x_1^k x_2^{n-k}$$

Applying this,

$$k_1 = 4 \cdot \frac{1}{6} = \frac{2}{3}$$

7.5 Experimentation

A certain quantity is measured n times with the results k_1, k_2, \dots, k_n . Assume the expected value of k is \bar{k} (unknown) and its standard deviation is σ_k (unknown).

$$k_{mean} = \frac{1}{n} \sum_{i=1}^n k_i$$

Note that $k_{mean} \neq \bar{k}$. However,

$$k_{mean} = \frac{1}{n} \sum_{i=1}^n k_i = \frac{1}{n} \sum_{i=1}^n \bar{k} = \bar{k}$$

Note that the expected value of both k and k_{mean} is \bar{k} . So, let's analyze the standard deviation,

$$\sigma_{k_1+k_2+\dots+k_n}^2 = \sum_{i=1}^n \sigma_i^2 = n\sigma_k^2 \Rightarrow \sigma_{\sum} = \sqrt{n}\sigma_k \Rightarrow \sigma_{mean} = \sqrt{n} \frac{\sigma_k}{n} = \frac{\sigma_k}{\sqrt{n}}$$

Thus, taking the mean keeps the same expected value but divides the std. dev. by \sqrt{n} . Note that we don't know the values of \bar{k} and σ_k . So, let's calculate

$\sigma_{k_{mean}}$.

$$\begin{aligned} \sum_{i=1}^n (k_i - k_{mean})^2 &= \sum_{i=1}^n (k_i - k_{mean})^2 = n(k_1 - k_{mean})^2 \\ &= n(k_1 - \bar{k})^2 - 2(k_1 - \bar{k})(k_{mean} - \bar{k}) + (k_{mean} - \bar{k})^2 \\ &= n \left[\sigma_k^2 + \frac{\sigma_k^2}{n} - 2(k_1 - \bar{k})(k_{mean} - \bar{k}) \right] \end{aligned}$$

Since k_1 and k_{mean} are dependent, let's look at k_2 .

$$(k_1 - \bar{k})(k_{mean} - \bar{k}) = \frac{\sigma_k^2}{n}$$

Plugging this in,

$$\sum_{i=1}^n (k_i - k_{mean})^2 = n \left[\sigma_k^2 + \frac{\sigma_k^2}{n} - 2 \frac{\sigma_k^2}{n} \right] = (n-1) \sigma_k^2$$

So,

$$\frac{1}{n-1} \sum_{i=1}^n (k_i - k_{mean})^2$$

7.6 Large n

Suppose we roll a fair six-sided die 6000 times. What is the probability a 2 comes up between 990 and 1050 times?

$$P = \sum_{k=990}^{1050} \binom{6000}{k} \left(\frac{1}{6}\right)^k \left(\frac{5}{6}\right)^{6000-k}$$

This is computationally intensive, so we can approximate this instead with an integral. Generalizing, say there are n rolls and a p probability. Using Sterling's approximation, $\ln n! \approx n \ln n - n + \frac{1}{2} \ln(2\pi n)$,

$$\begin{aligned} \ln \binom{n}{k} p^k (1-p)^{n-k} &= \ln n! - \ln k! - \ln(n-k)! + k \ln p + (n-k) \ln(1-p) \\ &\approx n \ln n - n + \frac{1}{2} \ln(2\pi n) - k \ln k + k - \frac{1}{2} \ln(2\pi k) - (n-k) \ln(n-k) \\ &\quad + n - k - \frac{1}{2} \ln(2\pi(n-k)) + k \ln p + (n-k) \ln(1-p) \end{aligned}$$

We want to look at this for large n . Let $k = xn$.

$$\begin{aligned} \ln P_k &\approx n \ln n - xn \ln(xn) - n(1-x) \ln(n-xn) + \frac{1}{2} \ln \frac{n}{2\pi xn^2(1-x)} \\ &\quad + xn \ln p + n(1-x) \ln(1-p) \\ &= n \ln n - xn \ln n - xn \ln x - n(1-x) \ln n - n(1-x) \ln(1-x) \\ &\quad + \frac{1}{2} \ln \frac{1}{2\pi x(1-x)} - \frac{1}{2} \ln n + xn \ln p + n(1-x) \ln(1-p) \end{aligned}$$

Cancelling and rearranging,

$$\begin{aligned} &= n [x \ln p - x \ln x + (1-x) \ln(1-p) - (1-x) \ln(1-x)] + \frac{1}{2} \ln \frac{1}{2\pi nx(1-x)} \\ &= n \left[x \ln \frac{p}{x} + (1-x) \ln \frac{1-p}{1-x} \right] + \frac{1}{2} \ln \frac{1}{2\pi nx(1-x)} \end{aligned}$$

Similar to asymptotic expansions, let's look at the maximum. For large n , the last term is negligible. Note that when $x = p$, the derivative and this expression vanish.

$$\frac{\partial^2}{\partial x^2} \Rightarrow -\frac{1}{x} - \frac{1}{1-x} = \frac{-1}{x(1-x)}$$

So,

$$\ln P_k \approx -\frac{n}{2} \frac{(x-p)^2}{p(1-p)} + \frac{1}{2} \ln \frac{1}{2\pi np(1-p)}$$

Substituting back to k ,

$$= -\frac{1}{2n} \frac{(k-pn)^2}{p(1-p)} + \frac{1}{2} \ln \frac{1}{2\pi n(p)(1-p)}$$

Remember that $\sigma_k = np(1-p)$ from the binomial distribution:

$$P_k \approx \frac{\exp\left[-\frac{(k-np)^2}{2\sigma_k^2}\right]}{\sqrt{2\pi\sigma_k^2}}$$

This is the bell curve and is valid for large n . We also note that $np = k$. Rewriting this, we get

$$\approx \frac{1}{\sigma_k \sqrt{2\pi}} e^{-\frac{1}{2} \cdot \left(\frac{k-k}{\sigma_k}\right)^2}$$

So, back to our example,

$$P = \sum_{k=990}^{1050} \binom{6000}{k} \left(\frac{1}{6}\right)^k \left(\frac{5}{6}\right)^{6000-k} \approx \int_{989.5}^{1050.5} \frac{1}{\sigma_k \sqrt{2\pi}} e^{-\frac{1}{2} \cdot \left(\frac{k-1000}{\sigma_k}\right)^2} dk$$

Since numerical integrations don't work that well with large values, we can substitute to rescale with $u = \frac{k-k}{\sigma_k}$; $du = \frac{dk}{\sigma_k}$. Recall that this u is the z^* score from statistics.

$$= \int_{z_{min}}^{z_{max}} \frac{e^{-\frac{u^2}{2}}}{\sqrt{2\pi}} du$$

7.7 Birthday Problem

There are n people in a room with random birthdays (none born on Feb. 29). How large must n be in order that the probability that at least two share the same birthday exceeds $\frac{1}{2}$.

7.7.1 Solution

Suppose we choose some fixed birthdays and then assign them:

$$P = 1 - \binom{365}{n} n! \left(\frac{1}{365}\right)^n$$

From a multinomial perspective, the probability of all different days is

$$\binom{365}{n, 365-n} \binom{n}{1, 1, \dots, 1} \left(\frac{1}{365}\right)^n$$

This generalizes well. Consider the case for one pair,

$$\binom{365}{1, n-2, 366-n} \binom{n}{2, 1, 1 \dots 1} \left(\frac{1}{365}\right)^n$$

For two pairs,

$$\binom{365}{2, n-4, 367-n} \binom{n}{2, 2, 1, 1 \dots 1} \left(\frac{1}{365}\right)^n$$

Chapter 8

Thermodynamics

8.1 Introduction

A **state variable** is a quantity that depends only on the state of a system. There are two kinds of state variables. **Intensive** variables do not scale with system size while **extensive** variables do scale. Combining systems in equilibrium preserves intensive state variables but adds extensive variables.

$$\Delta U = Q_{in} - W_{out}$$

The **First Law of Thermodynamics** states that the change in internal energy is equal to the amount of heat that is delivered to the system minus the work done by the system on the environment. From physics, we know $W = F\Delta h = pA\Delta h = p\Delta V$ (think about a piston). Graphing pressure vs. volume, the area under the curve defines work, so work does not just depend on the initial and final states but the path taken. Thus, work is not a change in a state variable. Note that this is not a change in work so dW is inappropriate. So, dW or δW sometimes used to still indicate that the work is small but not a change. Note that if we rearrange to $\frac{W}{P} = dV$, this is a change in a state variable, so pressure is an **integrating denominator** for work.

8.2 Ideal Gas Law

The gas molecules colliding is what imparts a force and gives the gas a pressure. These collisions can be considered as elastic. Consider a piston; the momentum imparted on the piston in time Δt is $\sum_{v_z > 0} 2mv_z n_{hit}$ where n_{hit} is the number of molecules with a positive v_z that hit the piston in time Δt .

$$= \sum_{v_z > 0} 2mv_z \frac{Av_z \Delta t}{V} N p_{v_z}$$

where p_{v_z} is the probability that the z component of a molecule is v_z . So,

$$p = \frac{F}{A} = \frac{\Delta p}{A \Delta t} = 2 \frac{N}{V} \sum_{v_z > 0} m v_z^2 p_{v_z}$$

Using symmetry,

$$= \frac{N}{V} \sum_{v_z} m v_z^2 p_{v_z}$$

Assuming that the gas is **isotropic**, same in all directions, we can simplify the following. Note that gravity does act only in the z directions, however this effect is negligible.

$$= \frac{N}{3V} \sum_v m v^2 p_v = \frac{2N}{3V} \sum_v \frac{1}{2} m v^2 p_v = \frac{2N}{3V} K$$

Rearranging,

$$pV = N \cdot \frac{2}{3} K$$

Popularly,

$$pV = nRT = N \frac{R}{\eta} T = N k_B T$$

Remember that n is in moles while N is a constant. k_B is known as the Boltzmann Constant and is $1.3806488(13) \times 10^{-23} \frac{J}{K}$. Equating,

$$K = \frac{3}{2} k_B T$$

Notice this 3 comes from the 3 directions that the particle can travel in. This is known as the **Equipartition of energy**. Overall, for l degrees of freedom,

$$U = \frac{l}{2} N k_B T = \frac{l}{2} pV$$

For monotomic gases, $l = 3$ but diatomic gases can spin if the temperature is high enough.

8.3 Heat Capacity

The heat capacity C is the heat required per Kelvin increase in temperature, $\frac{Q}{\Delta T}$. Note that C is extensive, so we can divide by mass. At **isobaric** (constant pressure) conditions,

$$\Delta U = \frac{l}{2} p \Delta V = Q - p \Delta V \Rightarrow Q = \left(\frac{l}{2} + 1 \right) p \Delta V$$

So,

$$C_p = \left(\frac{3}{2} + 1 \right) N k_B$$

At **isochoric** (constant volume) conditions, $W = 0$ and $\Delta U = Q$. Using ideal gas,

$$C_V = \frac{l}{2} N k_B$$

At **isothermal** (constant temperature), heat capacity doesn't make sense neither do non-infinitesimal changes in volume. So,

$$W = \int p dV = \int_{V_i}^{V_f} N k_B T \frac{dV}{V} = N k_B T \ln \frac{V_f}{V_i}$$

Additionally, $\Delta U = 0 \Rightarrow Q = W$, so isothermic processes are 100% efficient. An **adiabatic** or **isentropic** (constant entropy) has no heat flow. Here $Q = 0 \Rightarrow \Delta U = -W$. Substituting,

$$\frac{l}{2} d(pV) = -p dV \Rightarrow \left(\frac{l}{2} + 1 \right) p dV = -\frac{l}{2} V dp$$

Rearranging,

$$\frac{\frac{l}{2} + 1}{\frac{l}{2}} \frac{dV}{V} = -\frac{dp}{p}$$

Note that this ratio is $\frac{C_p}{C_v} = \frac{c_p}{c_v} = \gamma$ and is the ratio of specific heats (gamma is not Euler-Mascheroni). Integrating,

$$\gamma \ln V = -\ln P + \text{const}$$

$$pV^\gamma = \text{const}$$

The speed of sound through an ideal gas is

$$\text{speed of sound} = \sqrt{\frac{\gamma R T}{\text{molar mass}}}$$

A **Carnot cycle** uses only isothermal and adiabatic processes. The efficiency of this cycle

$$e_c = 1 - \frac{T_{\text{cold}}}{T_{\text{hot}}}$$

It is the most efficient possible for an engine between these temperature extremes.

8.4 Laws of Thermodynamics

The **Zeroth Law** states that if A is in thermal equilibrium with B and B is in TE with C , then A is in TE with C . The **First Law** states that energy is conserved.

8.5 Lagrange Multipliers

Lagrange multipliers are a technique for optimize a multivariate scalar function under a constraint. Suppose we need to maximize $f(x, y)$ under the constraint $g(x, y) = 0$. Note that if we draw level curves of $f(x, y)$, we see that to optimize this, $\nabla f = \lambda \nabla g$. We can build a function

$$F(x, y; \lambda) = f(x, y) + \lambda g(x, y)$$

Taking derivatives,

$$F_x = f_x(x, y) + \lambda g_x(x, y) = 0$$

$$F_y = f_y(x, y) + \lambda g_y(x, y) = 0$$

$$F_\lambda = g(x, y) = 0$$

Note that the derivative with respect to λ is the constraint. Solving these three equations with three variables should optimize $f(x, y)$ under $F_\lambda = g(x, y) = 0$.

8.6 Pfaffian Expressions

We know $dU = Q - W$. But, work is *not* an exact differential and it cannot be understood as a change in a state variable. Instead, the work is a sum of state variables times changes in state variables. A **Pfaffian Expression** is a sum of multiples of differentials. Consider the Pfaffian expression $(1 - xy)dx - x^2dy$. By Clairaut's, $\frac{\partial Q}{\partial x} = -2x \neq \frac{\partial P}{\partial y} = -x$. So, The expression cannot be the differential of some function, $\neq df$.

8.6.1 Integrating Denominator

However, if we divide the expression by e^{xy} , $\frac{\partial Q}{\partial x} \neq \frac{\partial P}{\partial y} = (x^2y - 2x)e^{-xy}$. This is an **integrating denominator** as it makes the expression an exact differential. The integrating denominator allows us to write a Pfaffian expression in terms of an exact differential. For work, P is an integrating denominator as $\frac{W}{P} = -dV$.

8.6.2 Canatheodory

A mathematician named **Canatheodory** tells us that a Pfaffian expression admits an integrating denominator iff there are points in the state space in every neighborhood of our initial point *inaccessible* to the initial point while the Pfaffian expression = 0. Notice that every expression in 2 dimensions has an integrating denominator. An example that doesn't have an integrating denominator is $ydx + dy - dz$. Suppose we start at $(0, 0, 0)$. We can transition to the following point while keeping the Pfaffian expression = 0.

$$(0, 0, 0) \rightarrow (a - \frac{c-b}{b}, 0, 0) \rightarrow (a - \frac{c-b}{b}, b, b) \rightarrow (a, b, c)$$

With $b \neq 0$ (special case), any point (a, b, c) is accessible. So, there is no integrating denominator.

8.7 Maximum Entropy

Suppose N atoms with total energy E have m accessible states with energies $\{\epsilon_k\}_{k=1}^m$. Determine the occupation numbers $\{n_k\}_{k=1}^m$ that extremize the entropy $S = k_B \ln \Omega = k_B \ln \frac{N!}{\prod_{k=1}^m n_k!}$. So, we maximize $\ln N! - \sum_{k=1}^m \ln n_k!$ subject to $\sum_{k=1}^m n_k = M$. Using Lagrange Multipliers,

$$F = \ln N! - \sum_{k=1}^m \ln n_k! + \lambda \left(N - \sum_{k=1}^m n_k \right) + \beta \left(E - \sum_{k=1}^m \epsilon_k n_k \right)$$

We can consider all n_k to be independent of each other. Taking a derivative,

$$\frac{\partial F}{\partial n_j} = -\frac{\partial}{\partial n_j} \ln n_j! - \lambda - \beta \epsilon_j = 0$$

Using Sterling's Approximation,

$$\frac{\partial}{\partial n} \ln n! \approx \frac{\partial}{\partial n} \left(n \ln n - n + \frac{1}{2} \ln(2\pi n) \right) = \ln n + \frac{1}{2n}$$

Plugging in,

$$\frac{\partial F}{\partial n_j} \approx \ln n_j - \lambda - \beta \epsilon_j = 0$$

In thermal equilibrium, $\ln n_j + \beta \epsilon_j = -\lambda$ and $\ln(n_j e^{\beta \epsilon_j})$ is independent of j . So, $n_j \propto e^{-\beta \epsilon_j}$. This is known as the **Boltzmann Factor**.

8.7.1 Thermal Contact

Suppose two systems are in thermal contact and System 1 gives $\epsilon_j - \epsilon_k$ energy to System 2 by moving a single atom from state k to state j . Then, $\Delta E_2 = \epsilon_j - \epsilon_k$. For entropy,

$$\begin{aligned} \Delta S_2 &= k_B \ln \frac{N!}{n_1 \cdots (n_k - 1)!(n_j + 1)! \cdots n_m!} - k_B \ln \frac{N!}{n_1 \cdots n_k! \cdots n_j \cdots n_m!} \\ &= k_B \ln \left(\frac{n_k! n_j!}{(n_k - 1)!(n_j + 1)!} \right) = k_B \ln \frac{n_k}{n_j + 1} \end{aligned}$$

Since the occupation numbers are extremely large, we can approximate and use the Boltzmann factor,

$$\approx k_B \ln \frac{n_k}{n_j} = k_B \beta (\epsilon_j - \epsilon_k) = k_B B \Delta E_2$$

If this is a reversible process, $\Delta E_2 = Q$ so

$$k_B \beta Q = \Delta S$$

Note that $k_B B$ is an integrating denominator for heat and is the same for systems in thermal equilibrium. So,

$$k_B \beta = \frac{1}{T} \Rightarrow \beta = \frac{1}{k_B T}$$

8.7.2 Finding Entropy

Let $N = 3 \times 10^{20}$ atoms be in three accessible states $\epsilon_1 = 0, \epsilon_2 = \epsilon, \epsilon_3 = 4\epsilon$ and let $E = \frac{1}{2}N\epsilon$. Entropy is

$$S = k_B(\ln N! - \ln n_1! - \ln n_2! - \ln n_3!)$$

Using Stirling's Approximation and simplifying,

$$S \approx k_B \left(- \sum_{k=1}^3 n_k \ln \frac{n_k}{N} + \frac{1}{2} \ln \frac{N}{4\pi^2 n_1 n_2 n_3} \right)$$

8.8 State Variable Derivatives

We know $dU = Q - W$. From previous analysis, we know $\frac{W}{p} = dV$ and $\frac{Q}{T} = S$.

$$dU = TdS - pdV$$

From multivariate calculus, we know $df = \nabla f \cdot d\vec{r}$. So, $U = U(S, V)$, $T = \left(\frac{\partial U}{\partial S}\right)_V$, and $p = -\left(\frac{\partial U}{\partial V}\right)_S$. Using Clairaut's,

$$\left(\frac{\partial T}{\partial V}\right)_S = -\left(\frac{\partial p}{\partial S}\right)_V$$

This is known as a **Maxwell relation**. The following values are easiest to measure.

$$B = -\left(\frac{\partial p}{\partial V/V}\right)_T = -V\left(\frac{\partial p}{\partial V}\right)_T$$

The **isothermal bulk modulus** is the pressure required for a fractional volume change.

$$\alpha = \left(\frac{\partial V/V}{\partial T}\right)_P = \frac{1}{V} \left(\frac{\partial V}{\partial T}\right)_P$$

The **isobaric thermal expansion coefficient** is the fractional volume change per temperature change.

$$C_p = T \left(\frac{\partial S}{\partial T}\right)_P$$

The **heat capacity** at constant pressure is the heat required per change in temperature.

8.8.1 Other Potentials

We know $U = U(S, V)$. What if we wanted something that is naturally in terms of S and p ? Consider $H = U + pV$. Then, $dH = dU + p dV + V dp = T dS + V dp$ (this H is known as the **enthalpy**). From the regular representation of dU ,

$$\left(\frac{\partial T}{\partial V}\right)_S = -\left(\frac{\partial P}{\partial S}\right)_V$$

From the differential of enthalpy,

$$\left(\frac{\partial T}{\partial P}\right)_S = \left(\frac{\partial V}{\partial S}\right)_P$$

The **Helmholtz free energy** is defined as $A = U - TS$. This gives $dA = -S dT - p dV$ and

$$\left(\frac{\partial S}{\partial V}\right)_T = \left(\frac{\partial P}{\partial T}\right)_V$$

The **Gibb's free energy** is defined as $G = U - TS + pV$ giving $dG = -S dT + V dp$ and

$$\left(\frac{\partial S}{\partial P}\right)_T = -\left(\frac{\partial V}{\partial T}\right)_P = -\alpha V$$

8.8.2 Example

Suppose we wanted to find $\left(\frac{\partial P}{\partial T}\right)_V$. We consider V as a function of p and T .

$$dV = \left(\frac{\partial V}{\partial p}\right)_T dp + \left(\frac{\partial V}{\partial T}\right)_P dT$$

Manipulating the three values,

$$= -\frac{V}{B} dp + \alpha V dT$$

Since the value we want to find occurs at constant volume we set LHS to 0 and solve giving αB .

8.9 Systems

8.9.1 Absolute Maximum Entropy

Using Lagrange multipliers, we can see that without regard for the total energy $\beta = 0$. Then, $n_j \propto e^{-\beta \epsilon_j} = 1$. So, the occupation numbers are evenly distributed.

8.9.2 Three Accessible States

Consider N atoms in thermal equilibrium with 3 accessible states of energies $0, \epsilon, 3\epsilon$. Then, by the Boltzmann factor,

$$N = A + Ae^{-\beta\epsilon} + Ae^{-3\beta\epsilon} = A(1 + x + x^3)$$

If the total energy is $N\epsilon$,

$$N\epsilon = A(0 + x\epsilon + x^3 \cdot 3\epsilon) \Rightarrow 1 + x + x^3 = x + 3x^3$$

We can find the roots of this equation to solve for the occupation numbers. Manipulating the Boltzmann factor, we get

$$T = -\frac{1}{\ln x} \cdot \frac{\epsilon}{k_B}$$

8.9.3 Temperature

In Thermodynamics, temperature is defined as follows.

$$T = USV$$

It is the integrating denominator for heat.

$$dS = \frac{Q}{T}$$

Consider two substances exchanging heat (T_1 passes heat Q to T_2).

$$\Delta S_1 = -\frac{Q}{T_1}, \Delta S_2 = \frac{Q}{T_2}$$

$$\Delta S = Q \left(\frac{1}{T_2} - \frac{1}{T_1} \right)$$

If $T_2 < T_1$, the change in entropy is positive and the process is **spontaneous**. Considering energy and entropy, we see that maximal entropy occurs at some point. In lasers, energy is added so that the occupation numbers in the excited states are larger than those in the regular states. For positive T , $k_B T$ is a measure of how much ambient energy is available at some temperature T . Note from the definition of temperature given above, temperature can be negative theoretically though this is hard in practice. Processes that require less than $k_B T$ can take place freely, but processes that require more than this do not happen.

8.10 Velocity/Speed Distribution

In classical mechanics, there are a continuum of energy states. Let's consider non-relativistic velocities only. Atoms of mass m with speed \vec{v} require energy

$\frac{1}{2}mv^2$. Additionally, the probability of velocity $\vec{v} \propto e^{-\frac{1}{2}\beta mv^2}$. However, since the velocity is a continuum, the probability of an atom having exactly some velocity is 0. Instead consider the probability of some velocity between \vec{v} and $\vec{v} + d\vec{v}$. So, instead we can write the probability as $\propto e^{-\frac{1}{2}\beta mv^2} dv_x dv_y dv_z$. A **phase space** represent a set of quantities that determine the state of the object. Note this is a volume in phase space. Solving for the constant of proportionality A ,

$$\begin{aligned} 1 &= A \int_{-\infty}^{\infty} dv_x \int_{-\infty}^{\infty} dv_y \int_{-\infty}^{\infty} dv_z e^{-\frac{1}{2}\beta mv^2} \\ &= A \left(\int_{-\infty}^{\infty} dv_x e^{-\frac{1}{2}\beta mv_x^2} \right) \left(\int_{-\infty}^{\infty} dv_y e^{-\frac{1}{2}\beta mv_y^2} \right) \left(\int_{-\infty}^{\infty} dv_z e^{-\frac{1}{2}\beta mv_z^2} \right) \end{aligned}$$

Recognizing these integrals as Gaussian integrals,

$$= A \left(\sqrt{\frac{2\pi}{\beta m}} \right)^3$$

Solving for A ,

$$P(\vec{v}, d\vec{v}) = \left(\frac{m}{2\pi k_B T} \right)^{\frac{3}{2}} e^{-\frac{1}{2}\beta mv^2} d^3v$$

This is known as the **Maxwell-Boltzmann velocity distribution**. This gives us a Gaussian distribution with highest value at 0. To get a speed distribution, we multiply by the volume of phase space associated with speed between v and $v + dv$.

$$P(v, dv) = \left(\frac{m}{2\pi k_B T} \right)^{\frac{3}{2}} e^{-\frac{1}{2}\beta mv^2} \cdot 4\pi v^2 dv$$

This is known as the **Maxwell-Boltzmann speed distribution**. Consider the expectation value of the speed. We can do this by integrating. In the integral, we first substitute $u = \sqrt{\beta mv^2}$ to scale it:

$$\begin{aligned} \left(\frac{\beta m}{2\pi} \right)^{\frac{3}{2}} e^{-\frac{u^2}{2}} \cdot 4\pi \cdot \frac{u^2}{\beta m} \cdot \frac{du}{\sqrt{\beta m}} &= \sqrt{\frac{2}{\pi}} e^{-\frac{u^2}{2}} u^2 du \\ v &= \int_0^{\infty} \sqrt{\frac{2}{\pi}} e^{-\frac{u^2}{2}} u^2 du = \sqrt{\frac{2k_B T}{\pi m}} \int_0^{\infty} u^3 e^{-\frac{u^2}{2}} du \end{aligned}$$

Using $s = \frac{u^2}{2}$, we can get,

$$v = \sqrt{\frac{2k_B T}{\pi m}} \int_0^{\infty} 2s e^{-s} ds = \sqrt{\frac{8k_B T}{\pi m}}$$

We can also find the expected value of the square of the speed.

$$v^2 = \int_0^{\infty} \sqrt{\frac{2}{\pi}} e^{-\frac{u^2}{2}} \cdot u^2 \cdot \frac{u^2}{\beta m} du = \sqrt{\frac{2}{\pi}} \cdot \frac{k_B T}{m} \cdot \int_0^{\infty} u^4 e^{-\frac{u^2}{2}} du$$

We know $\int_0^\infty e^{-\alpha u^2} = \frac{1}{2}\sqrt{\frac{\pi}{\alpha}}$. Taking two derivatives with respect to α ,

$$v^2 = \sqrt{\frac{3k_B T}{m}}$$

This is commonly known as the **rms speed** (root-mean-square). The most probable speed is where $u^2 e^{-\frac{u^2}{2}}$ is maximum. Taking derivatives, we can find $u = \sqrt{s}$. So, the **most probable speed** is

$$v_{mp} = \sqrt{\frac{2k_B T}{m}}$$

Notice that the substitution being used is

$$u = \sqrt{Bm}v = \sqrt{\frac{\text{molar mass}}{RT}}v$$

8.11 Rayleigh Jeans Law

Let's analyze the number of different states an electromagnetic wave has. Waves can be described in terms of their wave number k as $\sin(kx - \omega t)$. Consider some distance L that is an integer number of wavelengths. In other words,

$$\sin(kx - \omega t) = \sin(k(x + L) - \omega t) \Rightarrow kL = 2\pi n \Rightarrow k_n = \frac{2\pi n}{L}$$

To count this, we just sum

$$\sum \Delta n \rightarrow \sum \frac{L \Delta k}{2\pi}$$

This is the number of states between k and $k + \Delta k$. Similarly, in three dimensions,

$$\frac{L^3 d^3 k}{(2\pi)^3}$$

Notice that this is a volume in phase space. We can see that the **state density** is $\frac{d^3 k}{(2\pi)^3}$. So the energy of waves with wave number between k and $k + dk$ is

$$E = 2 \cdot 4\pi k^2 \cdot \frac{d^3 k}{(2\pi)^3} \cdot k_B T$$

This 2 comes from polarization, the $4\pi k^2$ comes from the volume of phase space between k and $k + dk$, and the $k_B T$ gives us the energy for each state. It turns out this is easier to write in terms of the wavelength, $k = \frac{2\pi}{\lambda}$. So, the energy density required by EM waves with wavelength between λ and $\lambda + d\lambda$ is

$$\frac{8\pi k_B T}{\lambda^4} d\lambda$$

This is the **Rayleigh-Jeans Law**.

8.12 Ultraviolet Catastrophe

To get the total amount of energy that an EM waves need, we would integrate the Rayleigh-Jeans Law quantity over λ . However, this is not integrable around 0, so it seems that EM waves require "all" energy at any temperature other than $T = 0$. The theory supports this, but experimental data does not. This is what is known as the **Ultraviolet Catastrophe**. Plank resolved this by changing the energy per state from $k_B T$ to

$$\frac{h \cdot \frac{c}{\lambda}}{e^{\beta \cdot \frac{hc}{\lambda}} - 1}$$

Notice that for large λ , the expansion of the exponent gives us $\approx k_B T$. Here, c is the speed of light in a vacuum. h is Planck's constant which, at the time, was fit to experimental data. Many theorists prefer working with this in terms of frequency, ν : $\lambda\nu = c \Rightarrow \lambda = \frac{c}{\nu}$. Plugging this in, the energy per state is

$$\Rightarrow \frac{h\nu}{e^{\beta h\nu} - 1} = h\nu e^{-\beta h\nu} \cdot \frac{1}{1 - e^{-\beta h\nu}} = h\nu (e^{-\beta h\nu} + e^{-2\beta h\nu} + \dots)$$

This is an infinite sum of Boltzmann factors associated with energies of $n h\nu$. The reason this solves the catastrophe is that there is a minimum amount of energy $h\nu$ to excite an EM wave. If $h\nu \ll k_B T$, the EM waves are easily excited, but if opposite, they are hard to excite. For EM waves, the **photons** are occupying these states. With this resolution, let's get the total energy density in EM waves in thermal equilibrium.

$$= \int_0^\infty 2 \cdot \frac{h\nu}{e^{\beta h\nu} - 1} \cdot \frac{4\pi\nu^2}{c^3} d\nu$$

Using $u = \beta h\nu$,

$$= \frac{8\pi}{(\beta hc)^3} \cdot \frac{1}{\beta} \int_0^\infty \frac{u^3}{e^u - 1} du$$

Notice this is the zeta-gamma integral.

$$= \frac{8\pi}{(\beta hc)^3} \cdot \frac{1}{\beta} \cdot \Gamma(4) \cdot \zeta(4) = \frac{8\pi^5 k_B^4}{15h^3 c^3} T^4$$

For low temperatures, the energy is contained in the matter. But as temperature increases, the energy in EM waves will overtake the matter until it is radiation dominated. Each photon carries energy $h\nu$, so the photon density is

$$= \int_0^\infty 2 \cdot \frac{1}{e^{\beta h\nu} - 1} \cdot \frac{4\pi\nu^2 d\nu}{c^3} = \frac{8\pi}{(\beta h\nu)^3} \int_0^\infty \frac{u^2 du}{e^u - 1} = \frac{16\pi}{(hc)^3} \zeta(3) k_B^3 T^3$$

8.13 Stefan-Boltzmann Law

Consider a surface and the amount of radiation escaping the surface. So, the energy that escapes in time Δt is,

$$2 \cdot \frac{h\nu}{e^{\beta h\nu} - 1} \cdot \frac{d^3 k}{(2\pi)^3} \cdot dS \cdot c \cos \phi \Delta t$$

Here, ϕ is the angle between \vec{k} and \vec{n} . The angular integration gives

$$\int_0^{\frac{\pi}{2}} \sin \phi d\phi \int_0^{2\pi} \cos \theta d\theta = \pi$$

So, the original integral is

$$\begin{aligned} &= 2 \int_0^\infty \frac{h\nu}{e^{\beta h\nu} - 1} \cdot \frac{\pi k^2 dk}{(2\pi)^3} dS \cdot c\Delta t = 2\pi \int_0^\infty \frac{h\nu}{e^{\beta h\nu} - 1} \cdot \frac{\nu^2 d\nu}{c^3} dS \cdot c\Delta t \\ &= (\text{total energy density}) \frac{c}{4} \cdot dS\Delta t \end{aligned}$$

The total power emitted will then be

$$\frac{2\pi^5 k_B^4}{15h^3 c} \cdot AT^4$$

This is the **Stefan-Boltzmann constant**.