Stochastic Equations and Processes in Physics and Biology

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Probability: basic concepts and definitions



 $X \dots$ a discrete random variable $P(X) \dots$ probability distribution function

$$P(X_i) = \lim_{n \to \infty} \frac{1}{n} \# \{ X = X_i \}, \quad P(X_i) \in [0, 1]$$

with

 $\#\{X = X_i\}\dots$ number of outcomes with $X = X_i$. Normalization condition

$$\sum_{X_i \in \Omega} P(X_i) = 1,$$

 $\Omega \ldots$ set of all possible values of X

 $X \dots$ continuous random variable from $X \in [a, b]$ $x \dots$ specific value of X $\rho(x) \dots$ probability density function (pdf)

$$\rho(x) = \lim_{n \to \infty, \ dx \to 0} \frac{\#\{X \in [x, x + dx]\}}{n \, dx}.$$

Probability to find X in a narrow interval $[x, x + \delta x]$

$$\Pr(X \in [x, x + \delta x]) = \rho(x) \,\delta x.$$

Normalization condition

$$\int_{a}^{b} \rho(x) \, dx = 1.$$

cumulative distribution function (cdf): F(x)

$$F(x) = \Pr(X \le x) = \int_{-\infty}^{x} \rho(x) \, dx.$$

This shows that

$$\rho(x) = \frac{dF(x)}{dx}.$$

Note that F(x) and $\rho(x)$ are defined on the whole line $x \in (-\infty, +\infty)$.

If
$$x \in [a, b]$$

 $\rho(x) = 0, \quad x \notin [a, b]$

F(x) is monotonically increasing with

$$F(-\infty) = 0$$
, and $F(+\infty) = 1$

 $X\sim$ uniformly distributed on $\left[0,1\right]$

pdf:
$$\rho(x) = \begin{cases} 1, & x \in [0, 1] \\ 0, & x \notin [0, 1] \end{cases}$$
 cdf: $F(x) = \begin{cases} 0, & x \le 0 \\ x, & x \in [0, 1] \\ 1, & x \ge 1 \end{cases}$

Expected value (average or mean)

In theory for a discrete rv X

$$E(X) = \langle X \rangle = \sum_{X_i \in \Omega} P(X_i) X_i$$

In theory for a continuous $\operatorname{rv} X$

$$E(X) = \langle X \rangle = \int_{-\infty}^{+\infty} x \rho(x) \, dx$$

For any given function Y = f(X)

$$E(Y) = \langle Y \rangle = \sum_{X_i \in \Omega} f(X_i) P(X_i) \Rightarrow \text{discrete},$$
$$E(Y) = \langle Y \rangle = \int_{-\infty}^{+\infty} f(x) \rho(x) \, dx \Rightarrow \text{continuous}$$

Expected value in an experiment

In a random experiment with n tries

$$\langle X \rangle = \frac{1}{n} \sum_{i=1}^{n} X_i$$

Unbiased estimator for the mean

 $X_i \dots$ independent and identically distributed (iid) rvs with

$$E(X_i) = \mu$$

Show that

$$E\left(\frac{1}{n}\sum_{i=1}^{n}X_{i}\right) = \mu$$

$$E\left(\frac{1}{n}\sum_{i=1}^{n}X_{i}\right) = \frac{1}{n}\sum_{i=1}^{n}E(X_{i}) = \frac{n}{n}\mu = \mu$$

In theory for a discrete rv \boldsymbol{X}

$$\operatorname{Var}(X) = \sum_{X_i \in \Omega} P(X_i) (X_i - E(X))^2$$

In theory for a continuous $\mathbf{rv} \ X$

$$\operatorname{Var}(X) = \int_{-\infty}^{+\infty} (x - E(X))^2 \rho(x) \, dx = \int_{-\infty}^{+\infty} x^2 \rho(x) \, dx - (\langle X \rangle)^2$$

Standard deviation σ

$$\sigma = \sqrt{\operatorname{Var}(X)}$$

Proof of $Var(X) = E(X^2) - E(X)^2$

$$\begin{aligned} \operatorname{Var}(X) &= \int_{-\infty}^{+\infty} (x - E(X))^2 \rho(x) \, dx \\ &= \int_{-\infty}^{+\infty} [x^2 + E(X)^2 - 2xE(X)] \rho(x) \, dx \\ &= \int_{-\infty}^{+\infty} x^2 \rho(x) \, dx + E(X)^2 \int_{-\infty}^{+\infty} \rho(x) \, dx - 2E(X) \int_{-\infty}^{+\infty} x \, \rho(x) \, dx \\ &= \int_{-\infty}^{+\infty} x^2 \rho(x) \, dx + E(X)^2 - 2E(X)^2 = E(X^2) - E(X)^2 \end{aligned}$$

Relation between E(X) and $E(X^2)$:

 $\langle X^2 \rangle \geq \langle X \rangle^2$

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Expected value (average or mean)

For a uniform distribution

$$E(X) = \int_0^1 x \, dx = \frac{1}{2}$$

Var(X) = $\int_0^1 x^2 \, dx - (E(X))^2 = \frac{1}{3} - \frac{1}{4} = \frac{1}{12}$
standard deviation = $\sigma = \sqrt{\operatorname{Var}(X)} = \frac{1}{\sqrt{12}}$

$$E(\sin(X)) = \int_0^1 \sin(x) \, dx = -\cos(x) \Big|_0^1 = 1 - \cos(1)$$

Variance and standard deviation in an experiment

In a random experiment with n tries

$$\operatorname{Var}(X) = \frac{1}{n-1} \sum_{i=1}^{n} (X_i - \langle X \rangle)^2, \text{ with } \langle X \rangle = \frac{1}{n} \sum_{i=1}^{n} X_i$$

Example

Let X_i be iid with $E(X_i) = \mu$ and $Var(X) = \sigma^2$. Show that

$$\frac{1}{n-1}\sum_{i=1}^{n} (X_i - \langle X \rangle)^2$$

is an unbiased estimator for σ^2 .

For this, show that

$$E\left(\frac{1}{n-1}\sum_{i=1}^{n}(X_i-\langle X\rangle)^2\right)=\sigma^2$$

Normal distribution

The <u>normal</u> rv X is a continuous rv with pdf

$$f(x) = \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{(x-\mu)^2}{2\sigma^2}}, \quad (-\infty < x < \infty)$$

$$X \sim N(\mu, \sigma^2), \quad E(X) = \mu, \quad \operatorname{Var}(X) = \sigma^2$$

Basic integrals to solve

$$\int_{-\infty}^{\infty} \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{(x-\mu)^2}{2\sigma^2}} dx = 1$$
$$\int_{-\infty}^{\infty} \frac{x}{\sqrt{2\pi\sigma^2}} e^{-\frac{(x-\mu)^2}{2\sigma^2}} dx = \mu$$
$$\int_{-\infty}^{\infty} \frac{x^2}{\sqrt{2\pi\sigma^2}} e^{-\frac{(x-\mu)^2}{2\sigma^2}} dx = \sigma^2 + \mu^2$$

Normal distribution

Graph of the pdf f(x) and the cdf F(x) for a normal rv $X \sim N(1,1)$.



Z-score and standard normal distribution

$$X \sim N(\mu, \sigma^2)$$

then

$$Z = \frac{X - \mu}{\sigma}$$

follows the standard normal distribution, i.e. $Z \sim N(0, 1)$

$$pdf(z) = f(z) = \frac{1}{\sqrt{2\pi}}e^{-\frac{z^2}{2}}, \quad (-\infty < z < \infty)$$

cdf: F(z)

$$F(z) = \int_{-\infty}^{z} \operatorname{pdf}(z) \, dz = \frac{1}{2} \left(\operatorname{erf}(z/\sqrt{2}) + 1 \right)$$

Error function $\operatorname{erf}(z) = 2/\sqrt{\pi} \int_0^z e^{-x^2} dx$ is tabulated

Change of variables (continuous case): Given a pdf for X, what is the pdf for Y = f(X) ?

 $\rho(x) \dots \text{ pdf of } X \text{ on } x \in [a, b]$ $Y = f(X) \dots \text{ one-to-one function on } [a, b]$ $p(y) \dots \text{ pdf of } Y \text{ on } y \in [f(a), f(b)] \text{ to be found}$



Change of variables (continuous case)

Probability for Y to be in $[y,y+\Delta y]$ $\Pr(Y\in[y,y+\Delta y])=p(y)\,\Delta y$ Probability for X to be in $[x,x+\Delta x]$

$$\Pr(X \in [x, x + \Delta x]) = \rho(x) \, \Delta x$$

These probabilities are identical

$$p(y) \Delta y = \rho(x) \Delta x, \Rightarrow \qquad p(y) = \rho(x) \frac{\Delta x}{\Delta y}$$
$$p(y) = \rho(x) \frac{1}{(\Delta y / \Delta x)} = \rho(x) \frac{1}{f'(x)}$$

Using $x = f^{-1}(y)$, we find

$$p(y) = \rho(f^{-1}(y)) \frac{1}{f'(f^{-1}(y))}.$$

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Example

Generate random numbers $y \ge 0$, with a given pdf p(y), using a uniformly distributed random numbers x from $x \in [0, 1]$.

Change of variables: solution

Looking for y = f(x) such that

$$p(y) = \frac{\rho(x)}{f'(x)} = \frac{1}{f'(x)}$$
, with $\rho(x) = 1$

with f'(x) = dy/dx, we find

$$p(y)\,dy = dx$$

integrating

$$\int_0^y p(y) \, dy = \int_0^x dx = x,$$

Recalling the definition of the cdf G(y) of y

$$G(y) = \int_{-\infty}^{y} p(y) \, dy = \int_{0}^{y} p(y) \, dy$$

solution: continued

Transformation formulae

$$x = G(y) \Rightarrow y = G^{-1}(x)$$



For exponential distribution: $p(y) = \alpha \exp(-\alpha y)$, $y \ge 0$

$$G(y) = \int_0^y \alpha \exp(-\alpha y) \, dy = 1 - \exp(-\alpha y)$$

inverting the cdf

$$y = -\alpha^{-1}\ln\left(1 - x\right)$$

Generating a Gaussian rv

cdf of $Z \sim N(0,1)$

$$G(z) = (1/2) \left(\operatorname{erf}(z/\sqrt{2}) + 1 \right) = X, \quad X \text{ uniform on } [0,1]$$

Solving for z

$$z = \sqrt{2} \operatorname{erf}^{-1}(2X - 1)$$

Inverse error function method

Computationally slow, as one needs to evaluate $\mathrm{erf}^{-1}(\dots)$

Box-Muller algorithm

Let U_1 and U_2 are independent and uniform on (0,1). Then

$$Z_1 = \sqrt{-2 \ln U_1} \cos (2\pi U_2)$$
, and $Z_2 = \sqrt{-2 \ln U_1} \sin (2\pi U_2)$

are independent with standard normal distribution $(Z_1, Z_2) \sim N(0, 1)$.

Probability and events

mutually disjoint events A and B are such that

 $A \cap B = \emptyset,$

where \emptyset denotes an empty set. If A_i , i = 1, 2, 3, 4, ... are mutually disjoint, then

 $P(A_1 \cup A_2 \cup A_3 \cup \dots) = P(A_1) + P(A_2) + P(A_3) + \dots$

For any A and B, we have

 $P(A \cup B) = P(A) + P(B) - P(A \cap B)$



Probability and events

<u>Conditional probability</u> Pr(A|B) is defined for any two events A and B as the probability of the event A given that the event B has certainly occurred.

$$\Pr(A|B) = \frac{\Pr(A \cap B)}{\Pr(B)}.$$

Example: roll of a die

• a)

$$A = \{1, 2, 3\}, B = \{1, 2, 5, 6\}, P(A|B) = \frac{P(\{1, 2\})}{P(\{1, 2, 5, 6\})} = \frac{2/6}{4/6} = 0.5$$

• b)

$$A = \{1, 2\}, \quad B = \{5, 6, 4, 3\}, \quad P(A|B) = \frac{P(\emptyset)}{P(\{5, 6, 4, 3\})} = 0$$

Probability

Example

Your neighbor has two children. You know that the name of one of them is John. What is the probability that your neighbor has two boys?

Solution: construct a table with all possible outcomes

Event	first child	second child	probability
(b,b)	boy	boy	1/4
(b,g)	boy	girl	1/4
(g,b)	girl	boy	1/4
(g,g)	girl	girl	1/4

Denote A = (two boys) = P(b, b) and $B = (\text{one is a boy}) = P(\{(b, b), (b, g), (g, b)\}).$ Then $A \cap B = A$. Consequently

$$P(A|B) = \frac{P(A \cap B)}{P(B)} = \frac{P(A)}{P(B)} = \frac{1/4}{3/4} = \frac{1}{3}$$

Independent events

Joint distribution

Any two events A and B are <u>independent</u> if the joint distribution can be factorized

$$P(A \cap B) = P(A)P(B)$$

As a consequence

$$P(A|B) = \frac{P(A \cap B)}{P(B)} = \frac{P(A)P(B)}{P(B)} = P(A).$$

and

$$P(B|A) = \frac{P(B \cap A)}{P(A)} = \frac{P(A)P(B)}{P(A)} = P(B).$$

Sum of two normal rv $Y = X_1 + X_2$

Example

Let
$$X_1 \sim N(\mu_1, \sigma_1^2)$$
, $X_2 \sim N(\mu_2, \sigma_2^2)$ find $Y \sim N(E(Y) = ?, Var(Y) = ?)$
 $E(Y) = E(X_1 + X_2) = E(X_1) + E(X_2) = \mu_1 + \mu_2$

$$Var(Y) = E((X_1 + X_2)^2) - (\mu_1 + \mu_2)^2$$

= $E(X_1^2 + X_2^2 + 2X_1X_2) - (\mu_1 + \mu_2)^2$
= $E(X_1^2) + E(X_2^2) + 2E(X_1X_2) - (\mu_1 + \mu_2)^2$
= $\sigma_1^2 + \mu_1^2 + \sigma_2^2 + \mu_2^2 + 2\mu_1\mu_2 - (\mu_1^2 + \mu_2^2 + 2\mu_1\mu_2)$
= $\sigma_1^2 + \sigma_2^2$

Only works if X_1 and X_2 are independent

 $E(X_1X_2) = E(X_1)E(X_2)$

Example

A particle moves with a constant absolute velocity V in a direction that changes randomly in time. For a gas of such active particles with a given concentration ρ_0 , the distribution of the direction of motion is uniform.

- Find the pressure in the gas
- Determine the distribution of the relative velocity $U = |\boldsymbol{u}_1 \boldsymbol{u}_2|$

1D case:

$$u_x = \pm V$$

$$\Pr(u_x = -V) = 1/2 \qquad \Pr(u_x = V) = 1/2$$

$$\longleftrightarrow \qquad x \rightarrow x$$

Ideal gas of active particles: 1D

Number of hits dN per unit area in time dt

$$dN = \frac{1}{2}\rho_0 V dt$$

Pressure *P*

$$P = \frac{m\Delta V}{dt}dN = \frac{\alpha}{2}m\rho_0 V^2, \ \alpha = \begin{cases} 2 & \text{elastic} \\ 1 & \text{inelastic} \end{cases}$$

Distribution of the relative velocity $U = |u_1 - u_2|$

$$\Pr(U=0) = \frac{1}{2}, \qquad \Pr(U=2V) = \frac{1}{2}$$

Ideal gas of active particles: 2D



Number of hits dN per unit area in time dt

$$dN = \rho_0 dt \int_0^V f(u_x) u_x \, du_x, \quad f(u_x) \dots \text{pdf of } u_x$$

Associated problem:

Find the distribution of the projection of the velocity onto any given direction

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Projection onto x axis

$$u_x = V \cos \phi$$

Distribution of the angle ϕ is uniform on $[0,2\pi]$

$$pdf(\phi) = \frac{1}{2\pi}$$

Changing variables: $\phi \Rightarrow u_x$

Note that the mapping $u_x = V \cos \phi$ is not one-to-one!



Ideal gas of active particles: 2D

pdf of u_x

$$f(u_x) du_x = -\frac{2}{2\pi} d\phi \Rightarrow f(u_x) = \frac{1}{\pi} \left| \frac{1}{du_x/d\phi} \right|$$

Using

$$u_x = V \cos \phi, \qquad \frac{du_x}{d\phi} = -V \sin \phi = -V \sqrt{1 - \cos^2 \phi}$$

we obtain

$$f(u_x) = \frac{1}{\pi V \sqrt{1 - \cos^2 \phi}} = \frac{1}{\pi \sqrt{V^2 - u_x^2}}.$$

Number of hits per unit area in time dt

$$\frac{dN}{dt} = \rho_0 \int_0^V \frac{u_x du_x}{\pi \sqrt{V^2 - u_x^2}} = \rho_0 \frac{V}{\pi}$$

Pressure

$$P = \rho_0 \int_0^V du_x \frac{2mu_x^2}{\pi\sqrt{V^2 - u_x^2}} = \frac{\rho_0 mV^2}{2} = \frac{\rho_v V^2}{2}$$

Relative velocity

$$U = |\boldsymbol{u}_1 - \boldsymbol{u}_2|$$

Associated problem:

Distribution of the distance between two random points on a circle

Distribution of $\Psi = \phi_2 - \phi_1$

Because ϕ_1 and ϕ_2 are independent, we can fix one angle at an arbitrary value, e.g. ϕ_1 -fixed, and look at the distribution of ϕ_2 .

- Because ϕ_1 and ϕ_2 are uniform on $[0,2\pi]$
- $\Psi = \phi_2 \phi_1$ is also uniform on $[0, 2\pi]$



Ideal gas of active particles: 2D

$$\operatorname{cdf}(\Delta) = \operatorname{Pr}(0 \leq \Psi = \phi_2 - \phi_1 \leq \Delta)$$
$$= \int_0^{2\pi} d\phi_1 \operatorname{Pr}(\phi_2 \in [\phi_1, \phi_1 + \Delta] | \phi_1) \times \operatorname{pdf}(\phi_1)$$
$$= \int_0^{2\pi} d\phi_1 \operatorname{Pr}(\phi_2 \in [\phi_1, \phi_1 + \Delta]) \times \operatorname{pdf}(\phi_1)$$
$$= \int_0^{2\pi} d\phi_1 \left[\operatorname{cdf}(\phi_1 + \Delta) - \operatorname{cdf}(\phi_1)\right] \times \operatorname{pdf}(\phi_1)$$
$$= \int_0^{2\pi} d\phi_1 \left[\frac{\phi_1 + \Delta}{2\pi} - \frac{\phi_1}{2\pi}\right] \times \frac{1}{2\pi} = \frac{\Delta}{2\pi}$$

 Ψ is uniform on $[0,2\pi]$

$$\operatorname{cdf}(\Psi) = \frac{\Psi}{2\pi} \Rightarrow \operatorname{pdf}(\Psi) = \frac{1}{2\pi}$$

periodicity of angles

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 $\phi_2 - \phi_1$ is uniform only for periodic boundary conditions.

Convolution of probability distributions

If x and y are not periodic and independent on [0, a], then z = x - y and s = x + y are distributed according to:

 $f(z) = \int_0^a pdf(x)pdf(z+x) dx$ $f(s) = \int_0^a pdf(x)pdf(s-x) dx$

Sum of independent random variables

Sum (difference) of two uniform rvs $(x, y \in [0, 1])$



Example

Using the convolution formulae, show that the sum of two independent normal variables $X_1 \sim N(\mu_1, \sigma_1^2)$ and $X_2 \sim N(\mu_2, \sigma_2^2)$ is normally distributed with $E(X_1 + X_2) = \mu_1 + \mu_2$ and $Var(X_1 + X_2) = \sigma_1^2 + \sigma_2^2$.

Ideal gas of active particles: 2D

Distribution of $U = 2V \sin{(\Psi/2)}$, with Ψ uniform on $[0, 2\pi]$.

 $U = 2V \sin{(\Psi/2)}$ is not a one-to-one function on $[0, 2\pi]$



Ideal gas of active particles: 2D

$$pdf(U)\Delta U = \frac{2}{2\pi}\Delta\Psi \Rightarrow pdf(U) = \frac{1}{\pi} \left| \frac{1}{dU/d\Psi} \right|$$
$$pdf(U) = \frac{1}{\pi} \frac{1}{V\cos(\Psi/2)} = \frac{1}{\pi V\sqrt{1-\sin^2(\Psi/2)}}$$
$$pdf(U) = \frac{2}{\pi\sqrt{(2V)^2 - U^2}}$$

Average relative velocity

$$\langle U \rangle = \int_0^{2V} \frac{2U \, dU}{\pi \sqrt{(2V)^2 - U^2}} = \frac{4V}{\pi}$$

- Determine the pressure in the ideal gas of active particles in 3D
- Determine the relative velocity of the active particles in 3D
- Derive the equation of state of an ideal gas, with the Maxwell distribution of the velocities

$$p(\boldsymbol{v}) = \left(\frac{m}{2\pi kT}\right)^{3/2} \exp\left(-\frac{m\boldsymbol{v}^2}{2kT}\right)$$