Chapter 3

Random Process

&

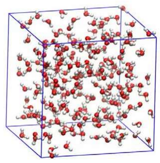
Partial Differential Equations

3.0 Introduction

Deterministic model (repeatable results)

Consider N particles with coordinates $\mathbf{r}_1, \mathbf{r}_2, \cdots \mathbf{r}_N$

- the interactions between particles modeled by potential $V(\mathbf{r}_1, \mathbf{r}_2, \cdots \mathbf{r}_N)$
- the dynamics of the system represented by ordinary differential equations



$$m_i \frac{d^2 \mathbf{r}_i}{dt^2} = \mathbf{f}_i, \qquad i = 1, 2, 3 \cdots N$$

$$\mathbf{f}_i = -\nabla_{\mathbf{r}_i} V(\mathbf{r}_1, \mathbf{r}_2, \cdots \mathbf{r}_N) = \left(-\frac{\partial V}{\partial x_i}, -\frac{\partial V}{\partial y_i}, -\frac{\partial V}{\partial z_i} \right)$$

These coupled equations can be solved using *numerical method*

3.0 Introduction

Verlet algorithm

Taylor expansion

$$\mathbf{r}(t+\Delta t) = \mathbf{r}(t) + \mathbf{v}(t)\Delta t + (1/2)\mathbf{a}(t)\Delta t^2 + (1/6)\mathbf{b}(t)\Delta t^3 + O(\Delta t^4)$$

$$\mathbf{r}(t-\Delta t) = \mathbf{r}(t) - \mathbf{v}(t)\Delta t + (1/2)\mathbf{a}(t)\Delta t^2 - (1/6)\mathbf{b}(t)\Delta t^3 + O(\Delta t^4)$$

相加 $\mathbf{r}(t+\Delta t) = 2\mathbf{r}(t) - \mathbf{r}(t-\Delta t) + \mathbf{a}(t)\Delta t^2 + O(\Delta t^4)$

相减 $\mathbf{v}(t) = \dfrac{\mathbf{r}(t+\Delta t) - \mathbf{r}(t-\Delta t)}{2\Delta t} + O\left(\Delta t^2\right)$

Verlet integrator is an order more accurate than integration by simple Taylor expansion alone, with the same term Δt^2

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3.0 Introduction

velocity Verlet algorithm

Verlet algorithm is not self-starting, we will use velocity Verlet algorithm in molecular dynamics simulations.

$$\mathbf{r}(t+\Delta t) = \mathbf{r}(t) + \mathbf{v}(t)\Delta t + (1/2)\mathbf{a}(t)\Delta t^2 + O\left(\Delta t^3\right)$$

$$\mathbf{v}(t+\Delta t) = \mathbf{v}(t) + \frac{\mathbf{a}(t) + \mathbf{a}(t+\Delta t)}{2}\Delta t + O\left(\Delta t^2\right)$$

Untitled.cdf

3.0 Introduction

Probabilistic model (unrepeatable results)

Consider the same system of N particles as before

- when there is uncetainty, say *random force* $\mathbf{R}_i$, which has a Gaussian probability distribution with correlation function

$$\left\langle \mathbf{R}_i(t) \cdot \mathbf{R}_i(t') \right\rangle = 6\gamma k_B T \delta(t - t') \qquad \gamma\text{: friction coefficient}$$

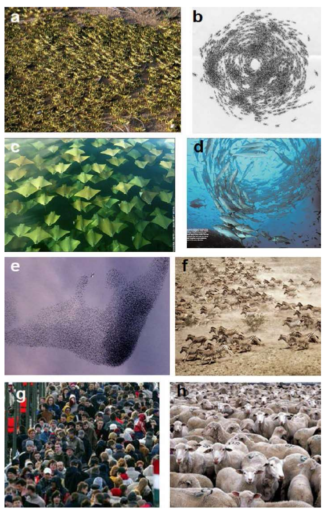
Langevin Equation:

$$m_i \frac{d^2 \mathbf{r}_i}{dt^2} + \gamma \frac{d\mathbf{r}_i}{dt} = \mathbf{f}_i + \mathbf{R}_i(t), \quad i = 1, 2, 3 \cdots N$$

$$\mathbf{f}_i = -\nabla_{\mathbf{r}_i} V(\mathbf{r}_1, \mathbf{r}_2, \cdots \mathbf{r}_N) = \left(-\frac{\partial V}{\partial x_i}, -\frac{\partial V}{\partial y_i}, -\frac{\partial V}{\partial z_i} \right)$$

Each particle's motion can be described by certain probabilities, derived from *Fokker- Planck Equation.*

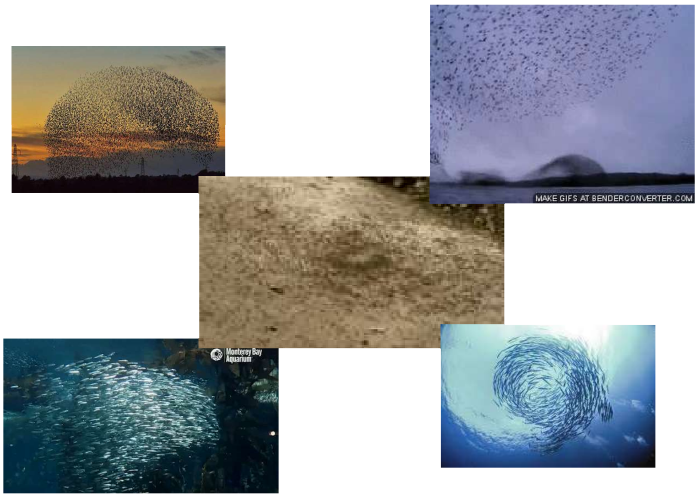
3.0 Introduction



(a) Wingless Locusts marching in the field.
(b) A rotating colony of army ants.
(c) A three-dimensional array of golden rays.
(d) Fish are known to produce such vortices.
(e) Before roosting, thousands of starlings producing a fascinating aerial display.
(f) A herd of zebra.
(g) People spontaneously ordered into traffic lanes as they cross a pedestrian bridge in large numbers.
(h) Although sheep are known to move very coherently, just as the corresponding theory predicts, when simply hanging around (no motion), well developed orientational patterns cannot emerge.

Tamás Vicsek, **Collective motion**, Physics Reports, Vol 517, 2012, Pages 71-140

3.0 Introduction



3.0 Introduction

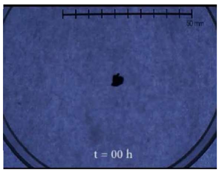
our primary goal:

- to investigate the connection between probabilistic and deterministic models of the same phenomenon.

Connection ?

probabilistic ⟷ deterministic

Micro view:
single random process



Macro view: (ensemble average)
definite distribution function

described by partial differential equation

- Looks paradoxical that a random process can be characterized by a definite equation
- But we know it is true from a lot of daily experience, such as coin tossing.

3.0 Introduction

coin tossing

~50% ~50%

many parameters unknown

- the initial orientation, velocity, and spin;
- the properties of the table surface;
- Various atomic defects, dislocations, grains, voids…

■ For single toss: no idea whether head or tail turns up.
■ After a large number of tosses, proportion of heads or tails is ~0.5.
■ With this example, it is not so surprising that there is a determinable distribution of probabilities which characterizes a random process.

3.0 Introduction

Probabilistic model originates from

- Incompleteness of information
  e.g. coin tossing
- Parameters sensitivity --- tiny perturbation in input induces huge variation in output.
  e.g. In kinetics of gases, a slight change in the initial conditions would result in a tremendous change after many collisions.

By an averaging of the solutions with varying initial conditions random processes can be modeled successfully.

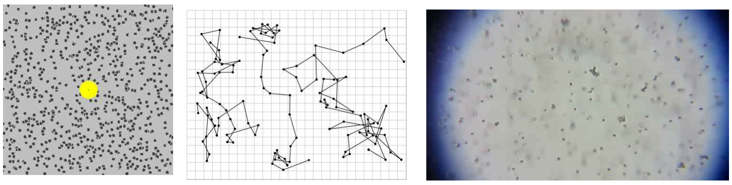
3.0 Introduction

in the following sections,

- Section 3.1
  1-D Brownian motion. An explicit expression of the probability *w(m, N).*
- Section 3.2
  Simplified expression of *w(m, N*). Asymptotic Series, Laplace's Method
- Section 3.3
  a difference equation for *w(m, N)* leads to a partial differential equation.
- Section 3.4
  The connection between probability and differential equations.

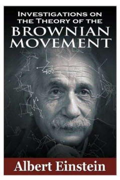
3.1 Random Walk in One Dimension; Langevin's Equation

In Brownian motion, small particles move about in liquid or gas.



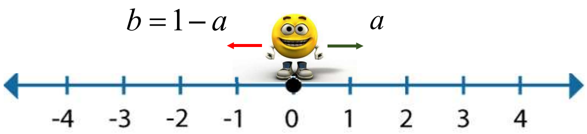
- no possibility and no interest of computing the trajectory of each molecule.
- one wishes to have an average understanding of the phenomenon.

- The Roman Lucretius's (卢克莱修) described Brownian motion of dust in his scientific poem "On the Nature of Things" (60 BC)
- Botanist Robert Brown in 1827 studied pollen grains suspended in water.
- Albert Einstein in 1905 solved this problem.



3.1.1 An one dimension random walk model

The minimum model of random walk: 1-D lattice model



Particle moves according to the following rules:

- Move in steps of a fixed length *dx* in a fixed time interval *dt*.
- The probability to the right *p* and to the left *q=1-p*.

Goal: to obtain the probability $w(m, N)$

- m steps to the right of the origin
- N the total steps

$$\text{Probability} = \frac{\text{number of observed events}}{\text{total number of events}}$$

3.1.1 An one dimension random walk model

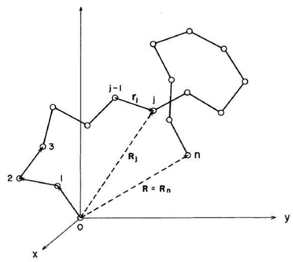
random walk model can be found in various situations

✓ a drunk staggering down a street

✓ a gambling game in which a coin is tossed

✓ Polymer Physics: Freely jointed chain model

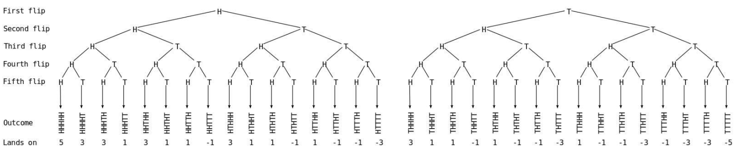
……

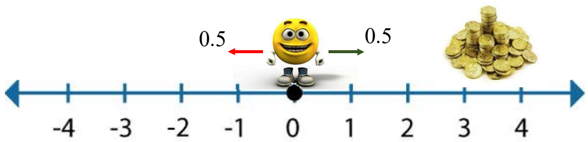


3.1.1 An one dimension random walk model

Fair coin tossing

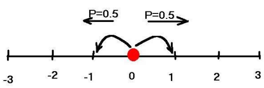
Head ~50%   Tail ~50%

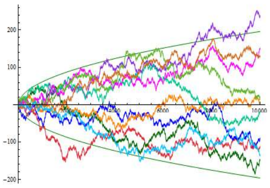


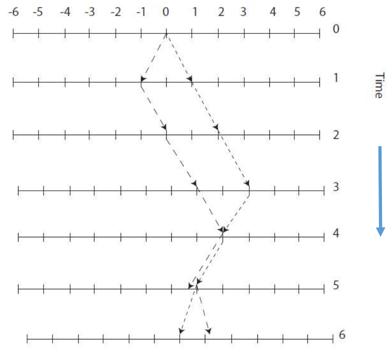


3.1.1 An one dimension random walk model

Random walk





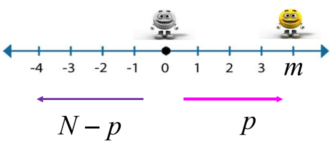


3.1.2 Explicit solution

To find *w(m, N)*, the probability that a particle at a point *m*∈[-*N*,*N*] steps to the right of its origin after total *N* steps.

Suppose that the particle

- *p* steps to the right, *p*>0
- *N-p* steps to the left



e.g. N=12 N-p=5 p=7 m=2

Displacment *m*

$m = p - (N-p) = 2p - N$

$p = (N + m)/2$

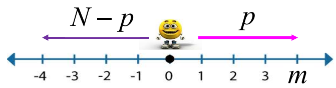
N is even $\rightarrow$ m is even. N is odd $\rightarrow$ m is odd

For example,

if N=3, the possible values of m = -3, -1, 1, 3.

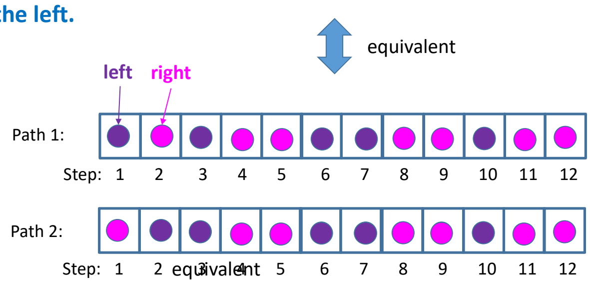
if N=4, the possible values of m = -4, -2, 0, 2, 4.

3.1.2 Explicit solution



To find out the number of paths with ***p* steps to the right** and ***N - p* to the left.**

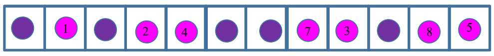
equivalent



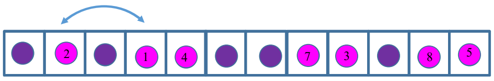
The number of choices with ***p*** indistinguishable **pink ball in *N* boxes**

3.1.2 Explicit solution

Consider p distinguishable balls, which can be placed in N boxes in the following number of ways:



$$N(N-1)(N-2)\cdots(N-p+1)=\frac{N!}{(N-p)!}$$



Interchanging distinguishable balls does not change the pattern.
There are $p!$ permutations of p balls.
排列

3.1.2 Explicit solution

number of ways p distinguishable balls can be placed in N boxes	=	number of full box empty box patterns	×	number of full permutations of distinguishable balls within a pattern
$\frac{N!}{(N-p)!}$	=	C_p^N	×	$p!$

binomial coefficient $$C_p^N=\frac{N!}{p!(N-p)!}$$

$$(x+y)^N=\sum_{p=0}^{N}C_p^N x^{N-p}y^p$$

3.1.2 Explicit solution

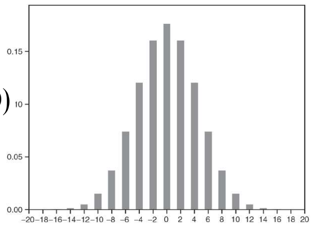
- The total number of possible path is 2^N
- the probability that a particle at a point m steps to the right of its origin after total N steps.

$$\boxed{w(m,N)=\frac{C_p^N}{2^N}} \qquad \text{where } p=(N+m)/2$$

The sum of all probabilities is unity

$$\sum_{m=-N}^{N}w(m,N)=\sum_{p=0}^{N}C_p^N\left(\frac{1}{2}\right)^N$$
$$=\sum_{p=0}^{N}C_p^N\left(\frac{1}{2}\right)^{N-p}\left(\frac{1}{2}\right)^p$$
$$=\left(\frac{1}{2}+\frac{1}{2}\right)^N=1$$

$w(m,20)$



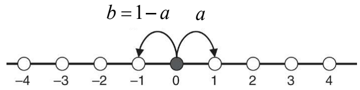
m

3.1.2 Explicit solution

Characteristic functions

- the **characteristic function** of any real-valued random variable defines its probability distribution.

Let $\lambda(\theta)=ae^{i\theta}+be^{-i\theta}$



$$\lambda^2(\theta)=\left(ae^{i\theta}+be^{-i\theta}\right)^2=a^2e^{i2\theta}\;+\;2abe^{i0}\;+\;b^2e^{-i2\theta}$$

	m=2	m=0	m=-2
$P_N(m)$	$P_2(2)$	$P_2(0)$	$P_2(-2)$
	$=a\cdot a$	$=2a\cdot b$	$=b\cdot b$

these coefficients are the probability

characteristic function $\lambda(\theta)=ae^{i\theta}+be^{-i\theta}=\left\langle e^{i\theta x}\right\rangle$ $\quad x=\pm1$

mean

3.1.2 Explicit solution

To extract the coefficient analytically , for example as m=2

$$\lambda^2(\theta)=\left(ae^{i\theta}+be^{-i\theta}\right)^2=a^2e^{i2\theta}\;+\;2abe^{i0}\;+\;b^2e^{-i2\theta}$$

$$P_2(2)=\frac{1}{2\pi}\int_{-\pi}^{\pi}\lambda^2(\theta)e^{-i2\theta}d\theta$$ Fourier transform

$$=\frac{1}{2\pi}\int_{-\pi}^{\pi}\left(a^2e^{i2\theta}\;+\;2abe^{i0}\;+\;b^2e^{-i2\theta}\right)e^{-i2\theta}d\theta$$
$$=\frac{1}{2\pi}\int_{-\pi}^{\pi}\left(a^2e^{i0\theta}\;+\;2abe^{-i2\theta}\;+\;b^2e^{-i4\theta}\right)d\theta$$
$$=\frac{1}{2\pi}\left(a^2\int_{-\pi}^{\pi}d\theta\;+2ab\int_{-\pi}^{\pi}e^{-i2\theta}d\theta+b^2\int_{-\pi}^{\pi}e^{-i4\theta}d\theta\right)$$
$$=a^2$$

3.1.2 Explicit solution

Generally, we extract the coefficient via Fourier transform

$$P_N(m)=\frac{1}{2\pi}\int_{-\pi}^{\pi}\lambda^N(\theta)e^{-i\theta m}d\theta$$
$$=\frac{1}{2\pi}\int_{-\pi}^{\pi}\left(ae^{i\theta}+be^{-i\theta}\right)^N e^{-i\theta m}d\theta$$
$$=\frac{1}{2\pi}\int_{-\pi}^{\pi}\sum_{k=0}^{N}C_k^N a^{N-k}e^{i\theta(N-k)}b^k e^{-i\theta k}e^{-i\theta m}d\theta$$
$$=\frac{1}{2\pi}\int_{-\pi}^{\pi}\sum_{k=0}^{N}C_{N-k}^N a^{N-k}e^{i\theta(N-k)}b^k e^{-i\theta k}e^{-i\theta m}d\theta$$
$$=\frac{1}{2\pi}\int_{-\pi}^{\pi}\sum_{p=0}^{N}C_p^N a^p e^{i\theta p}b^{N-p}e^{-i\theta(N-p)}e^{-i\theta m}d\theta$$
$$=\frac{1}{2\pi}\sum_{p=0}^{N}C_p^N a^p b^{N-p}\int_{-\pi}^{\pi}e^{i\theta(2p-N-m)}d\theta$$

$C_p^N=C_{N-p}^N$

$p=N-k$

3.1.2 Explicit solution

we notice

$$\frac{1}{2\pi}\int_{-\pi}^{\pi} e^{i\theta(2p-N-m)}d\theta = \begin{cases} 0, & if\ \ p \neq (N+m)/2 \\ 1, & if\ \ p = (N+m)/2 \end{cases}$$

Thus, we have

$$\boxed{P_N(m) = C_p^N a^p b^{N-p}, \quad p = (N+m)/2}$$

Specifically,

$$P_N(m) = w(m,N) = \frac{C_p^N}{2^N}$$

when $a = b = 1/2$

3.1.2 Explicit solution

General Characteristic function

- probability density function (PDF) $p(x)$.
- displacement x is continuous.
- the characteristic function is given by

$$\lambda(k) = \langle e^{ikx} \rangle = \int_{-\infty}^{\infty} p(x) e^{ikx} dx \qquad \lambda(\theta) = ae^{i\theta} + be^{-i\theta} = \langle e^{i\theta x} \rangle$$

Fourier transform of $p(x)$.

- One important property of the characteristic function

$$\lambda(0) = \int_{-\infty}^{\infty} p(x) dx = 1$$

3.1.2 Explicit solution

General random walk model

- Consider a continuous 1-D random walk process of n steps
- we have recursion relation:

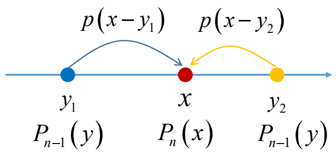
$$P_n(x) = \int_{-\infty}^{\infty} P_{n-1}(y) p(x-y) dy = P_{n-1}(x) * p(x)$$

convolution

$$f(x)*g(x) = \int_{-\infty}^{\infty} f(y) g(x-y) dy$$

This means that the probability $P_n(x)$ of a particle at x after *n* steps is

- $P_{n-1}(y)$ the probability of arriving at y in n −1 steps
- $p(x-y)$ the probability of displacements x-y in one step.



$$P_n(x) = \sum_i P_{n-1}(y_i) p(x-y_i)$$

$$\rightarrow P_n(x) = \int_{-\infty}^{\infty} P_{n-1}(y) p(x-y) dy$$

3.1.2 Explicit solution

Let us define

$$P_n(k) = \int_{-\infty}^{\infty} P_n(x) e^{ikx} dx$$

convolution theorem

$$f(x)*g(x) = \int_{-\infty}^{\infty} f(y) g(x-y) dy$$

$$F[f(x)*g(x)] = \frac{1}{2\pi} f(k)\cdot g(k)$$

$$P_n(x) = P_{n-1}(x) * p(x)$$

$$\lambda(k) = \int_{-\infty}^{\infty} p(x) e^{ikx} dx$$

$$\Downarrow$$

$$P_n(k) = P_{n-1}(k)\lambda(k)$$

$$\Downarrow$$

$$P_n(k) = P_{n-1}(k)\lambda(k) = P_{n-2}(k)\lambda^2(k) = \cdots = \lambda^n(k)$$

$$\Downarrow$$

$$\boxed{P_n(x) = \frac{1}{2\pi}\int_{-\infty}^{\infty} P_n(k) e^{-ikx} dx = \frac{1}{2\pi}\int_{-\infty}^{\infty} \lambda^n(k) e^{-ikx} dx}$$

3.1.3 Mean, Variance, and the Generating function

The expected value of function f is defined by

$$\langle f \rangle = \sum_{m=-N}^{N} f(m) w(m,N)$$

$$\langle p \rangle = \sum_{m=-N}^{N} p(m) w(m,N) = \sum_{p=0}^{N} p C_p^N \left(\frac{1}{2}\right)^N$$

n-th moment $\langle m^n \rangle = \sum_{m=-N}^{N} m^n w(m,N) = \sum_{m=-N}^{N} m^n C_p^N \left(\frac{1}{2}\right)^N$ where $p = (N+m)/2$

$\langle m \rangle$ mean displacement

$\langle m^2 \rangle$ mean square displacement or variance

3.1.3 Mean, Variance, and the Generating function

In order to evaluate the various moments, we introduce the generating function

$$G(u) = \sum_{p=0}^{N} u^p w(m,N)$$

or $G(u) = \sum_{p=0}^{N} u^p C_p^N \left(\frac{1}{2}\right)^N = \sum_{p=0}^{N} C_p^N u^p \left(\frac{1}{2}\right)^{N-p}\left(\frac{1}{2}\right)^p = (1+u)^N \left(\frac{1}{2}\right)^N$

Example: to calculate $\langle m \rangle$

$$G'(u) = \sum_{p=0}^{N} p u^{p-1} w(m,N) \Rightarrow G'(1) = \sum_{p=0}^{N} p w(m,N) = \langle p \rangle$$

$$G(u) = (1+u)^N \left(\frac{1}{2}\right)^N \Rightarrow G'(1) = N/2$$

$$\Rightarrow \langle p \rangle = N/2$$

since $p = (N+m)/2$

$$\langle p \rangle = \frac{1}{2}\sum_{p=0}^{N} (N+m) w(m,N)$$

$$= \frac{1}{2}\sum_{p=0}^{N} N w(m,N) + \frac{1}{2}\sum_{p=0}^{N} m w(m,N) = \frac{N}{2} + \frac{\langle m \rangle}{2} \Rightarrow \langle m \rangle = 0$$

3.1.3 Mean, Variance, and the Generating function

Example: $\langle m^2\rangle^{1/2}=?$

$$G'(u)=\sum_{p=0}^{N} p u^{p-1} w(m,N) \qquad G''(u)=\sum_{p=0}^{N} p(p-1)u^{p-2}w(m,N)$$

$$G''(1)=\sum_{p=0}^{N} p(p-1)w(m,N)=\langle p(p-1)\rangle=\langle p^2\rangle-\langle p\rangle$$

$$G(u)=(1+u)^N\left(\frac{1}{2}\right)^N \Rightarrow G''(u)=N(N-1)(1+u)^{N-2}\left(\frac{1}{2}\right)^N$$

$$\left.\begin{aligned}G''(1)&=\frac{N(N-1)}{4}\\ G''(1)&=\langle p^2\rangle-\langle p\rangle\end{aligned}\right\} \quad \langle p^2\rangle=\langle p\rangle+\frac{N(N-1)}{4}=\frac{N^2}{4}+\frac{N}{4}$$

$m=2p-N$

$$\langle m^2\rangle=\left\langle (2p-N)^2\right\rangle=4\langle p^2\rangle+N^2-4N\langle p\rangle=N^2+N+N^2-4N\frac{N}{2}=N$$

$$\boxed{\langle m^2\rangle^{1/2}=N^{1/2}}$$

3.1.3 Mean, Variance, and the Generating function

Generally, the nth- moment $\langle x^n\rangle=\int_{-\infty}^{\infty} p(x)x^n dx$

Its characteristic function

$$\lambda(k)=\langle e^{ikx}\rangle=\int_{-\infty}^{\infty} p(x)e^{ikx}dx=\int_{-\infty}^{\infty} dx\; p(x)\left(1+ikx-\frac{k^2x^2}{2!}+i\frac{k^3x^3}{3!}+\cdots\right)$$

$$=\sum_{n=0}^{\infty}\frac{i^n k^n}{n!}\langle x^n\rangle$$

We obtain n-th moments using characteristic function

$$\langle x^n\rangle=(-i)^n\left.\frac{d^n\lambda(k)}{dk^n}\right|_{k=0}$$

3.1.4 To determine Boltzmann's constant from Brownian Motion

Theory by Einstein, experiment by Perrin

Einstein

- Assume that the macroscopic resistance on the particle is proportional to the velocity - by classical hydrodynamics
- showed diffusion obey the statistical law

$$\langle x^2\rangle=\frac{1}{3}\left[\langle x^2\rangle+\langle y^2\rangle+\langle z^2\rangle\right]=\frac{1}{3}\langle r^2\rangle=2Dt$$ Verified by Perrin

the diffusion coefficient D is given by

$$D=kT/f$$

T: absolute temperature; K: Boltzmann's constant
f : the coefficient of resistance

$$f=6\pi\mu a \qquad \text{(Stokes' law)}$$

μ : viscosity coefficient; a : particle size

3.1.4 To determine Boltzmann's constant from Brownian Motion

The modern theory of the Brownian motion

Langevin's equation $\quad m\frac{d\mathbf{v}}{dt}=-f\mathbf{v}+\mathbf{F}(t)$

where $\boldsymbol{v}$ the velocity of the particle and m mass. The random force follows Fluctuation-dissipation relation

$$\langle \mathbf{F}_i(t)\cdot\mathbf{F}_i(t')\rangle=6fk_BT\delta(t-t')$$

3.1.4 To determine Boltzmann's constant from Brownian Motion

To solve $\quad m\frac{d\mathbf{v}}{dt}=-f\mathbf{v}+\mathbf{F}(t)$

multiply with $\mathbf{x}$, and take the ensemble average

$$m\left\langle \mathbf{x}\cdot\frac{d\mathbf{v}}{dt}\right\rangle=-f\langle\mathbf{x}\cdot\mathbf{v}\rangle+\langle\mathbf{x}\cdot\mathbf{F}(t)\rangle$$

$$\Downarrow$$

$$m\left(\frac{d\langle\mathbf{x}\cdot\mathbf{v}\rangle}{dt}-\langle v^2\rangle\right)=-f\langle\mathbf{x}\cdot\mathbf{v}\rangle+\langle\mathbf{x}\cdot\mathbf{F}(t)\rangle$$

$$\langle\mathbf{x}\cdot\mathbf{F}(t)\rangle=0$$

Not correlated

$$\Downarrow$$

$$\frac{d\langle\mathbf{x}\cdot\mathbf{v}\rangle}{dt}+\frac{f}{m}\langle\mathbf{x}\cdot\mathbf{v}\rangle-\langle v^2\rangle=0$$

$$\Downarrow$$

$$\langle\mathbf{x}\cdot\mathbf{v}\rangle=ce^{-\frac{f}{m}t}+\frac{m}{f}\langle v^2\rangle\rightarrow\frac{m}{f}\langle v^2\rangle \quad \text{stationary solution}$$

3.1.4 To determine Boltzmann's constant from Brownian Motion

$$\langle x^2\rangle=\frac{1}{3}\langle r^2\rangle=2Dt$$

$$\langle\mathbf{x}\cdot\mathbf{v}\rangle=\frac{1}{2}\frac{d\langle\mathbf{x}\cdot\mathbf{x}\rangle}{dt}=\frac{1}{2}\frac{d\langle r^2\rangle}{dt}=\frac{1}{2}\frac{d(6Dt)}{dt}=3D$$

$$\langle\mathbf{x}\cdot\mathbf{v}\rangle=\frac{m}{f}\langle v^2\rangle$$

$$\frac{1}{2}m\langle v^2\rangle=\frac{1}{2}f\langle\mathbf{x}\cdot\mathbf{v}\rangle=\frac{3}{2}fD$$

$$\frac{1}{2}m\langle v^2\rangle=\frac{3}{2}kT$$

energy equipartition principle

Boltzmann constant

$$\Rightarrow\quad k=D\frac{f}{T}=D\frac{6\pi\mu a}{T}$$

$$f=6\pi\mu a$$

作业： Ex. 4 Page 90

修正：Eq.(24) 应该为

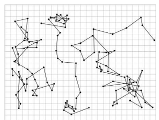
$$J_p(x)=\sum_{k=0}^{\infty}\frac{(-1)^k}{k!\,\Gamma(k+p+1)}\left(\frac{x}{2}\right)^{2k+p}$$

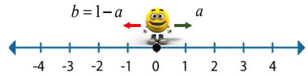
Recall what we did last time

probabilistic

Connection ?

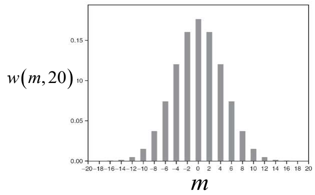
deterministic





random walk: 1-D lattice model

$$\boxed{w(m,N)=\frac{C_p^N}{2^N}}$$



Recall what we did last time

Characteristic function

$$\lambda(\theta)=ae^{i\theta}+be^{-i\theta}$$

$$P_N(m)=\frac{1}{2\pi}\int_{-\pi}^{\pi}\lambda^N(\theta)e^{-i\theta m}d\theta=w(m,N)=\frac{C_p^N}{2^N}$$

General characteristic function

$$\lambda(k)=\int_{-\infty}^{\infty}p(x)e^{ikx}dx \qquad P_N(x)=\frac{1}{2\pi}\int_{-\infty}^{\infty}\lambda^N(k)e^{-ikx}dx$$

3.1.3 Mean, Variance, and the Generating function

The expected value of function f is defined by

$$\langle f\rangle=\sum_{m=-N}^{N}f(m)w(m,N)$$

e.g. $$\langle p\rangle=\sum_{m=-N}^{N}p(m)w(m,N)=\sum_{p=0}^{N}pC_p^N 2^{-N}$$

$$\langle m^n\rangle=\sum_{m=-N}^{N}m^n w(m,N)$$ n-th moment

$\langle m\rangle$ mean displacement

$\langle m^2\rangle$ mean square displacement or variance

3.1.3 Mean, Variance, and the Generating function

In order to evaluate various moments, we introduce generating function

$$G(u)=\sum_{p=0}^{N}u^p w(m,N)$$

or

$$G(u)=\sum_{p=0}^{N}u^pC_p^N\left(\frac{1}{2}\right)^N=\sum_{p=0}^{N}C_p^N u^p\left(\frac{1}{2}\right)^{N-p}\left(\frac{1}{2}\right)^p$$

$$=(1+u)^N\left(\frac{1}{2}\right)^N$$

Their derivatives are related to n-th moments

3.1.3 Mean, Variance, and the Generating function

Example 1: $\langle m\rangle=?$

$$G'(u)=\sum_{p=0}^{N}pu^{p-1}w(m,N) \Rightarrow G'(1)=\sum_{p=0}^{N}pw(m,N)=\langle p\rangle$$

$$G'(u)=N(1+u)^{N-1}\left(\frac{1}{2}\right)^N \Rightarrow G'(1)=N/2$$

$$\boxed{\langle p\rangle=N/2}$$

$$\langle p\rangle=\frac{1}{2}\sum_{p=0}^{N}(N+m)w(m,N) \qquad p=(N+m)/2$$

$$=\frac{1}{2}\sum_{p=0}^{N}Nw(m,N)+\frac{1}{2}\sum_{p=0}^{N}mw(m,N)=\frac{N}{2}+\frac{\langle m\rangle}{2}$$

$$\boxed{\langle m\rangle=0}$$

3.1.3 Mean, Variance, and the Generating function

Example 2: $\langle m^2\rangle = ?$

$$G'(u)=\sum_{p=0}^{N} p u^{p-1} w(m,N) \qquad G''(u)=\sum_{p=0}^{N} p(p-1)u^{p-2} w(m,N)$$

$$G''(1)=\sum_{p=0}^{N} p(p-1)w(m,N)=\langle p(p-1)\rangle=\langle p^2\rangle-\langle p\rangle$$

$$G(u)=(1+u)^N\left(\frac{1}{2}\right)^N \Rightarrow G''(u)=N(N-1)(1+u)^{N-2}\left(\frac{1}{2}\right)^N$$

$$\Downarrow$$

$$G''(1)=\frac{N(N-1)}{4}$$

3.1.3 Mean, Variance, and the Generating function

$\langle p\rangle = N/2$

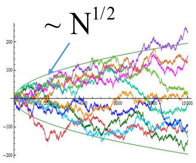
$$\left.\begin{aligned} G''(1)&=\langle p^2\rangle-\langle p\rangle \\ G''(1)&=\frac{N(N-1)}{4} \end{aligned}\right\} \langle p^2\rangle=\langle p\rangle+\frac{N(N-1)}{4}=\frac{N^2}{4}+\frac{N}{4}$$

$m = 2p - N$

$$\langle m^2\rangle=\langle(2p-N)^2\rangle=4\langle p^2\rangle+N^2-4N\langle p\rangle$$

$$=N^2+N+N^2-4N\frac{N}{2}=N$$

$$\boxed{\langle m^2\rangle^{1/2}=N^{1/2}}$$



3.1.3 Mean, Variance, and the Generating function

Generally the nth- moment $\langle x^n\rangle=\int_{-\infty}^{\infty} p(x)x^n dx$

Its characteristic function

$$\lambda(k)=\langle e^{ikx}\rangle=\int_{-\infty}^{\infty} p(x)e^{ikx}dx=\int_{-\infty}^{\infty} p(x)\sum_{m=0}^{\infty}\frac{(ikx)^m}{m!}dx$$

$$=\sum_{m=0}^{\infty}\frac{i^m k^m}{m!}\int_{-\infty}^{\infty} p(x)x^m dx=\sum_{m=0}^{\infty}\frac{i^m k^m}{m!}\langle x^m\rangle$$

n-th moments represented by characteristic function

$$\left.\frac{d^n\lambda}{dk^n}\right|_{k=0}=\left.\sum_{m=0}^{\infty} i^m\langle x^m\rangle\frac{m(m-1)\cdots(m-n+1)}{m!}k^{m-n}\right|_{k=0}=i^n\langle x^n\rangle$$

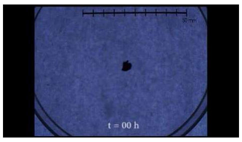
$$\Rightarrow \boxed{\langle x^n\rangle=-i^n\left.\frac{d^n\lambda(k)}{dk^n}\right|_{k=0}}$$

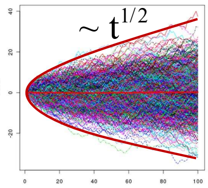
3.1.4 To determine Boltzmann's constant from Brownian Motion

Einstein (1905)

- assume that the macroscopic resistance on the particle is proportional to the velocity - using classical hydrodynamics
- predicated diffusion follows the statistical law

$$\langle x^2\rangle=\frac{1}{3}\left[\langle x^2\rangle+\langle y^2\rangle+\langle z^2\rangle\right]=\frac{1}{3}\langle r^2\rangle=2Dt$$





$\langle m^2\rangle^{1/2}=N^{1/2}$

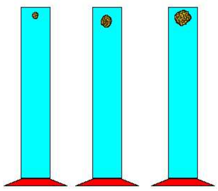
Perrin:
experiment in 1908.
Nobel Prize in 1926

3.1.4 To determine Boltzmann's constant from Brownian Motion

diffusion coefficient D

$$D = kT/f$$

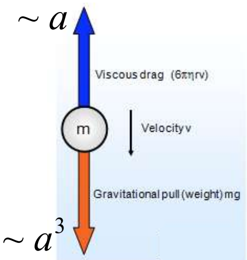
T: absolute temperature;
K: Boltzmann's constant
f: the coefficient of resistance



Stokes' law: the drag force F

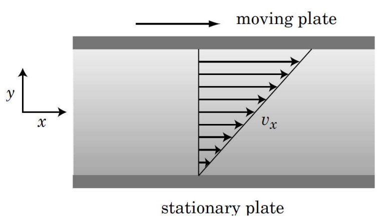
$$F = fV = 6\pi\eta a V$$

η: viscosity coefficient
a: particle size
V: velocity



3.1.4 To determine Boltzmann's constant from Brownian Motion

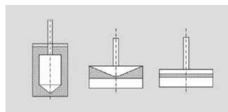
Viscosity of Solutions



$$\eta\frac{\partial v_x}{\partial y}=\sigma_{yx}$$

the unit of η is $N\cdot s/m^2$

Viscosity



Anton Paar Germany Inc

3.1.4 To determine Boltzmann's constant from Brownian Motion

The modern theory of the Brownian motion

Langevin's equation $$m\frac{d\mathbf{v}}{dt} = -f\mathbf{v} + \mathbf{F}(t)$$

- $\boldsymbol{v}$ the velocity of the particle and m mass.
- The random force follows Fluctuation-dissipation relation

$$\left\langle \mathbf{F}_i(t)\cdot\mathbf{F}_i(t')\right\rangle = 6 f k_B T\delta(t-t')$$

3.1.4 To determine Boltzmann's constant from Brownian Motion

To solve $$m\frac{d\mathbf{v}}{dt} = -f\mathbf{v} + \mathbf{F}(t)$$

multiply both sides with **x**, and take the average

$$m\left\langle \mathbf{x}\cdot\frac{d\mathbf{v}}{dt}\right\rangle = -f\left\langle \mathbf{x}\cdot\mathbf{v}\right\rangle + \left\langle \mathbf{x}\cdot\mathbf{F}(t)\right\rangle$$

$$\Downarrow$$

$$m\left(\frac{d\left\langle \mathbf{x}\cdot\mathbf{v}\right\rangle}{dt} - \left\langle v^2\right\rangle\right) = -f\left\langle \mathbf{x}\cdot\mathbf{v}\right\rangle + \left\langle \mathbf{x}\cdot\mathbf{F}(t)\right\rangle$$

$$\left\langle \mathbf{x}\cdot\mathbf{F}(t)\right\rangle = 0$$

Not correlated

$$\Downarrow$$

$$\frac{d\left\langle \mathbf{x}\cdot\mathbf{v}\right\rangle}{dt} + \frac{f}{m}\left\langle \mathbf{x}\cdot\mathbf{v}\right\rangle - \left\langle v^2\right\rangle = 0$$

3.1.4 To determine Boltzmann's constant from Brownian Motion

$$\frac{d\left\langle \mathbf{x}\cdot\mathbf{v}\right\rangle}{dt} + \frac{f}{m}\left\langle \mathbf{x}\cdot\mathbf{v}\right\rangle - \left\langle v^2\right\rangle = 0$$

$$\Downarrow$$

$$\left\langle \mathbf{x}\cdot\mathbf{v}\right\rangle = c\exp[-\frac{f}{m}t] + \frac{m}{f}\left\langle v^2\right\rangle$$

$$\rightarrow \frac{m}{f}\left\langle v^2\right\rangle \text{ stationary solution}$$

3.1.4 To determine Boltzmann's constant from Brownian Motion

$$\left\langle \mathbf{x}\cdot\mathbf{v}\right\rangle = \frac{1}{2}\frac{d\left\langle \mathbf{x}\cdot\mathbf{x}\right\rangle}{dt} = \frac{1}{2}\frac{d\left\langle r^2\right\rangle}{dt} = \frac{1}{2}\frac{d(6Dt)}{dt} = 3D$$

When in equilibrium

$$\left\langle \mathbf{x}\cdot\mathbf{v}\right\rangle = \frac{m}{f}\left\langle v^2\right\rangle \qquad \left\langle x^2\right\rangle = \frac{1}{3}\left\langle r^2\right\rangle = 2Dt$$

$$\left.\begin{aligned}&\frac{1}{2}m\left\langle v^2\right\rangle = \frac{1}{2}f\left\langle \mathbf{x}\cdot\mathbf{v}\right\rangle = \frac{3}{2}fD\\ &\boxed{\frac{1}{2}m\left\langle v^2\right\rangle = \frac{3}{2}kT}\end{aligned}\right\}$$

energy equipartition principle

Boltzmann constant

$$k = D\frac{f}{T} = D\frac{6\pi\eta a}{T}$$

Section 3.2

Asymptotic Series, Laplace's Method, Gamma Function, Stirling's Formula

3.2.0 Simplify probability function by Stirling's formula

- the exact form of $w(m, N)$ was obtained.
  m: position. N: total steps.

$$w(m,N) = \frac{C_p^N}{2^N} = \frac{N!}{2^N p!(N-p)!} \qquad p = (N+m)/2$$

- The calculation is tedious and heavy.
- James Stirling (*Scottish mathematician, 1692-1770*) presented a way to estimate it with enough accuracy.

3.2.0 Simplify probability function by Stirling's formula

Dominant term

$$\underline{\ln n! \sim \left(n+\frac{1}{2}\right)\ln n - n + \ln\sqrt{2\pi}} + \frac{1}{12n} - \frac{1}{360n^3} + \cdots$$

$$\Downarrow$$

$$n! \sim (2\pi n)^{1/2}\, n^n e^{-n}$$

Stirling's formula

will be proved later

3.2.0 Simplify probability function by Stirling's formula

$$\boxed{w(m,N) = \frac{N!}{2^N\, p!(N-p)!}} \qquad p = \frac{N+m}{2}$$

$$\ln n! \sim \frac{1}{2}\ln 2\pi n + n\ln n - n$$

$$\ln w(m,N) = \ln\frac{N!}{2^N\, p!(N-p)!}$$

$$= \ln N! - \ln p! - \ln(N-p)! - N\ln 2$$

$$= \ln\sqrt{\frac{2}{\pi N}} - \frac{1+N}{2}\ln\left[1-\left(\frac{m}{N}\right)^2\right] + \frac{m}{2}\ln\left[1-\frac{m}{N}\right] - \frac{m}{2}\ln\left[1+\frac{m}{N}\right]$$

$$\boxed{w(m,N) = \sqrt{\frac{2}{\pi N}}\left[1-\left(\frac{m}{N}\right)^2\right]^{-\frac{1+N}{2}}\left[1-\left(\frac{m}{N}\right)\right]^{\frac{m}{2}}\left[1+\left(\frac{m}{N}\right)\right]^{-\frac{m}{2}}}$$

3.2.0 Simplify probability function by Stirling's formula

$$w(m,N) = \frac{N!}{2^N\, p!(N-p)!} \qquad p = \frac{N+m}{2} \qquad \ln n! \sim \frac{1}{2}\ln 2\pi n + n\ln n - n$$

$$\ln w(m,N) = \ln\frac{N!}{2^N\, p!(N-p)!}$$

$$= \ln N! - \ln p! - \ln(N-p)! - N\ln 2$$

$$= \frac{1}{2}\ln 2\pi + \frac{1}{2}\ln N + N\ln N - N \quad -\frac{1}{2}\ln 2\pi - \frac{1}{2}\ln p - p\ln p + p$$

$$-\frac{1}{2}\ln 2\pi - \frac{1}{2}\ln(N-p) - (N-p)\ln(N-p) + (N-p) \quad - N\ln 2$$

$$= \frac{1}{2}\ln 2\pi + \frac{1}{2}\ln N + N\ln N - N \quad -\frac{1}{2}\ln 2\pi - \frac{1}{2}\ln\frac{N+m}{2} - \frac{N+m}{2}\ln\frac{N+m}{2} + \frac{N+m}{2}$$

$$-\frac{1}{2}\ln 2\pi - \frac{1}{2}\ln\frac{N-m}{2} - \frac{N-m}{2}\ln\frac{N-m}{2} + \frac{N-m}{2} \quad - N\ln 2$$

$$= \frac{1}{2}\ln N + N\ln N - \frac{1}{2}\ln\frac{N+m}{2} - \frac{N+m}{2}\ln\frac{N+m}{2} - \frac{1}{2}\ln\frac{N-m}{2} - \frac{N-m}{2}\ln\frac{N-m}{2} \quad - N\ln 2 - \frac{1}{2}\ln 2\pi$$

$$= \frac{1}{2}\ln N + N\ln N - \frac{1}{2}\ln\frac{N^2-m^2}{4} - \frac{N}{2}\ln\frac{N^2-m^2}{4} + \frac{m}{2}\ln\frac{N-m}{N+m} - N\ln 2 - \frac{1}{2}\ln 2\pi$$

$$= \frac{1}{2}\ln N + N\ln N - \frac{1+N}{2}\ln\frac{1-(m/N)^2}{4}N^2 + \frac{m}{2}\ln\frac{1-(m/N)}{1+(m/N)} - N\ln 2 - \frac{1}{2}\ln 2\pi$$

$$= \frac{1}{2}\ln N + N\ln N - N\ln 2 - \frac{1+N}{2}\ln\frac{N^2}{4} - \frac{1}{2}\ln 2\pi - \frac{1+N}{2}\ln\left(1-(m/N)^2\right) + \frac{m}{2}\ln\left(1-(m/N)\right) - \frac{m}{2}\ln\left(1+(m/N)\right)$$

$$= \ln\sqrt{\frac{2}{\pi N}} - \frac{1+N}{2}\ln\left(1-(m/N)^2\right) + \frac{m}{2}\ln\left(1-(m/N)\right) - \frac{m}{2}\ln\left(1+(m/N)\right)$$

3.2.0 Simplify probability function by Stirling's formula

$$w(m,N) = \sqrt{\frac{2}{\pi N}}\left[1-\left(\frac{m}{N}\right)^2\right]^{-\frac{1+N}{2}}\left[1-\left(\frac{m}{N}\right)\right]^{\frac{m}{2}}\left[1+\left(\frac{m}{N}\right)\right]^{-\frac{m}{2}}$$

$$\xrightarrow{N\to\infty}$$

$$= \sqrt{\frac{2}{\pi N}}\ \exp\left[\left(\frac{m}{N}\right)^2\frac{1+N}{2}\right]\ \exp\left[-\left(\frac{m}{N}\right)\frac{m}{2}\right]\ \exp\left[-\left(\frac{m}{N}\right)\frac{m}{2}\right]$$

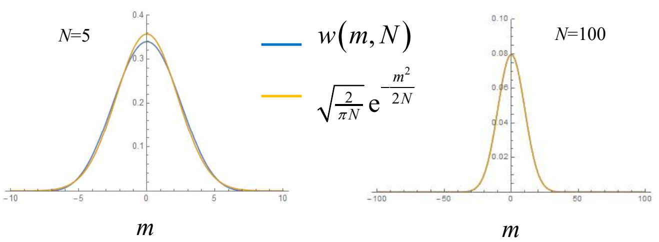
$$= \sqrt{\frac{2}{\pi N}}\exp\left[-\frac{(N-1)m^2}{2N^2}\right] \qquad \lim_{x\to\infty}\left(1+\frac{1}{x}\right)^x = e$$

$$\approx \sqrt{\frac{2}{\pi N}}\exp\left(-\frac{m^2}{2N}\right)$$

$$\boxed{w(m,N) \approx \sqrt{\frac{2}{\pi N}}\exp\left(-\frac{m^2}{2N}\right)}$$

3.2.0 Simplify probability function by Stirling's formula

$$\boxed{w(m,N) \approx \sqrt{\frac{2}{\pi N}}\exp\left(-\frac{m^2}{2N}\right)}$$



3.2.0 Simplify probability function by Stirling's formula

Stirling's formula

- 2 heuristic & 8 rigorous approaches to derive

In this book, via gamma function

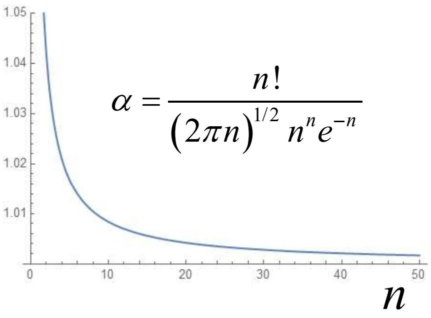
$$\ln n! \sim \left(n+\frac{1}{2}\right)\ln n - n + \ln\sqrt{2\pi} + \frac{1}{12n} - \frac{1}{360n^3} + \frac{1}{1260n^5} - \cdots$$

- Diverge for any value of n.
- Not a series in rigorous mathematical sense.

3.2.0 Simplify probability function by Stirling's formula

- But ! The dominant term works!

$$n! \sim (2\pi n)^{1/2} n^n e^{-n}$$



$$\alpha = \frac{n!}{(2\pi n)^{1/2} n^n e^{-n}}$$

n	α
5	1.01678
10	1.00837
50	1.00167
100	1.000837

Because it is an asymptotic series.

3.2.1 Examples of asymptotics

Jules Henri Poincaré introduced asymptotic expansion in 1886. This concept enables one to

- manipulate a large class of divergent series
- obtain numerical as well as qualitative results for many problems.

3.2.1 Examples of asymptotics

Example -1: ODE

$$\frac{dy}{dx} + y = \frac{1}{x} \qquad \text{for large x.}$$

we have a solution in the form

$$y = \frac{1}{x} + \frac{2!}{x^2} + \frac{3!}{x^3} + \cdots \frac{(n-1)!}{x^n} + \cdots$$

this divergent series is useful for numerical calculations, and called an asymptotic series

3.2.1 Examples of asymptotics

Example-2: regular quadratic

$$x^2 + \varepsilon x - 1 = 0$$

ε : a small constant, say ε =0.0000001.

Exact solutions $x = \dfrac{-\varepsilon \pm \sqrt{\varepsilon^2 + 4}}{2}$

As ε=0, we have the unperturbed solution

$$x^2 + \cancel{\varepsilon x} - 1 = 0 \Rightarrow x = \pm 1$$

3.2.1 Examples of asymptotics

- Taylor expansion of the exact solution:

$$x = \begin{cases} 1 - \dfrac{\varepsilon}{2} + \dfrac{\varepsilon^2}{8} - \dfrac{\varepsilon^4}{128} + O(\varepsilon^6) \\ -1 - \dfrac{\varepsilon}{2} - \dfrac{\varepsilon^2}{8} + \dfrac{\varepsilon^4}{128} + O(\varepsilon^6) \end{cases} \qquad \text{converge if } |\varepsilon| < 2$$

- Series method

power series expansion around $x = \pm 1$

$$x = \pm 1 + a_1 \varepsilon + a_2 \varepsilon^2 + a_3 \varepsilon^3 + \cdots$$

The same Taylor expansions can be reproduced.

3.2.1 Examples of asymptotics

Example-3: singular quadratic

$$\epsilon x^2 + x - 1 = 0$$

ε is a small constant, say ε =0.0000001.

Exact solutions $x = \dfrac{-1 \pm \sqrt{1 + 4\varepsilon}}{2\varepsilon}$

As ε=0, we have the unperturbed solution

$$\cancel{\epsilon x^2} + x - 1 = 0 \Rightarrow x = 1$$

Only one root !

■ Taylor expansion of the exact solution:

$$x = \begin{cases} 1-\varepsilon+2\varepsilon^2-5\varepsilon^3+O\left(\varepsilon^4\right) \\ -\frac{1}{\varepsilon}-1+\varepsilon-2\varepsilon^2+5\varepsilon^3+O\left(\varepsilon^4\right) \end{cases}$$

converge if $|\varepsilon|<1/4$

■ Expansion method

Assuming power series

Why? be patient

$$x = \frac{a_{-1}}{\varepsilon}+a_0+a_1\varepsilon+a_2\varepsilon^2+\cdots$$

Substituting into $\epsilon x^2 + x - 1 = 0$

$$\varepsilon^{-1}\left(a_{-1}^2+a_{-1}\right)+\varepsilon^0\left(2a_{-1}a_0+a_0-1\right)+\varepsilon\left(2a_{-1}a_1+a_0^2+a_1\right)+\cdots=0$$

Comparing coefficients of ε of same order

ε^{-1}: $a_{-1}^2+a_{-1}=0$ $\quad a_{-1}=-1$ or $a_{-1}=0$

ε^{0}: $2a_{-1}a_0+a_0-1=0$ $\quad a_0=-1$ $\quad a_0=1$

ε^{1}: $2a_{-1}a_1+a_0^2+a_1=0$ $\quad a_1=1$ $\quad a_1=-1$

$$\boxed{x=-\frac{1}{\varepsilon}-1+\varepsilon+\cdots} \qquad \boxed{x=1-\varepsilon+2\varepsilon^2\cdots}$$

Singular root Regular root

■ Rescaling method

balance the three terms $\varepsilon x^2+x-1=0$

(1) x and -1 is comparable, assuming εx^2 is smaller than other two terms.

$$x\sim O(1) \qquad \varepsilon x^2\sim o(1)$$

$$\varepsilon x^2+x-1=0 \Rightarrow x\approx 1$$

Good guess

(2) εx^2 and -1 is comparable, assuming x is smaller than other two terms.

$$\varepsilon x^2\sim O(1) \qquad x\sim o(1)$$

$$\varepsilon x^2+x-1=0 \Rightarrow |x|\approx\frac{1}{\sqrt{\varepsilon}}>>1$$

Bad guess

(3) εx^2 and x is comparable, assuming both terms >> 1.

$$\varepsilon x^2\sim O(x) >>1$$

$$\varepsilon x^2+x-1=0 \Rightarrow |x|\approx\frac{1}{\varepsilon}>>1$$

Self consistent

When εx^2 and x balance, x is very larger $x\sim O(\varepsilon^{-1})$

rescaling x, $x=\frac{X}{\varepsilon}$ with $X\sim O(1)$

We get a regular looking problem

$$X^2+X-\varepsilon=0$$

Using regular expansion

$$X=a_0+a_1\varepsilon+a_2\varepsilon^2+\cdots$$

Comparing coefficients of ε of same order, we get

$$\boxed{x=-\frac{1}{\varepsilon}-1+\varepsilon+\cdots}$$

Example-4: Asymptotic series by parts integration

Error function $\operatorname{Erf}(z) = \frac{2}{\sqrt{\pi}}\int_0^z e^{-t^2}dt$

- In the 19th century, error function from the theory of errors appeared in several contexts unrelated to probability, e.g. refraction and heat conduction.
- In 1871, J. W. Glaisher wrote that "Erf(*x*) may fairly claim at present to rank in importance next to the trigonometrical and logarithmic functions."
- Glaisher introduced the symbol Erf and the name it *error function*.

$$\operatorname{Erf}(z) = \frac{2}{\sqrt{\pi}}\int_0^z e^{-t^2}dt = \frac{2}{\sqrt{\pi}}\sum_{n=0}^{\infty}\frac{(-1)^n z^{2n+1}}{(2n+1)n!}$$

$$= \frac{2}{\sqrt{\pi}}\left(z - \frac{z^3}{3} + \frac{z^5}{10} - \frac{z^7}{42} + \frac{z^9}{216} - \frac{z^{11}}{1320} + \cdots\right)$$

D'Alembert's ratio test:

$$\lim_{n\to\infty}\left|\frac{a_{n+1}}{a_n}\right| = \lim_{n\to\infty}\left|\frac{(2n+1)n!z^{2n+3}}{(2n+3)(n+1)!z^{2n+1}}\right| = \lim_{n\to\infty}\left|\frac{(2n+1)z^2}{(2n+3)(n+1)}\right| = 0$$

This series is convergence.

Consider an alternative form of the error function

$$\operatorname{Erf}(z) = \frac{2}{\sqrt{\pi}}\int_0^z e^{-t^2}dt = \frac{2}{\sqrt{\pi}}\left(\int_0^\infty + \int_\infty^z\right)e^{-t^2}dt$$

$$= 1 - \frac{2}{\sqrt{\pi}}\int_z^\infty e^{-t^2}dt = 1 - \operatorname{Erfc}(z)$$

complementary error function

Integrating by parts

$$\int u\,dv = uv - \int v\,du$$

$$\frac{\operatorname{Erfc}(z)}{2/\sqrt{\pi}} = \int_z^\infty e^{-t^2}dt = -\int_z^\infty \frac{de^{-t^2}}{2t} = \frac{e^{-z^2}}{2z} - \int_z^\infty \frac{e^{-t^2}}{2t^2}dt$$

and 3 more times

$$\frac{\operatorname{Erfc}(z)}{2/\sqrt{\pi}} = \frac{e^{-z^2}}{2z}\left(1 - \frac{1}{2z^2} + \frac{1\cdot 3}{(2z^2)^2} - \frac{1\cdot3\cdot5}{(2z^2)^3} + \frac{1\cdot3\cdot5\cdot7}{(2z^2)^4}\cdots\right) + \int_z^\infty \frac{105e^{-t^2}}{16t^8}dt$$

the remainder can be bounded by

$$|R_5| = \int_z^\infty \frac{105e^{-t^2}}{16t^8}dt = \int_z^\infty \frac{105de^{-t^2}}{32t^9} < \frac{105}{32z^9}\int_z^\infty de^{-t^2} = \frac{105e^{-z^2}}{32z^9} = a_5$$

$$\boxed{|R_5| < a_5}$$

double factorial

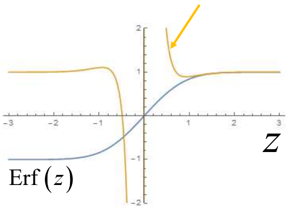
$$n!! \equiv \begin{cases} n\cdot(n-2)\dots5\cdot3\cdot1 & n>0 \text{ odd} \\ n\cdot(n-2)\dots6\cdot4\cdot2 & n>0 \text{ even} \\ 1 & n=-1,0. \end{cases}$$

Thus we have proven that as $z \longrightarrow \infty$

$$\operatorname{Erf}(z) = 1 - \operatorname{Erfc}(z) \approx 1 - \frac{e^{-t^2}}{z\sqrt{\pi}}\left(1 + \sum_{n=2}^{N}(-1)^{N+1}\frac{(2N-3)!!}{(2z^2)^{N-1}}\right) + O\left(z^{-2N+1}\right)$$

- This expansion for the error function diverges
- However, the truncated series, is useful

3 terms $1 - \frac{e^{-z^2}}{z\sqrt{\pi}}\left(1 - \frac{1}{2z^2}\right)$



	$z = 2.5$	$z = 3$
	$\operatorname{Erf}(z) = 0.999593$	$\operatorname{Erf}(z) = 0.999978$
	3 terms give 0.999599	3 terms give 0.9999778

This expansion has some important properties:
- the leading term is roughly correct
- further terms are corrections of decreasing size.

This property is called asymptoticness.

Example-5: from our book

To evaluate the integral

$$f(x) = \int_x^\infty t^{-1}e^{x-t}dt \qquad \text{as } x >> 1$$

Notice the incomplete gamma function reads

$$\Gamma(s,x) = \int_x^\infty t^{s-1}e^{-t}dt$$

$$\boxed{f(x) = e^x\int_x^\infty t^{-1}e^{-t}dt = e^x\Gamma(0,x)}$$

integration by parts, $\int u dv = uv - \int v du$

$$f(x) = \int_x^\infty t^{-1} e^{x-t} dt = -\int_x^\infty t^{-1} de^{x-t} = -t^{-1} e^{x-t} |_x^\infty + \int_x^\infty e^{x-t} t^{-2} dt$$

$$= \frac{1}{x} + \int_x^\infty e^{x-t} t^{-2} dt = \frac{1}{x} - \frac{1}{x^2} + 2\int_x^\infty e^{x-t} t^{-3} dt$$

by successive integration by parts,

$$\boxed{f(x) = S_n(x) + R_n(x)}$$

where $S_n(x) = \frac{1}{x} - \frac{1}{x^2} + \frac{2!}{x^3} - \cdots + \frac{(-1)^{n-1}(n-1)!}{x^n}$

$$R_n(x) = (-1)^n n! \int_x^\infty t^{-(n+1)} e^{x-t} dt = (-1)^n n! e^x \Gamma(-n, x)$$

We have some observations

- as $n \to \infty$, $S_n(x)$ diverges for a fixed x.

$$\lim_{n\to\infty} \left| \frac{a_{n+1}}{a_n} \right| = \lim_{n\to\infty} \left| \frac{n! x^n}{(n-1)! x^{n+1}} \right| = \lim_{n\to\infty} \left| \frac{n}{x} \right| = \infty$$

- as $x \to \infty$, $R_n(x) \to 0$, for a fixed n.

$$|R_n(x)| < n! x^{-(n+1)} \int_x^\infty e^{x-t} dt = n! x^{-(n+1)} = |a_{n+1}|$$

- The ratio of the remainder to the last term approaches zero, as $x \to \infty$

$$\left| \frac{R_n(x)}{a_n(x)} \right| < \left| \frac{a_{n+1}(x)}{a_n(x)} \right| = \frac{n! x^{-(n+1)}}{(n-1)! x^{-n}} = \frac{n}{x} < 1$$

- As $x \geq 2n$

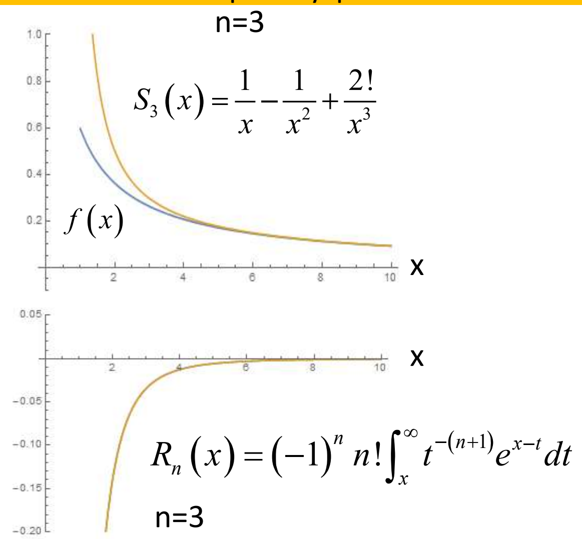
$$|R_n(x)| < |a_{n+1}(x)| = n! x^{-(n+1)} < n!(2n)^{-(n+1)}$$

$$= \frac{1}{2^{n+1} n} \cdot \frac{n!}{n^n} = \frac{1}{2^{n+1} n} \cdot \left[\frac{n}{n} \frac{n-1}{n} \cdots \frac{1}{n} \right] < \frac{1}{2^{n+1} n^2}$$

which is small even for moderate values of n.

for example, as n=3, $x = 2n \geq 6$

$$|R_n(x)| < \frac{1}{2^4 3^2} = \frac{1}{144} \approx 0.007$$



3.2.1 Examples of asymptotics

- As $x \geq 2n$

$$|R_n(x)| < |a_{n+1}(x)| = n! x^{-(n+1)} < n!(2n)^{-(n+1)}$$

$$= \frac{1}{2^{n+1} n} \cdot \frac{n!}{n^n} = \frac{1}{2^{n+1} n} \cdot \left[\frac{n}{n} \frac{n-1}{n} \cdots \frac{1}{n} \right] < \frac{1}{2^{n+1} n^2}$$

which is small even for moderate values of n.

for example, as n=3, $x = 2n \geq 6$

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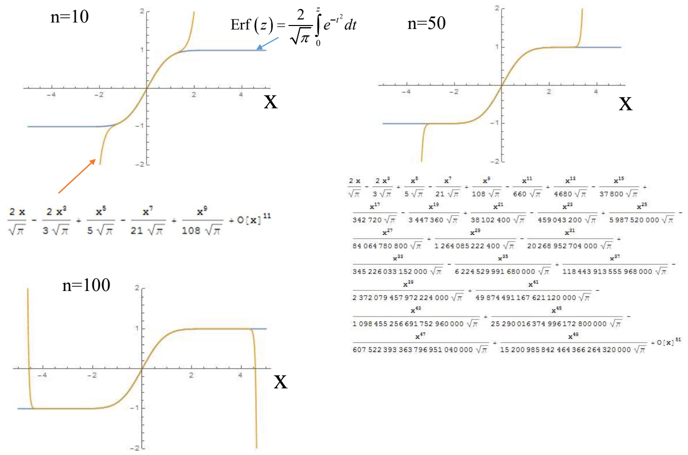


This convergent series is less useful in practice.

More asymptotic series

0-order Bessel functions

$$J_0(x) = \sum_{n=0}^{\infty}(-1)^n \frac{x^{2n}}{2^{2n}(n!)^2}$$
$$= 1 - \frac{1}{4}x^2 + \frac{1}{64}x^4 - \frac{1}{2304}x^6 + \frac{1}{147456}x^8 - \cdots$$

$$J_0(x) \sim \left(\frac{2}{\pi x}\right)^{\frac{1}{2}}\left[\left(1 - \frac{(3!!)^2}{2!(8x)^2} + \frac{(7!!)^2}{4!(8x)^4} - \cdots\right)\cos\left(x + \frac{1}{4}\pi\right)\right.$$
$$\left.+\left(\frac{1}{8x} - \frac{(5!!)^2}{3!(8x)^3} + \frac{(9!!)^2}{5!(8x)^5} - \cdots\right)\sin\left(x - \frac{1}{4}\pi\right)\right]$$

More asymptotic series

Laplace integral

$$T = \int_a^b g(t)e^{xh(t)}at \qquad I \sim g(a)e^{xh(a)}\sqrt{\frac{-\pi}{2xh''(a)}}$$

ODE

$$\frac{d}{dx}\left(p\frac{dy}{dx}\right) + (\lambda^2 q_0 + q_2)y = 0$$

$$y \sim C_1\frac{1}{(q_0 p)^{\frac{1}{4}}}\cos\left[\lambda\int_{x_0}^{x}\left(\frac{q_0}{p}\right)^{\frac{1}{2}}dx\right]$$
$$+C_2\frac{1}{(q_0 p)^{\frac{1}{4}}}\sin\left[\lambda\int_{x_0}^{x}\left(\frac{q_0}{p}\right)^{\frac{1}{2}}dx\right]$$

Consider function $f(\varepsilon)$, there are three possibilities

$$f(\varepsilon) = 0, \infty, A \qquad \text{as } \varepsilon \to 0, \quad 0 < A < \infty$$

- the speed at which $f(\varepsilon) \to \infty$ or $f(\varepsilon) \to 0$ can be expressed by comparing *gauge functions.*
- *gauge functions* may be

$$1, \varepsilon^{\pm n}, \varepsilon^{\pm 1/n}, \log\varepsilon^{-1}, \log\left(\log\varepsilon^{-1}\right), e^{\varepsilon^{-1}}, \sin\varepsilon, \sinh\varepsilon, \cdots$$

e.g.

$$\lim_{\varepsilon\to 0}\frac{f(\varepsilon)}{\varepsilon^{1/2}} = 0$$

This indicates $f(\varepsilon)$ goes to 0 in a speed faster than that of $\varepsilon^{1/2}$

The Symbol *O*

Definition: if there exists a positive constant *M* such that $|\phi(x)| \le M\,|\varphi(x)|$, as $x \to x_0$, we say

$$\phi(x) = O\left[\varphi(x)\right] \qquad \text{or} \qquad \phi(x) \sim \varphi(x)$$

ϕ is big-oh of φ $\qquad$ ϕ is asymptotic to φ

Meaning ϕ is of the same order of φ, or

$$\lim_{x\to x_0}\frac{\phi(x)}{\varphi(x)} = C \qquad C \text{ is a constant}$$

e.g. as x → 0 $\quad \cos x = O(1), \ x\sin x^2 = O(x^3)$

The Symbol *o*

Definition: if for every positive constant *M* such that $|\phi(x)| \le M\,|\varphi(x)|$, as $x \to x_0$, we say

$$\phi(x) = o\left[\varphi(x)\right] \qquad \text{or} \qquad \phi(x) << \varphi(x)$$

ϕ is small-oh of φ $\qquad$ ϕ is much less than φ

Meaning ϕ is of lower order of φ, or $\displaystyle\lim_{x\to x_0}\frac{\phi(x)}{\varphi(x)} = 0$

e.g., as x → 0 $\quad \sin x = o(1), \ \sin x^2 = o(x)$

e.g., as x → ∞ & any $a > 0$

$$e^{-x} = o\left(x^{-a}\right), \ x^a = o\left(e^x\right), \ \ln x = o\left(x^a\right), \ \ln\ln x = o(\ln x)$$

$$w(m,N) = \frac{N!}{2^N p!(N-p)!} \Rightarrow \sqrt{\frac{2}{\pi N}}\exp\left(-\frac{m^2}{2N}\right)$$

Stirling's formula $\ln n! \sim \left(n+\frac{1}{2}\right)\ln n - n + \ln\sqrt{2\pi} + \frac{1}{12n} - \frac{1}{360n^3} + \cdots$

$$x^2 + \varepsilon x - 1 = 0 \qquad x = \begin{cases} 1 - \frac{\varepsilon}{2} + \frac{\varepsilon^2}{8} - \frac{\varepsilon^4}{128} + O\left(\varepsilon^6\right) \\ -1 - \frac{\varepsilon}{2} - \frac{\varepsilon^2}{8} + \frac{\varepsilon^4}{128} + O\left(\varepsilon^6\right) \end{cases}$$

$$\epsilon x^2 + x - 1 = 0 \qquad x = \begin{cases} 1 - \varepsilon + 2\varepsilon^2 - 5\varepsilon^3 + O\left(\varepsilon^4\right) \\ -\frac{1}{\varepsilon} - 1 + \varepsilon - 2\varepsilon^2 + 5\varepsilon^3 + O\left(\varepsilon^4\right) \end{cases}$$

Review

convergent series

$$\mathrm{Erf}(z)=\frac{2}{\sqrt{\pi}}\int_0^z e^{-t^2}dt=\frac{2}{\sqrt{\pi}}\sum_{n=0}^{\infty}\frac{(-1)^n z^{2n+1}}{(2n+1)n!}$$

$\mathrm{Erf}(z)=1-\mathrm{Erfc}(z)$ asymptotic series

$$=1-\frac{e^{-t^2}}{z\sqrt{\pi}}\left(1+\sum_{n=2}^{N}(-1)^{N+1}\frac{(2N-3)!!}{(2z^2)^{N-1}}\right)+O\left(z^{-2N+1}\right)$$

$$\boxed{f(x)=S_n(x)+R_n(x)}$$

- as $n\to\infty$, $S_n(x)$ diverges for a fixed x.
- as $x\to\infty$, $R_n(x)\to 0$, for a fixed n.
- $\boxed{\text{as } x\to\infty,\ |R_n|<|a_n|}$

Review

$$\lim_{x\to x_0}\frac{\phi(x)}{\varphi(x)}=0 \qquad \phi(x)=o[\varphi(x)] \quad \text{or} \quad \phi(x)<<\varphi(x)$$

$$\lim_{x\to x_0}\frac{\phi(x)}{\varphi(x)}=C \qquad \phi(x)=O[\varphi(x)] \quad \text{or} \quad \phi(x)\sim\varphi(x)$$

3.2.2 Definition asymptotic expansion

- One can use a general sequence of gauge functions $\{\phi_n(\varepsilon)\}$ as *asymptotic sequence* as $\varepsilon\to 0$

  e.g. $\varphi_n(\varepsilon)=\varepsilon^n,\quad (\log\varepsilon)^{-n},\quad (\sin\varepsilon)^n \ldots$

- in the example of $\varepsilon x^2+x-1=0$, we see

  $x=1-\varepsilon+2\varepsilon^2+o(\varepsilon^2)$

  with asymptotic sequence $\{1,\varepsilon,\varepsilon^2,\ldots\}$

  $x=-\varepsilon^{-1}-1+\varepsilon-2\varepsilon^2+o(\varepsilon^2)$

  with asymptotic sequence $\{\varepsilon^{-1},1,\varepsilon,\varepsilon^2,\ldots\}$

3.2.2 Definition asymptotic expansion

- In terms of asymptotic sequences $\{\varphi_n(\varepsilon)\}$, we can expand functions $f(\varepsilon)$ in *asymptotic expansion* if constants a_n exist,

$$f(\varepsilon)=\sum_{n=0}^{N}a_n\phi_n(\varepsilon)+o[\phi_n(\varepsilon)] \qquad \text{as} \quad \varepsilon\to 0$$

or, $$f(\varepsilon)\sim\sum_{n=0}^{N}a_n\phi_n(\varepsilon) \qquad \text{as} \quad \varepsilon\to 0$$

- Usually, a function may depend on x and a small parameter ε. we may look for an expansion in the form

$$f(x,\varepsilon)\sim\sum_{n=0}^{N}a_n(x)\phi_n(\varepsilon) \qquad \text{as} \quad \varepsilon\to 0$$

3.2.2 Definition asymptotic expansion

Consider an expansion

$$A_0+\frac{A_1}{x}+\frac{A_2}{x^2}+\cdots+\frac{A_n}{x^n}+\frac{A_{n+1}}{x^{n+1}}+\cdots\equiv S_n(x)+\frac{A_{n+1}}{x^{n+1}}+\cdots$$

$S_n(x)$ is an asymptotic expansion of $f(x)$, if

$$\lim_{x\to\infty}\frac{f(x)-S_n(x)}{A_nx^{-n}}=0 \quad \text{with fixed } n \qquad |R_n|<|a_n|$$

or

$$f(x)-S_n(x)=o(x^{-n}) \quad \text{with } x\to\infty, \text{ fixed } n$$

we then say $\boxed{f(x)\sim\sum_{i=0}^{n}A_ix^{-i},\quad x\to\infty}$

asymptotic to

3.2.2 Definitions in asymptotic expansion

If for any n, we always have

$$f(x)\sim\sum_{i=0}^{n}A_ix^{-i},\quad x\to\infty$$

then we say $f(x)$ has an asymptotic power series

$$f(x)\sim\sum_{i=0}^{\infty}A_ix^{-i},\quad x\to\infty$$

This asymptotic series is usually divergent for any fixed *x*.

3.2.2 Definitions in asymptotic expansion

Convergence

An expansion $\sum_N f_n(x)$ is said to converge at a fixed value of x if given an arbitrary $\varepsilon > 0$ it is possible to find a number $N_0(x, \varepsilon)$ such that

$$\left|\sum_{M}^{N} f_n(x)\right| < \varepsilon \qquad \text{for } M, N > N_0$$

This property of convergence is less useful in practice.

3.2.2 Definitions in asymptotic expansion

Asymptoticness

The sum $\sum^N f_n(\varepsilon)$ is said to be an ***asymptotic approximation*** to $f(\varepsilon)$ as $\varepsilon \to 0$, if for each $n \leq N$

$$\frac{R_n(\varepsilon)}{f_n(\varepsilon)} = \frac{f(\varepsilon) - \sum^{n} f_n(\varepsilon)}{f_n(\varepsilon)} \to 0 \qquad \text{as } \varepsilon \to 0$$

the remainder R_n is smaller than the last term f_n.

- If the sum has this asymptotic property, one writes

$$f(\varepsilon) \sim \sum^{N} f_n(\varepsilon) \qquad \text{as } \varepsilon \to 0$$

3.2.2 Definitions in asymptotic expansion

More comments on convergence and divergence

Let's look at Taylor series

$$f(x) = f(x_0) + f'(x_0)(x - x_0) + \frac{1}{2} f''(x_0)(x - x_0)^2 + o\left((x - x_0)^2\right)$$

- the sum converges to $f(x)$ as $n \to \infty$.
- Taylor series are *de facto* asymptotic expansions

There are two limiting processes for an asymptotic expansion, $n \to \infty$ and $\varepsilon \to 0$.

- An asymptotic expansion provide an accurate approximation as $\varepsilon \to 0$ for each n
- many useful expansions diverge as $n \to \infty$.

3.2.2 Definitions in asymptotic expansion

Optimal truncation

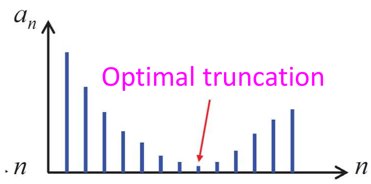
A famous example is the incomplete exponential integral

$$f(x) = \int_x^\infty t^{-1} e^{x-t} dt \sim \frac{1}{x} - \frac{1}{x^2} + \frac{2!}{x^3} - \cdots + \frac{(-1)^{n-1}(n-1)!}{x^n}$$

$$\frac{a_{n+1}}{a_n} = \frac{(n+1)!\varepsilon^{n+1}}{n!\varepsilon^n} = (n+1)\varepsilon > 1 \quad \Rightarrow \quad n_0 = \left[\frac{1}{\varepsilon}\right]$$

$$R_{n_0}(\varepsilon) = o\left(a_{n_0}\right)$$

increase as $n > n_0$



3.2.2 Definitions in asymptotic expansion

- **In practical problems**, it is difficult to calculate enough terms to decide whether the asymptotic series is divergent, as opposed to mathematical asymptotic problem.
- impossible to prove that the remainder after even one or two terms is small enough.
- Luckily, one or two terms is enough for most problems encountered in applied math.

3.2.3 Laplace's method

Laplace's method :

- to obtain the asymptotic expansion of certain integrals containing a large parameter.

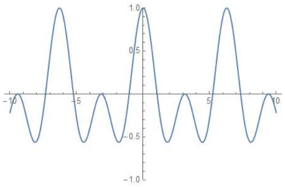
Consider

$$F(\lambda) = \int_\alpha^\beta g(t) e^{-\lambda f(t)} dt \qquad \lambda >> 1$$

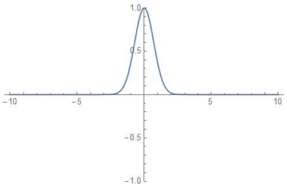
idea:

- the dominant contribution comes from a small portion。

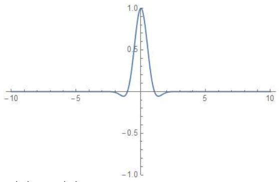
3.2.3 Laplace's method



$g(t) = 0.5(\cos x + \cos 2x)$

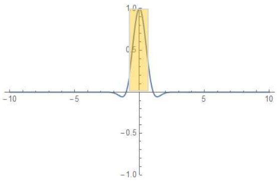


$f(t) = \exp(-x^2)$



$g(t)f(t)$

$= 0.5(\cos x + \cos 2x)\exp(-x^2)$



$F(\lambda) = \int_\alpha^\beta g(t) e^{-\lambda f(t)} dt$

3.2.3 Laplace's method

Let's stare at the integrand

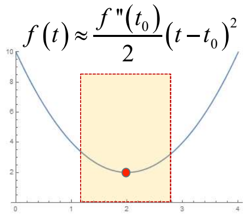
$$F(\lambda) = \int_\alpha^\beta g(t) e^{-\lambda f(t)} dt$$

a minimum at t_0

$$F(\lambda) \approx \int_{t_0-\delta}^{t_0+\delta} g(t) e^{-a(t-t_0)^2} dt$$

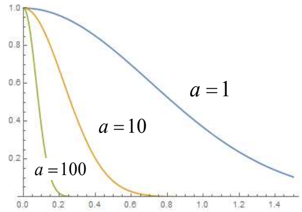
$$a = \frac{-\lambda f''(t_0)}{2}$$

$f(t) \approx \dfrac{f''(t_0)}{2}(t-t_0)^2$



$\alpha \quad t_0-\delta \quad t_0 \quad t_0+\delta \quad \beta$

$Q(t) = \exp\left[-a(t-t_0)^2\right]$



3.2.3 Laplace's method

Taylor expansion about t_0 .

Assuming $\quad f'(t_0) = 0 \quad f''(t_0) > 0$

$$f(t) = f(t_0) + f'(t_0)(t-t_0) + \frac{1}{2} f''(t_0)(t-t_0)^2 + o\left((t-t_0)^2\right)$$

$$\approx f(t_0) + \frac{1}{2} f''(t_0)(t-t_0)^2$$

thus

$$F(\lambda) = \int_\alpha^\beta g(t) e^{-\lambda f(t)} dt$$

$$\sim g(t_0) e^{-\lambda f(t_0)} \int_{-\infty}^{\infty} \exp\left[\frac{-\lambda f''(t_0)(t-t_0)^2}{2}\right] dt$$

3.2.3 Laplace's method

$$F(\lambda) = \int_\alpha^\beta g(t) e^{-\lambda f(t)} dt$$

$$\sim g(t_0) e^{-\lambda f(t_0)} \int_{-\infty}^{\infty} \exp\left[\frac{-\lambda f''(t_0)(t-t_0)^2}{2}\right] dt$$

$u = (t-t_0)\sqrt{\dfrac{f''(t_0)}{2}}$

$$= g(t_0) e^{-\lambda f(t_0)} \left[\frac{2}{f''(t_0)}\right]^{1/2} \int_{-\infty}^{\infty} \exp(-\lambda u^2) du$$

$$= g(t_0) e^{-\lambda f(t_0)} \left[\frac{2\pi}{\lambda f''(t_0)}\right]^{1/2}$$

Gauss integral

$\int_{-\infty}^{\infty} \exp(-u^2) du = \sqrt{\pi}$

3.3.4 Asymptotic Stirling series for Gamma function

Gamma function $\quad \Gamma(s) = \int_0^\infty x^{s-1} e^{-x} dx \qquad \mathrm{Re}(s) > 0$

$\Gamma\left(\frac{1}{2}\right) = \pi \qquad \Gamma(n) = (n-1)!$

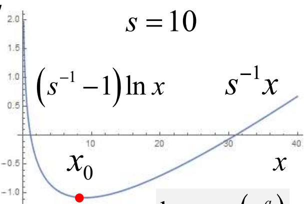
for s >>1, the gamma function can be reformed as

$$\Gamma(s) = \int_0^\infty e^{(s-1)\ln x} e^{-x} dx$$

$$= \int_0^\infty e^{-sF} dx$$

where

$$F(x,s) = (s^{-1}-1)\ln x + s^{-1}x$$



$\ln x = o(x^a)$

$$\frac{\partial F}{\partial x} = 0 \Rightarrow x_0 = s-1$$

3.3.4 Asymptotic Stirling series for Gamma function

The minimal $x_0 = s-1$ shifts with s . Let $\boxed{t = \dfrac{x}{s-1}}$

So that the minimal point $x_0 = s-1$ corresponds to

$t_0 = 1$. This leads to

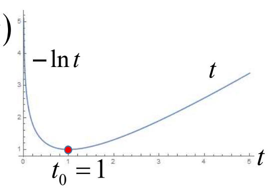
$$\Gamma(s) = \int_0^\infty e^{-sF} dx = (s-1)^s J(\lambda)$$

where

$$J(\lambda) = \int_0^\infty e^{-\lambda f(t)} dt$$

$$f(t) = t - \ln t$$

$$\lambda = s-1 \gg 1$$



$\left.\dfrac{df}{dt}\right|_{t_0=1} = 0 \qquad f(t_0) = 1$

In order to use Laplace's method, we modify the integrand

$$J=\int_0^\infty e^{-\lambda f(t)}dt=\int_0^\infty e^{-\lambda\left[f(t_0)+f(t)-f(t_0)\right]}dt$$

$$=e^{-\lambda f(t_0)}\int_0^\infty e^{-\lambda w^2(t)}dt$$

where

$$w^2(t)=f(t)-f(t_0)=t-\ln t-1$$

define $w(t)$ as continuous and monotonic

$$\begin{cases} w(t)=-\sqrt{f(t)-f(t_0)} & 0\le t\le t_0 \\ w(t)=\sqrt{f(t)-f(t_0)} & t>t_0 \end{cases}$$

$$w\in(-\infty,\infty) \quad \leftrightarrow \quad t\in(0,\infty)$$

$$F(\lambda)=\int_\alpha^\beta g(t)e^{-\lambda f(t)}dt$$

Rewrite

$$J=e^{-\lambda f(t_0)}\int_{-\infty}^\infty e^{-\lambda w^2(t)}\frac{dt}{dw}dw \qquad \boxed{\frac{dt}{dw}=?}$$

We now try to expand w(t) around $t_0=1$

$$w^2(t)=t-1-\ln t$$
$$=(t-1)-\ln\left[1+(t-1)\right]$$
$$=(t-1)-\left[(t-1)-\frac{1}{2}(t-1)^2+\frac{1}{3}(t-1)^3+O\left[(t-1)^4\right]\dots\right]$$
$$=\frac{1}{2}(t-1)^2-\frac{1}{3}(t-1)^3+O\left[(t-1)^4\right]$$

w: a small number

Using the first order $\quad w^2(t)=\frac{1}{2}(t-1)^2-\frac{1}{3}(t-1)^3+O\left[(t-1)^4\right]$

$$w^2(t)=\frac{1}{2}(t-1)^2\Rightarrow t-1=\sqrt{2}w$$

assume an asymptotic series

$$\boxed{t-1=u_0+u_1w+u_2w^2+\dots}$$

$$\Rightarrow\quad u_0=0,\qquad u_1=\sqrt{2}$$

rewrite $\quad t-1=\sqrt{2}w\left(1+a_1w+a_2w^2\dots\right)$

substituting into the Taylor expansion

$$w^2(t)=\frac{1}{2}(t-1)^2-\frac{1}{3}(t-1)^3+o\left((t-1)^3\right)$$

comparing term by term, we have

$$a_1=\frac{\sqrt{2}}{3},\qquad a_2=\frac{1}{18},\qquad a_3=-\frac{11\sqrt{2}}{27},\quad \dots \qquad \boxed{b_0=\sqrt{2}}$$

Then $\quad \frac{dt}{dw}=\frac{d}{dw}\left[\sqrt{2}w\left(1+a_1w+a_2w^2\dots\right)\right]=\sum_{m=0}^\infty b_mw^m$

If term-by-term integration is valid, $\quad \frac{dt}{dw}=\sum_{m=0}^\infty b_mw^m$

$$J(\lambda)=e^{-\lambda f(t_0)}\int_{-\infty}^\infty e^{-\lambda w^2(t)}\frac{dt}{dw}dw=e^{-\lambda f(t_0)}\sum_{m=0}b_mI_m(\lambda)$$

where

$$I_m(\lambda)=\int_{-\infty}^\infty e^{-\lambda w^2}w^m dw$$

$$I_m(\lambda)=0,\quad m \text{ is odd}$$

$$I_m(\lambda)=\frac{(m-1)!!}{2^{m/2}\lambda^{m/2}}\sqrt{\frac{\pi}{\lambda}},\quad m \text{ is even}$$

3.3.4 Asymptotic Stirling series for Gamma function

As m is odd

$$I_1(\lambda)=\int_{-\infty}^{\infty} e^{-\lambda w^2} w\,dw=\frac{-1}{2\lambda}e^{-\lambda w^2}\Big|_{-\infty}^{\infty}=0$$

$$I_3=\int_{-\infty}^{\infty} e^{-\lambda w^2} w^3 dw=-\frac{d}{d\lambda}I_1=0$$

$$I_5=\int_{-\infty}^{\infty} e^{-\lambda w^2} w^5 dw=-\frac{d}{d\lambda}I_3=0$$

$$I_m=0$$

3.3.4 Asymptotic Stirling series for Gamma function

As m is even

$$I_0=\int_{-\infty}^{\infty} e^{-\lambda w^2} dw=\sqrt{\pi/\lambda}$$

$$I_2=\int_{-\infty}^{\infty} e^{-\lambda w^2} w^2 dw=-\frac{d}{d\lambda}I_0$$

$$I_4=\int_{-\infty}^{\infty} e^{-\lambda w^2} w^4 dw=-\frac{d}{d\lambda}I_2=(-1)^2\frac{d^2}{d\lambda^2}I_0$$

$$I_m=(-1)\frac{dI_{m-2}}{d\lambda}=(-1)^{m/2}\frac{d^{m/2}I_0}{d\lambda^{m/2}}=\frac{(m-1)!!}{2^{m/2}\lambda^{m/2}}\sqrt{\frac{\pi}{\lambda}}$$

3.3.4 Asymptotic Stirling series for Gamma function

To the first order approximation

$$J(\lambda)=e^{-\lambda f(t_0)}\sum_{m=0} b_m I_m(\lambda)\approx e^{-\lambda f(t_0)}\left[b_0 I_0(\lambda)+O\left(\lambda^{-3/2}\right)\right]$$

$$=e^{-\lambda}\sqrt{2\pi/\lambda}\left[1+O\left(\lambda^{-1}\right)\right]$$

$b_0=\sqrt{2}$ $\quad I_0=\sqrt{\pi/\lambda}$

$\Gamma(s)=(s-1)^s J(\lambda)$

$s=\lambda+1$

$$\ln\Gamma(s)=\ln(s-1)^s J(\lambda)$$

$$=s\ln(s-1)+\ln e^{-(s-1)}\sqrt{\frac{2\pi}{s-1}}\left[1+O\left(\lambda^{-1}\right)\right]$$

$$=s\ln(s-1)-(s-1)+\ln\sqrt{\frac{2\pi}{s-1}}+\ln\left[1+O\left(\lambda^{-1}\right)\right]$$

$$=\left(s-\frac{1}{2}\right)\ln(s-1)-(s-1)+\frac{1}{2}\ln 2\pi+O\left(\frac{1}{s-1}\right)$$

3.3.4 Asymptotic Stirling series for Gamma function

$$\ln\Gamma(s)=\left(s-\frac{1}{2}\right)\ln(s-1)-(s-1)+\frac{1}{2}\ln 2\pi+O\left(\frac{1}{s-1}\right)$$

In the case of integer, i.e. $s=n+1$

$$\boxed{\begin{aligned}&\ln n!=\ln\Gamma(n+1)\\&=\left(n+\frac{1}{2}\right)\ln n-n+\frac{1}{2}\ln 2\pi+O\left(n^{-1}\right)\end{aligned}}$$

$\Gamma(n+1)=n!$

Stirling's approximation ☐

Section 3.3

A Difference Equation and Its Limit

3.3.1 Difference equation for the probability function

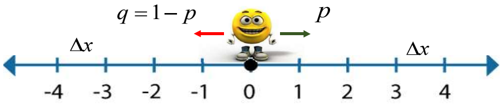
An essential practice of approaching the same problem in different ways, enabling a deeper understanding.

Here is a new way to study random walk:
- Start with a difference equation
- Reach to a PDE solution.

$$w(m,N)=\frac{N!}{2^N p!(N-p)!}\approx\sqrt{\frac{2}{\pi N}}\exp\left(-\frac{m^2}{2N}\right)$$

3.3.1 Difference equation for the probability function

$\overline{w}(x,t)$: the probability that the particle is found at point x at time t.



$x = m\Delta x \qquad t = N\Delta t \qquad \Delta m = 2$

N is even $\longrightarrow$ m is even. $\quad N$ is odd $\longrightarrow m$ is odd

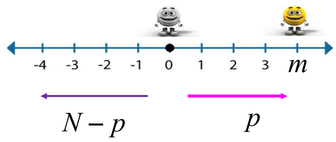
$$w(m,N) = \frac{N!}{2^N p!(N-p)!} = w\left(\frac{x}{\Delta x}, \frac{t}{\Delta t}\right)$$

$$= \frac{(t/\Delta t)!}{2^{t/\Delta t}\left(\frac{t/\Delta t + x/\Delta x}{2}\right)!\left(\frac{t/\Delta t - x/\Delta x}{2}\right)!} = \overline{w}(x,t)$$

3.1.2 Explicit solution

To find $w(m, N)$, the probability that a particle at a point $m\in[-N,N]$ steps to the right of its origin after total N steps.

Suppose that the particle
- p steps to the right, p>0
- N-p steps to the left



Displacement m

$m = p - (N-p) = 2p - N$

$p = (N + m)/2$

N is even $\longrightarrow$ m is even. $\quad N$ is odd $\longrightarrow m$ is odd

For example,

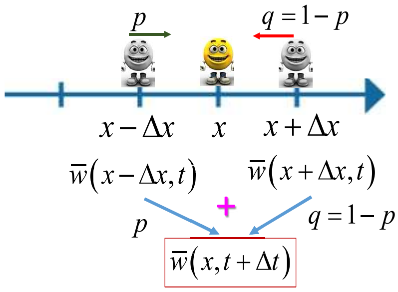
if N=3, the possible values of m = -3, -1, 1, 3.

if N=4, the possible values of m = -4, -2, 0, 2, 4.

3.3.1 Difference equation for the probability function

the probability of the particle at point x at $t + \Delta t$

$$\overline{w}(x,t+\Delta t) = p\,\overline{w}(x-\Delta x,t) + q\,\overline{w}(x+\Delta x,t)$$



as $\quad p = q = 1/2$

$$\overline{w}(x,t+\Delta t) = \frac{1}{2}\overline{w}(x-\Delta x,t) + \frac{1}{2}\overline{w}(x+\Delta x,t)$$

3.1.2 Explicit solution

General random walk model

- Consider a continuous 1-D random walk process of n steps
- we have recursion relation:

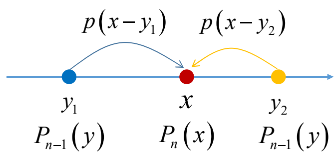
$$P_n(x) = \int_{-\infty}^{\infty} P_{n-1}(y)\,p(x-y)\,dy = P_{n-1}(x) * p(x)$$

convolution

$$f(x)*g(x) = \int_{-\infty}^{\infty} f(y)\,g(x-y)\,dy$$

This means that the probability $P_n(x)$ of a particle at x after n steps is

- $P_{n-1}(y)$ the probability of arriving at y in n −1 steps
- $p(x-y)$ the probability of displacements x-y in one step.



$$P_n(x) = \sum_i P_{n-1}(y_i)\,p(x-y_i)$$

$$\rightarrow P_n(x) = \int_{-\infty}^{\infty} P_{n-1}(y)\,p(x-y)\,dy$$

3.3.1 Difference equation for the probability function

Evolution equation of $\overline{w}(x,t)$:

$$\overline{w}(x,t+\Delta t) = \frac{1}{2}\overline{w}(x-\Delta x,t) + \frac{1}{2}\overline{w}(x+\Delta x,t)$$

Conditions in the begining

$$\overline{w}(0,0) = 1$$

$$\overline{w}(x,0) = 0, \quad x \neq 0$$

It is easy to verify that the solution is

$$\overline{w}(x,t) = \frac{(t/\Delta t)!}{2^{t/\Delta t}\left(\frac{t/\Delta t + x/\Delta x}{2}\right)!\left(\frac{t/\Delta t - x/\Delta x}{2}\right)!}$$

3.3.2 Approximated by differential equation

Apply Taylor's formula about (x,t)

$$\begin{cases} \overline{w}(x,t+\Delta t) = \overline{w}(x,t) + \dfrac{d\overline{w}}{dt}\Delta t + \dfrac{1}{2}\dfrac{d^2\overline{w}}{dt^2}(\Delta t)^2 + O\left((\Delta t)^3\right) \\ \overline{w}(x-\Delta x,t) = \overline{w}(x,t) - \dfrac{d\overline{w}}{dx}\Delta x + \dfrac{1}{2}\dfrac{d^2\overline{w}}{dx^2}(\Delta x)^2 + O\left((\Delta x)^3\right) \\ \overline{w}(x+\Delta x,t) = \overline{w}(x,t) + \dfrac{d\overline{w}}{dx}\Delta x + \dfrac{1}{2}\dfrac{d^2\overline{w}}{dx^2}(\Delta x)^2 + O\left((\Delta x)^3\right) \end{cases}$$

$$\overline{w}(x,t+\Delta t) = \frac{1}{2}\overline{w}(x-\Delta x,t) + \frac{1}{2}\overline{w}(x+\Delta x,t)$$

$$\Downarrow$$

$$\overline{w}_t\Delta t + \frac{1}{2}\overline{w}_{tt}(\Delta t)^2 + O(\Delta t^3) = \frac{1}{2}\overline{w}_{xx}(\Delta x)^2 + O\left((\Delta x)^3\right)$$

$$\Downarrow$$

3.3.2 Approximated by differential equation

$$\overline{w}_t+\frac{1}{2}\overline{w}_{tt}\Delta t+O(\Delta t)=\overline{w}_{xx}\frac{(\Delta x)^2}{2\Delta t}+O\left(\frac{(\Delta x)^2}{\Delta t}(\Delta x)\right)$$

Consider two limits

$$N\to\infty,\quad N\Delta t=t\ \text{ fixed},\quad \Rightarrow\ \Delta t\to 0$$

$$m\to\infty,\quad m\Delta x=x\ \text{ fixed},\quad \Rightarrow\ \Delta x\to 0$$

Recall diffusion coefficient *D*, we may assume

$$\lim_{\Delta x,\Delta t\to 0}\frac{(\Delta x)^2}{2\Delta t}=D\qquad D\neq 0$$

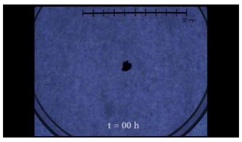
3.1.4 To determine Boltzmann's constant from Brownian Motion

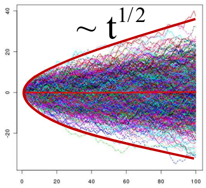
Einstein (1905)

- assume that the macroscopic <u>resistance</u> on the particle is proportional to the <u>velocity</u> - using classical hydrodynamics
- predicated diffusion follows the statistical law

$$\langle x^2\rangle=\frac{1}{3}\left[\langle x^2\rangle+\langle y^2\rangle+\langle z^2\rangle\right]=\frac{1}{3}\langle r^2\rangle=2Dt$$

$$\langle m^2\rangle^{1/2}=N^{1/2}$$





Perrin:
experiment in 1908.
Nobel Prize in 1926

3.3.2 Approximated by differential equation

We obtain the differential equation of random walk

$$\boxed{\overline{w}_t=D\,\overline{w}_{xx}}$$

So far so good. But … !

the probability density function *u*

$$u(x,t)=\frac{\overline{w}(x,t)}{2\Delta x}$$

$m=\pm1,\pm3,\pm5,\ldots$
or $m=\pm2,\pm4,\pm6\ldots$

$$\boxed{\Delta m=2}$$

3.3.2 Approximated by differential equation

The probability of finding a particle between $a=i\Delta x$ and $b=k\Delta x$ at time *t* can be expressed by

$$\sum_{m=i}^{k}\overline{w}(x,t)=\sum_{m=i}^{k}u(m\Delta x,t)\cdot 2\Delta x$$

Therefore, we get the PDE in terms of probability density *u*

$$\overline{w}_t=D\overline{w}_{xx}\ \Rightarrow\ \boxed{u_t=Du_{xx}}$$

The probability between a and b at time t

$$U(a,b;t)=\int_a^b u(x,t)\,dx$$

3.3.3 Solution of the PDE for the probability distribution function

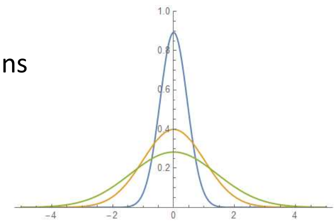
Partial differential equation for random walk

$$\frac{\partial u}{\partial t}=D\frac{\partial^2 u}{\partial x^2}$$

Initial and normalized conditions

$$\int_{-\infty}^{\infty}u(x,t)\,dx=1$$

$$\lim_{t\to 0^+}u(x,t)=0,\qquad x\neq 0$$



$Dt=0.1,\ 0.5,1.0$

Solution from self-similar form

$$u(x,t)\approx u_0(x,t)=\sqrt{\frac{1}{4\pi Dt}}\exp\left(-\frac{x^2}{4Dt}\right)$$

3.3.3 Solution of the PDE for the probability distribution function

$$u(x,t)\approx\sqrt{\frac{1}{4\pi Dt}}\exp\left(-\frac{x^2}{4Dt}\right)\ \Leftrightarrow\ w(m,N)\approx\sqrt{\frac{2}{\pi N}}\exp\left(-\frac{m^2}{2N}\right)$$

$$N\Delta t=t\qquad m\Delta x=x\qquad \lim_{\Delta x,\Delta t\to 0}\frac{(\Delta x)^2}{2\Delta t}=D\qquad u=\frac{\overline{w}}{2\Delta x}$$

$$\sqrt{\frac{1}{4\pi Dt}}=\sqrt{\frac{1}{4\pi}\frac{2\Delta t}{(\Delta x)^2}\frac{1}{N\Delta t}}=\frac{1}{\Delta x}\sqrt{\frac{1}{2N\pi}}$$

$$\exp\left(-\frac{x^2}{4Dt}\right)=\exp\left(-\frac{(m\Delta x)^2}{4N\Delta t}\frac{2\Delta t}{(\Delta x)^2}\right)=\exp\left(-\frac{m^2}{2N}\right)$$

$$2\Delta x u(x,t)\approx\sqrt{\frac{2}{N\pi}}\exp\left(-\frac{m^2}{2N}\right)=w(m,N)$$

1. Dimensional analysis

$$\frac{\partial u}{\partial t}=D\frac{\partial u}{\partial^2 x} \qquad 1=\int_{-\infty}^{\infty}u(x,t)\,dx$$

$$[x]=\mathrm{L},\quad [t]=\mathrm{T},\quad [u]=\mathrm{L}^{-1},\quad [D]=\mathrm{L}^2\mathrm{T}^{-1},\quad [Dt]=\mathrm{L}^2$$

Two Dimensionless quantities

$$\Pi_1=u(x,t)\sqrt{D\,t} \qquad \Pi_2=\frac{x}{\sqrt{Dt}}$$

The solution must be of the form

$$\Pi_1=f(\Pi_2)$$

$$\Downarrow$$

$$u=\frac{f(s)}{\sqrt{D\,t}} \qquad \text{define} \quad s=\frac{x}{\sqrt{Dt}}$$

the number of independent variables reduced from 2 to 1.

2. From PDE to ODE

$$u=\frac{f(s)}{\sqrt{D\,t}} \qquad s=\frac{x}{\sqrt{D\,t}}$$

The partial derivatives

$$\frac{\partial u}{\partial t}=\frac{f'}{\sqrt{Dt}}\frac{-x}{2\sqrt{Dt^3}}-\frac{f}{2\sqrt{Dt^3}}=-\frac{xf'}{2Dt^2}-\frac{f}{2t\sqrt{Dt}}$$

$$\frac{\partial u}{\partial x}=\frac{f'}{\sqrt{Dt}}\frac{1}{\sqrt{Dt}}=\frac{f'}{Dt}$$

$$\frac{\partial^2 u}{\partial x^2}=\frac{\partial}{\partial x}\frac{f'}{Dt}=\frac{f''}{(Dt)^{3/2}}$$

inserting into the PDE, we get ODE

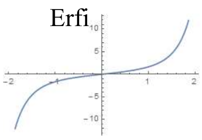
$$\frac{\partial u}{\partial t}=D\frac{\partial u}{\partial^2 x} \;\Rightarrow\; \boxed{f''+\frac{s}{2}f'+\frac{1}{2}f=0}$$

the solution

$$f(s)=c_1e^{-s^2/4}+c_2e^{-s^2/4}\sqrt{\pi}\,\mathrm{Erfi}[s/2]$$

imaginary error function

$$\mathrm{Erfi}[x]=\frac{2}{\sqrt{\pi}}\int_0^x e^{t^2}\,dt$$



From initial and normalized conditions

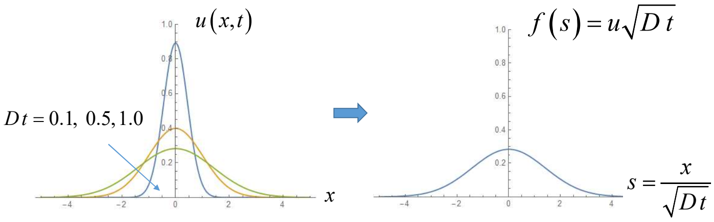
$$\lim_{t\to 0^+}u(x,t)=0,\quad x\neq 0 \;\Rightarrow\; c_2=0$$

$$\int_{-\infty}^{\infty}u(x,t)\,dx=1 \;\Rightarrow\; c_1=\frac{1}{\sqrt{4\pi}}$$

Final solution

$$\boxed{u(x,t)=\frac{1}{\sqrt{4\pi Dt}}e^{-\frac{x^2}{4Dt}}}$$

why can we turn a PDE to an ODE ?



- All different curves collapse onto one master curve with the rescaling.
- called self-similar solution.
- *x* and *t* are not really 2 independent variables

- Self-similar solutions are coincidences in physical processes.
- We cannot always find self-similar solutions for a PDE.
- Self-similar solutions exists only when there is no characteristic length scale and characteristic time scale in the PDE problem. i.e.

$$\cancel{\tilde{x}=\frac{x}{l},\quad \tilde{t}=\frac{t}{\tau}} \qquad s=\frac{x}{\sqrt{Dt}}$$

Two ways to find the approximate solution

1. Stirling's formula applied to the exact solution

$$w(m,N)\sim\left(\frac{2}{\pi N}\right)^{1/2}\exp\left(\frac{-m^2}{2N}\right) \qquad N\Delta t=t \quad m\Delta x=x$$

$$\overline{w}(x,t)\equiv w\left(\frac{x}{\Delta x},\frac{t}{\Delta t}\right)\sim\left(\frac{2\Delta t}{\pi t}\right)^{1/2}\exp\left(\frac{-x^2\Delta t}{2t(\Delta x)^2}\right)$$

$$u(x,t)=\frac{\overline{w}}{2\Delta x}=\lim_{\substack{\Delta t\to 0,\Delta x\to 0\\ \frac{(\Delta x)^2}{2\Delta t}\to D}}\left(\frac{1}{4\pi t}\frac{2\Delta t}{(\Delta x)^2}\right)^{1/2}\exp\left(-\frac{x^2}{4t}\frac{2\Delta t}{(\Delta x)^2}\right)=\frac{\exp\left(-\frac{x^2}{4Dt}\right)}{\sqrt{4\pi Dt}}$$

2. by solving the partial differential equation

$$\frac{\partial u}{\partial t}=D\frac{\partial u}{\partial^2 x} \;\Rightarrow\; u(x,t)=\frac{1}{\sqrt{4\pi Dt}}e^{-\frac{x^2}{4Dt}}$$

3.3.4 Further examination of the limiting process

- Stirling's formula requires N, p and N-p all large.
- Small p : most steps to the left, $m \sim -N$.
- Small N-p, most of the steps to the right, $m \sim +N$.
- Thus, those cases where $|m| \sim N$ is excluded.

$$m = p-(N-p) = 2p - N \sim \cancel{\pm N}$$

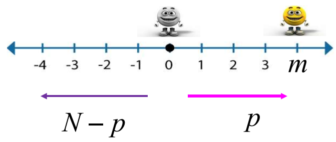
$$m \sim N^{\alpha} \qquad \alpha = 1/2 \text{ or } 1/3 \text{ or} \cdots ?$$

$$\langle m^2 \rangle = N$$

3.1.2 Explicit solution

To find $w(m, N)$, the probability that a particle at a point $m\in[-N,N]$ steps to the right of its origin after total N steps.

Suppose that the particle
- p steps to the right, $p>0$
- N-p steps to the left



e.g. N=12 N-p=5 p=7 m=2

Displacment m

$m = p - (N\text{-}p) = 2p - N$

$p = (N + m)/2$

N is even $\longrightarrow$ m is even. N is odd $\longrightarrow$ m is odd

For example,

if N=3, the possible values of m = -3, -1, 1, 3.

if N=4, the possible values of m = -4, -2, 0, 2, 4.

3.3.4 Further examination of the limiting process

This requirement was not mentioned in the limiting differential equation. Why?

$$\Delta x \to 0, \quad \Delta t \to 0, \quad m \to \infty, \quad N \to \infty,$$

$$m\Delta x \to x, \quad N\Delta t \to t, \quad \frac{(\Delta x)^2}{2\Delta t} \to D$$

speed

$$\frac{\Delta x}{\Delta t} \sim \frac{2D}{\Delta x} \to \infty \quad \Rightarrow \quad \Delta t = \mathrm{o}(\Delta x) \qquad \Delta t = (\Delta x)^2$$

$$\frac{m}{N} = \frac{m\Delta x}{N\Delta t}\frac{\Delta t}{\Delta x} = \frac{x}{t}\frac{\Delta t}{\Delta x} \to 0 \quad \Rightarrow \quad |m| \ll N, \quad x = m\Delta x \ll N\Delta x$$

try

$$\frac{m}{N^{1/2}} = \frac{x}{\Delta x}\left(\frac{\Delta t}{t}\right)^{1/2} = x\sqrt{\frac{2\Delta t}{2t(\Delta x)^2}} = \frac{x}{\sqrt{2Dt}} \sim 1 \quad \Rightarrow \quad m \sim N^{1/2}$$

3.3.5 Reflecting and absorbing barriers

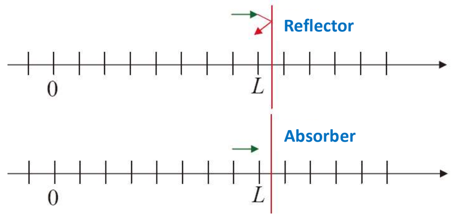
the probability of the particle reaching position L at $t+\Delta t$

Reflecting barrier

$$\overline{w}(L, t+\Delta t) = \frac{1}{2}\overline{w}(L-\Delta x, t) + \frac{1}{2}\overline{w}(L, t)$$

Absorbing barrier

$$\overline{w}(L, t+\Delta t) = \frac{1}{2}\overline{w}(L-\Delta x, t) + 0$$



3.3.5 Reflecting and absorbing barriers

Reflecting barrier

$$\overline{w}(L, t+\Delta t) = \frac{1}{2}\overline{w}(L-\Delta x, t) + \frac{1}{2}\overline{w}(L, t)$$

$$\overline{w}(L, t+\Delta t) = \overline{w}(L, t) + \overline{w}_t\Delta t + O(\Delta t^2)$$

$$\overline{w}(L-\Delta x, t) = \overline{w}(L, t) - \overline{w}_x\Delta x + O(\Delta x^2)$$

$$\Downarrow$$

$$\overline{w}_t\Delta t + O(\Delta t^2) = -\frac{1}{2}\overline{w}_x\Delta x + O(\Delta x^2)$$

$$\Downarrow$$

$$\boxed{u_x(L, t) = 0} \qquad u = \frac{\overline{w}}{2\Delta x} \qquad \frac{\Delta t}{\Delta x} \to 0$$

3.3.5 Reflecting and absorbing barriers

Absorbing barrier

$$\overline{w}(L, t+\Delta t) = \frac{1}{2}\overline{w}(L-\Delta x, t)$$

$$\overline{w}(L, t+\Delta t) = \overline{w}(L, t) + \overline{w}_t\Delta t + O(\Delta t^2)$$

$$\overline{w}(L-\Delta x, t) = \overline{w}(L, t) - \overline{w}_x\Delta x + O(\Delta x^2)$$

$$\Downarrow$$

$$\overline{w}(L, t) + \overline{w}_t\Delta t + O(\Delta t^2) = \frac{1}{2}\overline{w}(L, t) - \frac{1}{4}\overline{w}_x\Delta x + O(\Delta x^2)$$

$$\Downarrow$$

$$\boxed{u(L, t) = 0} \qquad u = \frac{\overline{w}}{2\Delta x} \qquad \frac{\Delta t}{\Delta x} \to 0$$

3.3.5 Reflecting and absorbing barriers

Reflecting barrier

$$\begin{cases} \dfrac{\partial u}{\partial t} = D\dfrac{\partial^2 u}{\partial x^2} \\ \int_{-\infty}^{L} u(x,t)dx = 1 \\ \lim\limits_{t\to 0^+} u(x,t) = 0, \qquad x \neq 0 \\ u_x(L,t) = 0 \end{cases}$$

$$u = u_R(x,t) = u_0(x,t) + u_0(x-2L,t)$$

Absorbing barrier

$$\begin{cases} \dfrac{\partial u}{\partial t} = D\dfrac{\partial^2 u}{\partial x^2} \\ \cancel{\int_{-\infty}^{L} u(x,t)dx = 1,} \\ \lim\limits_{t\to 0^+} u(x,t) = 0, \qquad x \neq 0 \\ u(L,t) = 0 \end{cases}$$

$$u = u_A(x,t) = u_0(x,t) - u_0(x-2L,t)$$

Section 3.4

Further Considerations Pertinent to the Relationship Between Probability and Partial Differential Equations

3.4.0 Introduction

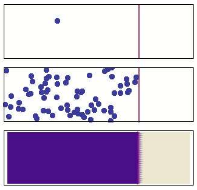
The partial differential equation of Brownian motion is common to various different phenomena

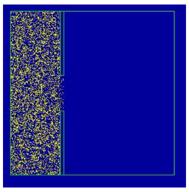
- heat conduction
- diffusion of gas

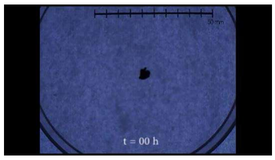
In this section, we will

- continue to study the relations between random walk and partial differential equations from a continuum viewpoint.
- examine various solution techniques for the diffusion equation.

3.4.1 More on diffusion equation and random walk







$$\boxed{J \propto -\nabla u}$$

- There is flow from high concentration to low concentration.
- The simplest hypothesis: such flow is due to difference in concentration.
- The magnitude of *flow* is proportional to *gradient.* This is Fick's first law.

3.4.1 More on diffusion equation and random walk

To derivation from a continuum viewpoint

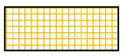
$$\boxed{\frac{\partial u}{\partial t} = D\frac{\partial^2 u}{\partial x^2}}$$

We start with

- $u(x, t)$ concentration: the amount per unit volume of some quantity interested.
- $J(x, t)$ flux: measuring the amount of substance that flow through a unit area during a unit time. Its dimension

[flux]=[quantity] / ([time]·[area])

3.4.1 More on diffusion equation and random walk

Flux $J(x,t) \Rightarrow$  $\Rightarrow J(x+\Delta x,t)$

$x \qquad x+\Delta x$

mass conservation:

$$\frac{\partial}{\partial t}\int_x^{x+\Delta x} u(x,t)dx = J(x,t) - J(x+\Delta x,t)$$

$$\frac{\partial}{\partial t}\left[u(x,t)\Delta x\right] = J(x,t) - J(x+\Delta x,t)$$

$$\frac{\partial}{\partial t}u(x,t) = -\frac{J(x+\Delta x,t) - J(x,t)}{\Delta x}$$

$$\Delta x \to 0 \qquad \boxed{\frac{\partial u}{\partial t} = -\frac{\partial J}{\partial x}}$$

constitutive relation: Fick's first law

$$J=-D\frac{\partial u}{\partial x}$$

D diffusion constant.

$$\frac{\partial u}{\partial t}=-\frac{\partial J}{\partial x}$$

$$J=-D\frac{\partial u}{\partial x}$$

$$\Rightarrow \boxed{\frac{\partial u}{\partial t}=D\frac{\partial^2 u}{\partial x^2}}$$

diffusion equation

u can be
- Temperature
- Concentration
- …

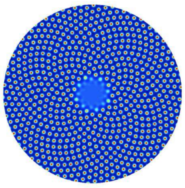
Comments

- macro diffusion time $t \gg$ particle collision time τ
- macro diffusion distance $\gg$ particle mean free path
- macro diffusion velocity $\ll$ particle velocity

Nonlinear Diffusion Models

$$\frac{\partial u}{\partial t}=D\frac{\partial^2 u}{\partial x^2}+f(u)$$

Phyllotaxis



$$\frac{\partial u}{\partial t}=\mu u-(\nabla^2+1)^2u-\frac{\beta}{3}(|\nabla u|^2+2u\nabla^2 u)-u^3,$$

Alan C. Newell. PRL 110, 248104 (2013)

We seek the solution of

$$\frac{\partial u}{\partial t}=D\frac{\partial^2 u}{\partial x^2}+f(u)\xrightarrow{x\to x/\sqrt{D}}\frac{\partial u}{\partial t}=\frac{\partial^2 u}{\partial x^2}+f(u)$$

normal (Fourier) modes

$$u(k)=A(k)e^{i(kx-\omega t)}$$

the solution

$$u(x,t)=\int_{-\infty}^{\infty}A(k)\exp[ikx-i\omega t]\,dk$$

- When $f(u)=0$ $\quad u_t=u_{xx}$

$$u_t=-i\omega u \quad u_{xx}=-k^2u \Rightarrow$$

Dispersion relation $\omega=-ik^2$

Phase velocity $c=\mathrm{Re}(\omega)/k=0$

$$u(k)=A(k)\exp(ikx-k^2t)=A\exp(-k^2t)\exp(ikx)$$

decay quickly as k>>1

$\Downarrow$

$u\to 0 \quad as\ t>>1$

Called: dissipation

No constant wave in diffusion equation

- When $f(u)=au_x+bu$ $\quad u_t=u_{xx}+au_x+bu$

$a,b>0$

Dispersion relation $\omega=-ak-i\left(k^2-b\right)$

Phase velocity $c=\mathrm{Re}(\omega)/k=-a$

$$u(k)=Ae^{-(k^2-b)t}\exp\left[ik(x+at)\right]$$

decay quickly as $\boxed{k\neq\pm b}$

$t>>1$

$k=\pm b$

$\Downarrow$

$$u=A\exp\left[\pm ib(x+at)\right]$$

Two constant waves

Nonlinear reaction diffusion models

$$\frac{\partial u}{\partial t} = D\frac{\partial^2 u}{\partial x^2} + f(u,v) \qquad \frac{\partial v}{\partial t} = D\frac{\partial^2 v}{\partial x^2} + g(u,v)$$

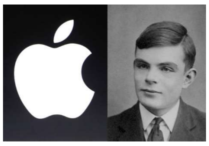
Turing Patterns

THE CHEMICAL BASIS OF MORPHOGENESIS

By A. M. TURING, F.R.S. *University of Manchester*

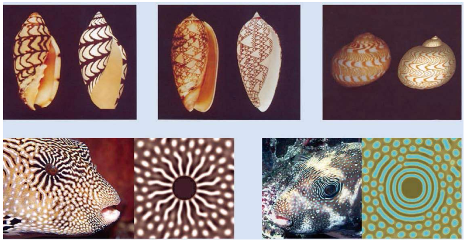
(*Received* 9 *November* 1951—*Revised* 15 *March* 1952)

It is suggested that a system of chemical substances, called morphogens, reacting together and diffusing through a tissue, is adequate to account for the main phenomena of morphogenesis. Such a system, although it may originally be quite homogeneous, may later develop a pattern or structure due to an instability of the homogeneous equilibrium, which is triggered off by random disturbances. Such reaction-diffusion systems are considered in some detail in the case of an isolated ring of cells, a mathematically convenient, though biologically unusual system. The investigation is chiefly concerned with the onset of instability. It is found that there are six essentially different forms which this may take. In the most interesting form stationary waves appear on the ring. It is suggested that this might account, for instance, for the tentacle patterns on *Hydra* and for whorled leaves. A system of reactions and diffusion on a sphere is also considered. Such a system appears to account for gastrulation. Another reaction system in two dimensions gives rise to patterns reminiscent of dappling. It is also suggested that stationary waves in two dimensions could account for the phenomena of phyllotaxis.



23 June 1912
– 7 June 1954

Turing Patterns



Diffusion equation $\frac{\partial u}{\partial t} = D\frac{\partial^2 u}{\partial x^2}$

solution $u_0(x,t) = \frac{1}{\sqrt{4\pi Dt}}\exp\left(-\frac{x^2}{4Dt}\right)$

satisfy

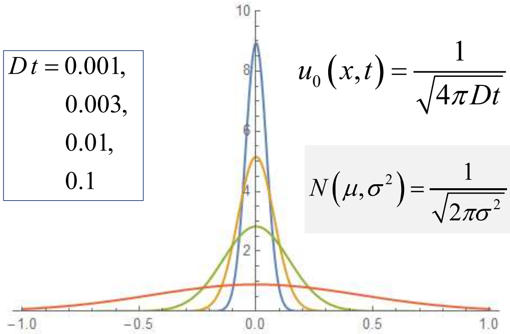
- delta function initial condition

$$\lim_{t\to 0^+} u_0(x,t) = 0, \qquad x \neq 0$$

$$\int_{-\infty}^{\infty} \delta(x)\,dx = 1$$

- normalization condition

$$\int_{-\infty}^{\infty} u_0(x,t)\,dx = 1$$



$$u_0(x,t) = \frac{1}{\sqrt{4\pi Dt}}\exp\left(-\frac{x^2}{4Dt}\right)$$

$$N(\mu,\sigma^2) = \frac{1}{\sqrt{2\pi\sigma^2}}\exp\left(-\frac{(x-\mu)^2}{2\sigma^2}\right)$$

- $u_0(x,t)$ called unit source solution or fundamental solution.
- general solution formed from its combinations.

Some properties of the diffusion equation

$$\frac{\partial u}{\partial t} = D\frac{\partial^2 u}{\partial x^2}$$

- Translation invariance

$u_0(x,t)$ is a solution

$$x \to x - \xi, \qquad t \to t - \tau$$

$u_0(x-\xi, t-\tau)$ also solution

an unit source initially placed at point ξ and time τ.

- Linearity and superposition

$$u(x,t) = c_1 u_1(x,t) + c_2 u_2(x,t)$$

The combination of solutions is also a solution.

$u_0(x,t)$ is a solution of $\frac{\partial u}{\partial t} = D\frac{\partial^2 u}{\partial x^2}$

$$u(x,t) = c_1 u_0(x-\xi_1,t) + c_2 u_0(x-\xi_2,t)$$

superposition of two sources

3.3.5 Reflecting and absorbing barriers

Reflecting barrier

$$\begin{cases} \dfrac{\partial u}{\partial t} = D\dfrac{\partial^2 u}{\partial x^2} \\ \int_{-\infty}^{L} u(x,t)dx = 1 \\ \lim_{t\to 0^+} u(x,t) = 0, \qquad x \neq 0 \\ u_x(L,t) = 0 \end{cases}$$

$$u = u_R(x,t) = u_0(x,t) + u_0(x-2L,t)$$

Absorbing barrier

$$\begin{cases} \dfrac{\partial u}{\partial t} = D\dfrac{\partial^2 u}{\partial x^2} \\ \cancel{\int_{-\infty}^{L} u(x,t)dx = 1,} \\ \lim_{t\to 0^+} u(x,t) = 0, \qquad x \neq 0 \\ u(L,t) = 0 \end{cases}$$

$$u = u_A(x,t) = u_0(x,t) - u_0(x-2L,t)$$

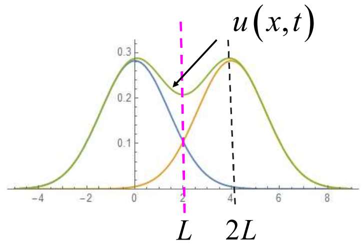
u_0 fundamental solution starting at x=0 and t=0

3.4.2 Superposition of fundamental solutions: the method of images

Method of image 镜像法

Reflecting barrier

Boundary condition $\quad u_x(L,t) = 0$

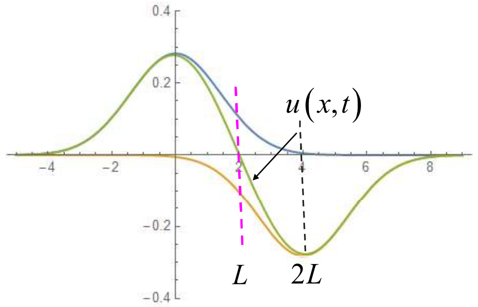


$$u(x,t) = u_0(x,t) + u_0(x-2L,t)$$

3.4.2 Superposition of fundamental solutions: the method of images

Absorbing barrier

Boundary condition $\quad u(L,t) = 0$



$$u(x,t) = u_0(x,t) - u_0(x-2L,t)$$

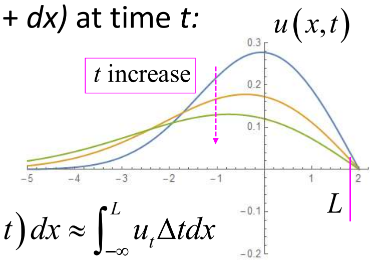
3.4.3 First passage time as a flux

Consider the leaking probability at the boundary x=L of absorbing barrier

$$u(x,t) = u_0(x,t) - u_0(x-2L,t) \qquad u(L,t) = 0$$

Probability between (*x*, *x* + *dx*) at time *t*:

$$\int_x^{x+\Delta x} u(x,t)dx$$



The total probability *U*(*t*)

$$\Delta U = \int_{-\infty}^{L} u(x,t+\Delta t) - u(x,t)dx \approx \int_{-\infty}^{L} u_t \Delta t dx$$

$$\frac{\partial U}{\partial t} = \int_{-\infty}^{L} \frac{\partial u}{\partial t}dx = \int_{-\infty}^{L} D\frac{\partial^2 u}{\partial x^2}dx = D\left(\frac{\partial u}{\partial x}\right)_L$$

3.4.3 First passage time as a flux

- Define *F(L, t) dt* the probability that a particle is absorbed (flow out) per unit time at *x* = *L* in the time interval *(t, t + dt)*

$$F(L,t)dt = -\frac{\partial U}{\partial t}dt = -D\left(\frac{\partial u}{\partial x}\right)_L dt$$

- An alternative interpretation of *F(L, t) :* the rate at which mass is leaving the system at *x* = *L*.

$$F(L,t) = -D\left(\frac{\partial u_A}{\partial x}\right)_L = J(L,t)$$

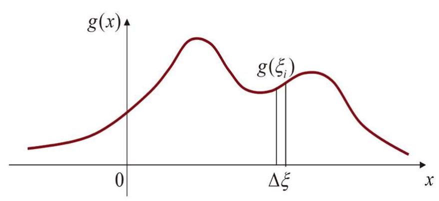
3.4.4 General initial value problem in diffusion

Consider $\dfrac{\partial u}{\partial t} = D\dfrac{\partial^2 u}{\partial x^2}$

with initial condition

$$u(x,0) = g(x)$$

with $-\infty < x < \infty$



The solution can be linear superposition of fundamental solution

$$u(x,t) = \int_{-\infty}^{\infty} u_0(x-\xi,t)g(\xi)d\xi$$

$$g(x) \to 0, \qquad \text{as } x \to \pm\infty$$

convolution

$$f(x)*g(x) = \int_{-\infty}^{\infty} g(x-\xi)f(\xi)d\xi$$

3.4.4 General initial value problem in diffusion

To check the initial condition $u(x,0)=g(x)$

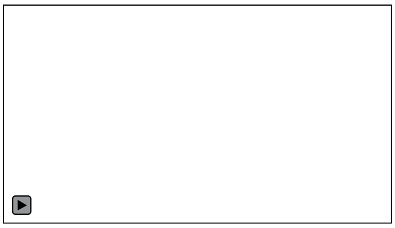
$$u(x,t)=\int_{-\infty}^{\infty}u_0(x-\xi,t)g(\xi)d\xi$$

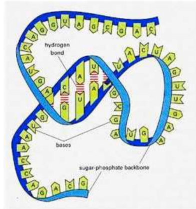
$$=\int_{-\infty}^{\infty}\frac{1}{\sqrt{4\pi Dt}}\exp\left(-\frac{(x-\xi)^2}{4Dt}\right)g(\xi)d\xi \qquad \eta^2=\frac{(x-\xi)^2}{4Dt}$$

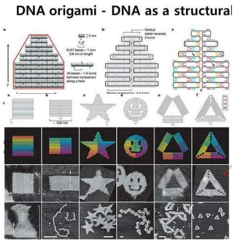
$$=\int_{-\infty}^{\infty}\frac{1}{\sqrt{\pi}}\exp(-\eta^2)g\left(x+\eta\sqrt{4Dt}\right)d\eta$$

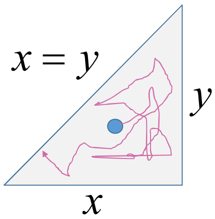
$$\lim_{t\to 0^+}u(x,t)=g(x)$$

3.4.5 DNA and The first passage in 2D

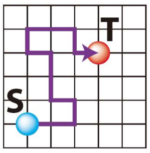




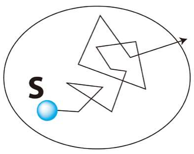




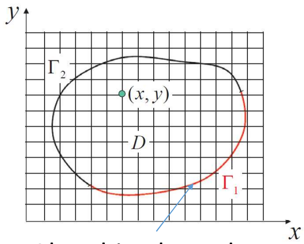
3.4.5 DNA and The first passage in 2D



first-passage



first-exit

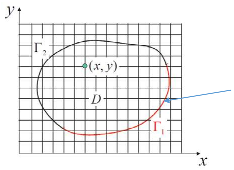


Absorbing boundary

To determine the probability *P(x, y):*

- *a particle* starting from a point (x,y) in region D
- first reaching the absorbing boundary Γ_1.

3.4.5 DNA and The first passage in 2D



Discrete boundary point (x_i, y_i)

we obtain the partial difference equation

$$P(x,y)$$
$$=\frac{1}{4}\left[P(x-\Delta,y)+P(x+\Delta,y)+P(x,y-\Delta)+P(x,y+\Delta)\right]$$

If the starting point (x,y) is a boundary point, we have

$$P(x,y)=\begin{cases}1, & (x,y)=(x_i,y_i)\\ 0, & (x,y)\neq(x_i,y_i)\end{cases}$$

3.4.5 DNA and The first passage in 2D

Taylor expansion

Laplace equation $\dfrac{\partial^2 P}{\partial x^2}+\dfrac{\partial^2 P}{\partial y^2}=0$

P: the probability density

Boundary conditions
$$\lim_{(x,y)\to\Gamma_1}P(x,y)=1$$
$$\lim_{(x,y)\to\Gamma_2}P(x,y)=0$$

$$\oint_{\Gamma}P(x,y)ds=\oint_{\Gamma_1}+\oint_{\Gamma_2}P(x,y)ds=\oint_{\Gamma_1}P(x,y)ds=1$$

3.4.5 DNA and The first passage in 2D

- Suppose f(x,y) the initial probability distribution function in *D*
- the probability that a particle leaving *D* along Γ_1 is

$$\overline{P}=\iint_D P(x,y)f(x,y)dxdy$$

Noticing the *Green's second theorem*

$$\iint_D\left(Q\nabla^2P-P\nabla^2Q\right)dxdy=\oint_{\Gamma}\left(Q\frac{\partial P}{\partial n}-P\frac{\partial Q}{\partial n}\right)ds$$

$\dfrac{\partial}{\partial n}$ denotes exterior normal derivative

3.4.5 DNA and The first passage in 2D

- P is the probability function defined above
- Q is defined as

$$\nabla^2 Q = f, \qquad Q = 0 \ \text{ on } \ \Gamma$$

Using the *Green's second theorem*

$$\iint_D \left(Q\cancel{\nabla^2 P} - P\nabla^2 Q \right) dxdy = \iint_D \left(-P\,f \right) dxdy$$

$$= \oint_\Gamma \left(\cancel{Q\frac{\partial P}{\partial n}} - P\frac{\partial Q}{\partial n} \right) ds = \oint_\Gamma \left(-P\frac{\partial Q}{\partial n} \right) ds$$

$$\Downarrow$$

$$\overline{P} = \iint_D P\,f\,dxdy = \oint_{\Gamma_1} P\frac{\partial Q}{\partial n} ds$$

3.4.5 DNA and The first passage in 2D

Now our questions becomes to solve Q

Poisson equation

$$\nabla^2 Q = f, \qquad Q = 0 \ \text{ on } \ \Gamma$$

Then we can determine

$$\overline{P} = \int_{\Gamma_1} P\left(\frac{\partial Q}{\partial n} \right) ds$$

3.4.5 DNA and The first passage in 2D

Example: Torsional Deformation

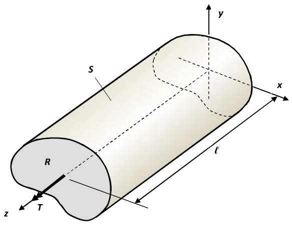
Stress Function $\phi = \phi(x,y)$

$$\tau_{xz} = \frac{\partial \phi}{\partial y}, \quad \tau_{yz} = -\frac{\partial \phi}{\partial x}$$

$$\nabla^2 \varphi = -2\mu\alpha$$

α *twist angle per length*

μ *Shear modulus*



3.4.6 Recurrence property in Brownian motion

A particle starts at a point *x* in the domain *D* described by

$$D: \varepsilon < x < R$$

1D Laplace equation $\quad \dfrac{d^2 P(x)}{dx^2} = 0$

Boundary conditions

$$P = 1, \ \ as \ \ |x| = \varepsilon$$
$$P = 0, \ \ as \ \ |x| = R$$

Solution $\quad P = \dfrac{R - |x|}{R - \varepsilon}$

3.4.6 Recurrence property in Brownian motion

$$P = \frac{R - |x|}{R - \varepsilon} \to 1, \quad as \ R \to \infty, \quad x, \varepsilon \ fixed$$