Stochastic Equations and Processes in Physics and Biology

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AMSI 2017

Probability: basic concepts and definitions

 X_{max} a discrete random variable $P(X) \ldots$ 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

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

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

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

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

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

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

$$
\sum_{\substack{1 \le x \le 1 \\ 0, \le x \le 1}}^{\infty} \sum_{\substack{1 \le x \le 1 \\ 0, \le x \le 1}}^{\infty
$$

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 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

 $X_i \ldots \,$ 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 X

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

In theory for a continuous rv X

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

Standard deviation σ

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

Proof of $\text{Var}(X) = E(X^2) - E(X)^2$

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

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

 $\langle X^2 \rangle \ge \langle X \rangle^2$

For a uniform distribution

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

\n
$$
Var(X) = \int_0^1 x^2 \, dx - (E(X))^2 = \frac{1}{3} - \frac{1}{4} = \frac{1}{12}
$$

\nstandard deviation = $\sigma = \sqrt{Var(X)} = \frac{1}{\sqrt{12}}$

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

Variance and standard deviation in an experiment

In a random experiment with n tries

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

Example

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

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

is an unbiased estimator for $\sigma^2.$

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 *normal* rv X is a continuous rv with pdf

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

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

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: $F(z)$

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

Error function $\mathrm{erf}(z)=2/\sqrt{\pi}\int_{0}^{z}e^{-x^{2}}\,dx$ is tabulated

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

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

$$
p(y) \Delta y = \rho(x) \Delta x, \Rightarrow p(y) = \rho(x) \frac{\Delta x}{\Delta y}
$$

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

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 $y \geq 0$, 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

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

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

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

Generating a Gaussian rv

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

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

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 Ø denotes an empty set. If A_i , $i = 1, 2, 3, 4, \ldots$ are mutually disjoint, then

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

For any A and B , we have

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

Probability and events

Conditional probability $Pr(A|B)$ 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

 \bullet a)

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

 \bullet 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

Denote $A =$ (two boys) = $P(b, b)$ and $B = \text{(one is a boy)} = P(\{(b, b), (b, q), (q, b)\}).$ 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 independent 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 $Y \sim N(E(Y) = ?$, $Var(Y) = ?$)

$$
E(Y) = E(X_1 + X_2) = E(X_1) + E(X_2) = \mu_1 + \mu_2
$$

$$
\begin{array}{rcl}\n\text{Var}(Y) & = & E((X_1 + X_2)^2) - (\mu_1 + \mu_2)^2 \\
& = & E(X_1^2 + X_2^2 + 2X_1X_2) - (\mu_1 + \mu_2)^2 \\
& = & E(X_1^2) + E(X_2^2) + 2E(X_1X_2) - (\mu_1 + \mu_2)^2 \\
& = & \sigma_1^2 + \mu_1^2 + \sigma_2^2 + \mu_2^2 + 2\mu_1\mu_2 - (\mu_1^2 + \mu_2^2 + 2\mu_1\mu_2) \\
& = & \sigma_1^2 + \sigma_2^2\n\end{array}
$$

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
Pr(u_x =V)=1/2
or

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 $U = |u_1 - u_2|$

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

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 $[0, 2\pi]$

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

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

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

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

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

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 $[0, 2\pi]$
- $\bullet \Psi = \phi_2 \phi_1$ is also uniform on $[0, 2\pi]$

Ideal gas of active particles: 2D

$$
cdf(\Delta) = Pr(0 \le \Psi = \phi_2 - \phi_1 \le \Delta)
$$

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

 Ψ is uniform on $[0, 2\pi]$

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

periodicity of angles

 \bullet

 \bullet

 $\phi_2 - \phi_1$ 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:

> $f(z) = \int^a$ 0 $pdf(x)pdf(z+x) dx$ $f(s) = \int_0^a$ $\int_0^{\infty} \text{pdf}(x) \text{pdf}(s-x) dx$

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

$$
pdf(U)\Delta U = 2\frac{1}{2\pi}\Delta \Psi \Rightarrow pdf(U) = \frac{1}{\pi} \left| \frac{1}{dU/d\Psi} \right|
$$

$$
pdf(U) = \frac{1}{\pi} \frac{1}{V \cos{(\Psi/2)}} = \frac{1}{\pi V \sqrt{1 - \sin^2{(\Psi/2)}}}
$$

$$
pdf(U) = \frac{2}{\pi \sqrt{(2V)^2 - U^2}}
$$

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

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