

Basic concepts – part 1

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Outline

Basics

- Sample measurements
- Error propagation
- Probabilities, Bayes Theorem
- Probability density function

Parameter estimation

- Maximum likelihood method
- Linear regression
- Least square fit

Model testings

- p-value and test statistics
- Chi2 and KS tests
- Hypothesis testing

Introductory books (non exhaustive)

Excellent book of reference

• G. Cowan, *Statistical Data Analysis* (Oxford Science Publication)

Introduction to Bayesian analysis

• D. Sivia, *Data Analysis: A Bayesian Tutorial* (Oxford Science Publication)

Classic textbook

 Louis Lyons, Statistics for Nuclear and Particle Physicists (Cambridge University Press)

En Français

 B. Clement, Analyse de données en sciences expérimentales (Dunod)

Population

- Let's consider a sample of values (e.g. experimental measurements)
 N measurement of a random variable X: {x_i} = {x₁, x₂, ..., x_N}
- There are several quantities that can be determined to characterize this population without any knowledge of the underlying model/theory

Measure of position

Arithmetic mean:
$$\bar{x} = \frac{1}{N} \sum_{i=1}^{N} x_i$$
 Median: value that separates sample in half

Quartiles (Q_1, Q_2, Q_3) : values that separates sample in four equal-size sample



Samples: basic basics

Measure of dispersion

Variance: if truth sample **mean** μ is known

$$v = \frac{1}{N} \sum_{i=1}^{N} (x_i - \bar{\mu})^2$$

But $\boldsymbol{\mu}$ is in general not know and sample mean is used instead

• Sample variance (biased):

$$v = \frac{1}{N} \sum_{i=1}^{N} (x_i - \bar{x})^2 = \overline{x^2} - \bar{x}^2$$

• Estimated variance (unbiased): $v = \frac{1}{N-1} \sum_{i=1}^{N} (x_i - \bar{x})^2 = \frac{N}{N-1} (\bar{x}^2 - \bar{x}^2)$

→ Bias is below α if N ≥ 1/ α − 1 (ex for 1% bias, N≥101)

Standard deviation (is of same unit as x): $\sigma = \sqrt{v}$

Standard deviation and error

In many situations **repeating an experiment** a large amount of time produces a spread of results whose distribution is approximately **Gaussian**.

This is a consequence of the **Central Limit Theorem**.

Gaussian (a.k.a normal) distribution

$$f(x) = \frac{1}{\sqrt{2\pi\sigma}} e^{-\frac{1}{2}\left(\frac{x-\mu}{\sigma}\right)^2}$$

Interval $\mu \pm \sigma$ contains 68.3% of distribution



A **measurement** = outcome of the **sum** of a large number of **effects**.

In general the distribution of this variable will be gaussian.

The **standard deviation** of the sample is associated to the standard deviation of the normal distribution.

The standard deviation is then interpreted as an **interval** that could contain the true value with a **68.3% confidence level**.

CLT at work

 x_i

Simple illustration of CLT

- let's consider x: a random variable uniformly distributed in [0,1]
- and the distribution of the sum of N values x:



Multidimensional samples

Case where N measurements are performed of M different variables

 $\rightarrow\,$ The sample then consists of N vectors of M measurements

$$\{\overrightarrow{x_i}\} = \{\overrightarrow{x_1}, \overrightarrow{x_2}, \dots, \overrightarrow{x_N}\} \quad \text{with} \quad \left\{ \begin{array}{c} \overrightarrow{x_1}: x_1^{(1)}, x_1^{(2)}, \dots, x_1^{(M)} \\ (\dots) \\ \hline \overrightarrow{x_N}: x_N^{(1)}, x_N^{(2)}, \dots, x_N^{(M)} \end{array} \right.$$

Mean and variance can be calculated for each variable $x_i^{(k)}$ but to quantify how of one variable behaves w.r.t another one uses the **covariance**:

For two variables x and y:
$$\operatorname{cov}(x, y) = \frac{1}{N} \sum_{i=1}^{N} (x_i - \bar{x})(y_i - \bar{y}) = \overline{xy} - \bar{x}\bar{y}$$

Correlation factor is defined as: $\rho_{xy} = \frac{\operatorname{cov}(x, y)}{\sigma_x \sigma_y}$ with $-1 \le \rho_{xy} \le 1$

 $\rho_{xy} = 1(-1) \rightarrow x$ and y are fully (anti)correlated $\rho_{xy} = 0 \rightarrow x$ and y are uncorrelated (\neq independent !)

Covariance matrix

Covariance matrix (aka error matrix) of sample $\{\vec{x_i}\}, i = 1..N$

• Real, symmetric, N×N matrix of the form:

$$C = \begin{pmatrix} \operatorname{cov}(x_1, x_1) & \cdots & \operatorname{cov}(x_1, x_N) \\ \vdots & \operatorname{cov}(x_i, x_j) & \vdots \\ \operatorname{cov}(x_N, x_1) & \cdots & \operatorname{cov}(x_N, x_N) \end{pmatrix} = \begin{pmatrix} \sigma_1^2 & \cdots & \rho_{1N} \sigma_1 \sigma_N \\ \vdots & \rho_{ij} \sigma_i \sigma_j & \vdots \\ \rho_{N1} \sigma_N \sigma_1 & \cdots & \sigma_N^2 \end{pmatrix}$$

Correlation matrix:
$$\rho = \begin{pmatrix} 1 & \cdots & \rho_{1N} \\ \vdots & 1 & \vdots \\ \rho_{N1} & \cdots & 1 \end{pmatrix}$$

Example of usage of covariance matrix:

- Transformation of input variables
- Error propagation
- Combination of correlated measurements

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Decorrelation

Decorrelation: choose a **basis** $\{\vec{y_i}\}$ where **C** becomes **diagonal**.

 \rightarrow transformation matrix **A** such that new covariance matrix **U** is diagonal

$$y_{i} = \sum_{j=1}^{N} A_{ij} x_{j}$$

$$U_{ij} = \operatorname{cov}(y_{i}, y_{j}) = \operatorname{cov}\left(\sum_{k=1}^{N} A_{ik} x_{k}, \sum_{l=1}^{N} A_{jl} x_{l}\right)$$

$$= \sum_{k,l=1}^{N} A_{ik} A_{jl} \operatorname{cov}(x_{l}, x_{k}) = \sum_{k,l=1}^{N} A_{ik} C_{kl} A_{lj}^{T}$$

$$U = ACA^{T}$$
(A is orthogonal A⁻¹=A^T)

Diagonalization of C: find orthonormal eigenvectors e_i such that $Ce_j = \lambda_j e_j$

$$A^{T} = \begin{pmatrix} e_{1}^{(1)} & e_{1}^{(2)} & \cdots & e_{1}^{(N)} \\ & \vdots & \vdots & \\ & & & \\ e_{N}^{(1)} & e_{N}^{(2)} & \cdots & e_{N}^{(N)} \end{pmatrix} \text{ and } \mathsf{U} = \begin{pmatrix} \lambda_{1} & 0 & \cdots & 0 \\ 0 & \lambda_{2} & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \lambda_{N} \end{pmatrix}$$

 λ_i = eigenvalues of C = σ_i^2 = variance of y_i

Decorrelation

2D example: variables x_1 and x_2 with correlation factor ρ

$$\lambda_{\pm} = \frac{1}{2} \Big(\sigma_1^2 + \sigma_2^2 \pm \sqrt{(\sigma_1^2 + \sigma_2^2)^2 - 4(1 - \rho^2)\sigma_1^2 \sigma_2^2} \Big)$$



Decorrelation: use cases

- Data pre-processing (for ML): remove correlation from input variables
- Reduce dimensionality of a problem: Principal Component Analysis (PCA)

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Consider only the M<N dominant eigenvalues (=variance) terms in U \rightarrow Reduced covariance matrix C: M×M
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Note: the decorrelation method is able to eliminate only **linear** correlations

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Error propagation

Function **f** of several variables $\mathbf{x} = \{x_1, \dots, x_N\}$

- Each variable x_i of mean μ_i and variance σ_i^2
- Perform 1st order Taylor expansion of *f* around mean value

$$f(\vec{x}) \approx f(\vec{\mu}) + \sum_{i=1}^{N} \frac{\partial f}{\partial x_i} (\vec{\mu}) (x_i - \mu_i)$$

$$f(\vec{x})^2 \approx f(\vec{\mu})^2 + 2f(\vec{\mu}) \sum_{i=1}^N \frac{\partial f}{\partial x_i} (\vec{\mu}) (x_i - \mu_i) + \sum_{i,j=1}^N \frac{\partial f}{\partial x_i} \frac{\partial f}{\partial x_j} (\vec{\mu}) (x_i - \mu_i) \Big(x_j - \mu_j \Big)$$

Variance of *f(x)*:

$$\sigma_f^2 = \overline{f(\vec{x})^2} - \left(\overline{f(\vec{x})}\right)^2 \approx \sum_{i,j=1}^N \frac{\partial f}{\partial x_i} \frac{\partial f}{\partial x_j} (\vec{\mu}) \times \operatorname{cov}(x_i, x_j)$$

Since $\overline{(x_i - \mu_i)} = 0$ $\overline{(x_i - \mu_i)^2} = \sigma_i^2$

 $\overline{(x_i - \mu_i)(x_j - \mu_j)} = \operatorname{cov}(x_i, x_j)$

Validity: up to 2nd order, linear case, small errors

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Error propagation

2D Example: x and y with correlation factor ρ

$$\sigma_f^2 = \left(\frac{\partial f}{\partial x}\sigma_x\right)^2 + \left(\frac{\partial f}{\partial y}\sigma_y\right)^2 + 2\frac{\partial f}{\partial x}\frac{\partial f}{\partial y}\operatorname{cov}(x,y)$$

$$f(x, y) = x + y \quad \Rightarrow \quad \sigma_f^2 = \sigma_x^2 + \sigma_y^2 + 2\rho\sigma_x\sigma_y$$
$$f(x, y) = xy \quad \Rightarrow \quad \sigma_f^2 = y\sigma_x^2 + x\sigma_y^2 + 2xy\rho\sigma_x\sigma_y$$

For a set of m function $f_1(\vec{x}), ..., f_m(\vec{x})$

- C is the covariance of variables x={x_i}
- We can build the covariance matrix of {f_i(x)}: U

$$U_{kl} = \operatorname{cov}(f_k, f_l) = \sum_{i,j=1}^{N} \frac{\partial f_k}{\partial x_i} \frac{\partial f_l}{\partial x_j} (\vec{\mu}) \times \operatorname{cov}(x_i, x_j)$$

This can be expressed as $| U = ACA^T |$

where
$$A_{ij} = \frac{\partial f_i}{\partial x_j} (\vec{\mu})$$

(Jacobian matrix)

Interlude



You are given a coin, you toss it and obtain "tail". What is the probability that both sides are "tail" ?



Interlude



It depends on the **prior** that the coin is **unfair** (and on the person that gave you the coin)

Who is more likely to give a fair coin ?







Probabilities

Sample space: Ω

- Set of all possible results of an experiment
- Populated by events



Probability

• Frequentist: related to frequency of occurrence

 $P(A) = \frac{\text{number of time event A occurs}}{\text{number of time experience is repeated}}$

 Subjectivist (Bayesian): degree of belief that A is true Introduces concepts of prior and posterior probability
 P(A|data) \propto P(data|A) \times P(A)

Knowledge on A increases using data

Axioms and rules

Mathematical formalization (Kolmogorov)

 $P(\Omega) = 1$ $0 \le P(A) \le 1$ $P(A \cap B) = P(A) + P(B) - P(A \cup B)$



Incompatible events: $P(A \cap B) = \emptyset \Rightarrow P(A \cup B) = P(A) + P(B)$

Conditional probability: $P(A|B) = \frac{P(A \cap B)}{P(B)}$

Independent events: $P(A \cap B) = P(A|B)P(B) = P(A)P(B)$

Bayes theorem



An Essay towards solving a Problem in the Doctrine of Chances. By the late Rev. Mr. Bayes, communicated by Mr. Price (1763) "If there be two subsequent events, the probability of the second b/N and the probability of both together P/N, and it being first discovered that the second event has also happened, from hence I guess that the first event has also happened, the probability I am right is P/b."

Thomas Bayes (?) c. 1701 –1761

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

If the sample space Ω can be divided in disjoint subsets A_i

$$P(B) = \sum_{i} P(B \cap A_i) = \sum_{i} P(B|A_i) P(A_i)$$

$$P(A|B) = \frac{P(B|A)P(A)}{\sum_{i} P(B|A_{i})P(A_{i})}$$



 $A_i \cap A_j = \emptyset \ (i \neq j)$

Bayes Theorem in everyday life

Example: 10 coins, **one** of which is **unfair** (two-sided tail): You flip a random coin and obtain **tail**. What is the probability that this is the unfair coin ?

A: event where the coin is unfair, B: event where the result is tail

You want
$$P(A|B)$$
: $P(A|B) = \frac{P(B|A)P(A)}{P(B)}$

where: $P(B) = P(B \cap A) + P(B \cap \overline{A}) = P(B|A)P(A) + P(B|\overline{A})P(\overline{A})$

$$P(B|A) = 1, P(A) = \frac{1}{10}$$

$$\Rightarrow P(A|B) = \frac{1 \times \frac{1}{10}}{1 \times \frac{1}{10} + \frac{1}{2} \times \frac{9}{10}} = \frac{2}{11}$$

In **Bayesian** language: P(A) is the **prior** probability and P(A|B) the **posterior**

Consequences of not knowing Bayes Th.

Estimates of probability (%)

Simple tools for understanding risks: from innumeracy to insight (2003)

G. Gigerenzer, A. Edwards, BMJ 327, 2003 <u>http://www.ncbi.nlm.nih.gov/pmc/articles/PMC200816/</u>

Conditional probabilities

The probability that a woman has breast cancer is 0.8%. If she has breast cancer, the probability that a mammogram will show a positive result is 90%. If a woman does not have breast cancer the probability of a positive result is 7%. Take, for example, a woman who has a positive result. What is the probability that she actually has breast cancer?

$$P(C|+) = \frac{P(+|C)P(C)}{P(+)} = \frac{0.9 \times 0.008}{0.9 \times 0.008 + 0.07 \times 0.992} = 9.4\%$$

Natural frequencies

Eight out of every 1000 women have breast cancer. Of these eight women with breast cancer seven will have a positive result on mammography. Of the 992 women who do not have breast cancer some 70 will still have a positive mammogram. Take, for example, a sample of women who have positive mammograms. How many of these women actually have breast cancer?

$$\mathbf{P}(\mathbf{C}|+)\simeq rac{7}{77}=9.1\%$$



"Bad presentation of medical statistics such as the risks associated with a particular intervention can lead to patients making poor decisions on treatment"

Bayes Theorem and statistical inference

Statistical inference

Estimate true parameters of a theory or a model using data

- Frequentist: perform measurement (or set limits)
- Bayesian: Improve prior knowledge using data



Probability distribution



Probability distribution

Random variable X

Discrete random variable: result (realizations) $x_i \in \Omega$ with probability $P(x_i)$

 \rightarrow **P** is the **probability distribution** and $\sum_{i} P(x_i) = 1$

For continuous variable: probability of observing x in infinitesimal interval \rightarrow Given by the probability density function (p.d.f) f(x) ^{f(x)}



Quantiles



Probability density function: **f(x)**

Cumulative distribution: F(x)=y

Inverse cumulative distribution: x=F⁻¹(y)

Median: x such that $F(x)=1/2 \rightarrow x_{1/2} = F^{-1}(1/2)$

Quantile of order α : $x_{\alpha} = F^{-1}(\alpha)$

• Ex: quartile, percentile, ...

Expectation value

Expectation value of a random variable X:

For a **function** of x, **a(x)**, the expectation value is: $E[a(x)] = \int_{-\infty}^{\infty} a(x)f(x)dx$

- mean of X:
$$E[x] = \int_{-\infty}^{\infty} xf(x)dx = \mu$$

- nth order moment: $E[x^n] = \int_{-\infty}^{\infty} x^n f(x) dx = \mu_n$

- Characteristic function Φ(t):

$$\phi(t) = E[e^{itx}] = \int e^{itx} f(x) dx = FT^{-1}(f) \text{ where } \mu_n = (-i)^n \frac{d^n \phi}{dt^n}(0)$$

- Variance:
$$V[x] = E[(x - E[x])^2] = \int_{-\infty}^{\infty} (x - \mu)^2 f(x) dx$$
$$= E[x^2] - E[x]^2$$

- Standard deviation:
$$\sigma = \sqrt{V[x]}$$

Some common distributions

Binomial law: efficiency, trigger rates, ...

$$B(k;n,p) = \mathcal{C}_k^n p^k (1-p)^{n-k}$$
, $\mu = np$, $\sigma = \sqrt{np(1-p)}$

Poisson distribution: counting experiments, hypothesis testing

$$P(n;\lambda) = rac{\lambda^n e^{-\lambda}}{n!}, \mu = \lambda, \sigma = \sqrt{\lambda}$$

Gauss distribution (aka normal): many use-case (asymptotic convergence)

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

Cauchy distribution (aka Breit-Wigner): particle decay width,

$$f(x; x_0, \gamma) = \frac{1}{\pi \gamma \left[1 + \left(\frac{x - x_0}{\gamma}\right)^2\right]}$$

 μ and σ not defined (divergent integral)

Cumulative distribution and p-value



One can choose any x_{sel} to compute F(x) or p-value, that is x_{sel} does not have a preferred value: it follows the **uniform** distribution

 \rightarrow The distributions of F(x_{sel}) and p-value are also uniform [proof next page]

→ Important for MC sample generation and hypothesis testing

Cumulative distribution and p-value



[proof] Given any random continuous variable X, define $Y = F_X(X)$

Then:
$$F_Y(y) = P(Y \le y)$$

 $= P(F_X(X) \le y)$
 $= P(X \le F_X^{-1}(y))$
 $= F_X(F_X^{-1}(y))$
 $= y$

 F_Y is just the cumulative distribution function of a uniform U(0,1) variable.

 \rightarrow Thus, Y has a **uniform distribution** on the interval [0,1]

(Silly) use case

Grading copies:



$$f(x) = \frac{1}{\pi \gamma \left[1 + \left(\frac{x - x_0}{\gamma}\right)^2\right]}$$

Try Cauchy distribution

$$F(x) = \frac{1}{\pi} \arctan\left(\frac{x - x_0}{\gamma}\right) + \frac{1}{2}$$

- 100 copies, grades: 0-20
- Peaked distribution at 10

$$F^{-1}(y) = x = \gamma \tan\left(\pi\left(y - \frac{1}{2}\right)\right) + x_0$$



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(Silly) use case

Grading copies:



Try Cauchy distribution

$$f(x) = \frac{1}{\pi \gamma \left[1 + \left(\frac{x - x_0}{\gamma}\right)^2\right]}$$

$$F(x) = \frac{1}{\pi} \arctan\left(\frac{x - x_0}{\gamma}\right) + \frac{1}{2}$$

- 100 copies, grades: 0-20
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Data uniformization

(Inverse) cumulative distribution is naturally useful to uniformize data distributions



For **Machine Learning**: data preprocessing is usually the 1^{st} step \rightarrow Uniformization of all input variables can sometime be a good idea.

To know more about **data transformation** see for example: https://scikit-learn.org/stable/modules/preprocessing.html

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χ^2 distribution

<u>Pearson's χ^2 test</u>: estimate global compatibility between data and a model

- The data is regrouped in an histogram of N bins
- A goodness-of-fit test K² is computed as follows

$$K^{2} = \sum_{i=1}^{N} \frac{(n_{i} - \nu_{i})^{2}}{\nu_{i}}$$

 n_i : number of observed events in bin i v_i : expected number of events in bin i

If the data n_i are **Poisson** distributed with mean values v_i and $n_i > \sim 5$ then: K² is a random variable following a χ^2 **distribution** with **N** degrees of freedom.

A variant of this test statistics is the <u>Neyman's χ^2 </u>

$$K^{2} = \sum_{i=1}^{N} \frac{(n_{i} - \nu_{i})^{2}}{n_{i}}$$

Easier to code (in particular for fits) Asymptotically equivalent to Pearson's χ^2 Follows χ^2 with N-1 degrees of freedom

χ^2 distribution

Probability density function k degrees of freedom, x>0

$$\chi^{2}(x;k) = \frac{x^{\frac{k}{2}-1}e^{-\frac{x}{2}}}{2^{\frac{k}{2}}\Gamma\left(\frac{k}{2}\right)}$$

Cumulative distribution

$$F(x;k) = \frac{\gamma\left(\frac{k}{2}, \frac{x}{2}\right)}{\Gamma\left(\frac{k}{2}\right)}$$

With:
$$\gamma(s, x) = \int_0^x t^{s-1} e^{-t} dt$$

$$\Gamma(s) = \int_0^{+\infty} t^{s-1} e^{-t} dt$$

Mean = k, variance = 2k



The **p-value** of a χ^2 test is obtained by integrating the χ^2 distribution **above** the measured K² value.

$$p-value = \int_{K^2}^{+\infty} \chi^2(x;k) \, dx$$

Example



Multi-dimensional p.d.f

An experiment can perform a set of measurement

 \rightarrow Vector of N measurements $\vec{x} = \{x_1, x_2, ..., x_N\}$

Probability of observing \vec{x} in infinitesimal interval $\vec{x} + d\vec{x}$ given by joint p.d.f

 $f(\vec{x})d\vec{x} = f(x_1, \dots, x_N)dx_1 \dots dx_N$

Ex: for a measurement of 2 values x and y

Probability of x in [x, x + dx] and y in [y, y + dy] is f(x, y)dxdy



$$\iint_{\Omega} f(x,y) dx dy = 1$$

Marginal and conditional p.d.f

Marginal distribution: p.d.f of one variable regardless of the others

$$f_x(x) = \int_{-\infty}^{\infty} f(x, y) \, dy \qquad f_y(y) = \int_{-\infty}^{\infty} f(x, y) \, dx$$



Conditional distribution: p.d.f of one variable given a constant other



$$k(y|x) = \frac{f(x,y)}{f_x(x)} = \frac{f(x,y)}{\int f(x,y')dy'}$$
$$g(x|y) = \frac{f(x,y)}{f_y(y)} = \frac{f(x,y)}{\int f(x',y)dx'}$$

Note: k and g are both functions of x and y

Marginal and conditional p.d.f

Bayes theorem for continuous variables

$$f(x,y) = g(x|y)f_y(y) = k(y|x)f_x(x) \quad \rightarrow$$

$$g(x|y) = \frac{k(y|x)f_x(x)}{f_y(y)}$$

Marginal p.d.f can also be expressed with conditional probabilities:

$$f_x(x) = \int_{-\infty}^{\infty} g(x|y) f_y(y) \, dy \qquad f_y(y) = \int_{-\infty}^{\infty} k(y|x) f_x(x) \, dx$$

Note: this is a generalization of the relation $P(B) = \sum_{i} P(B|A_i)P(A_i)$ to continuous variables

Independent variables: if x and y are independent $f(x, y) = f_y(y)f_x(x)$

Ex: 2D Gaussian function with uncorrelated variables

$$Gaus(x, y) = \frac{1}{2\pi\sigma_x\sigma_y} \exp\left(\frac{-(x-\mu_x)^2}{2\sigma_x^2}\right) \exp\left(\frac{-(y-\mu_y)^2}{2\sigma_y^2}\right)$$



Interlude: counting experiment



What is the meaning of error bars on **observed** data ?