

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)

Nice approach

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

En Français

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

Samples: basic basics

Population

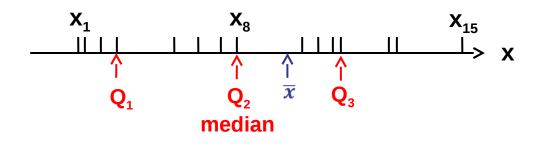
- Let's consider a sample of values (e.g. experimental measurements)
 N measurement of a variable X: {x_i} = {x₁, x₂, ..., x_N}
- There are several quantities that can be determined to characterize this population without any knowledge of the underlying model/theory

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): $v = \frac{1}{N}$

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

→ 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

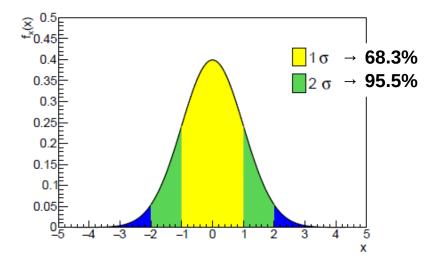
In many situations repeating an experiment a large amount of time produces a spread of results whose distribution is approximately Gaussian.

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

Gaussian 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.

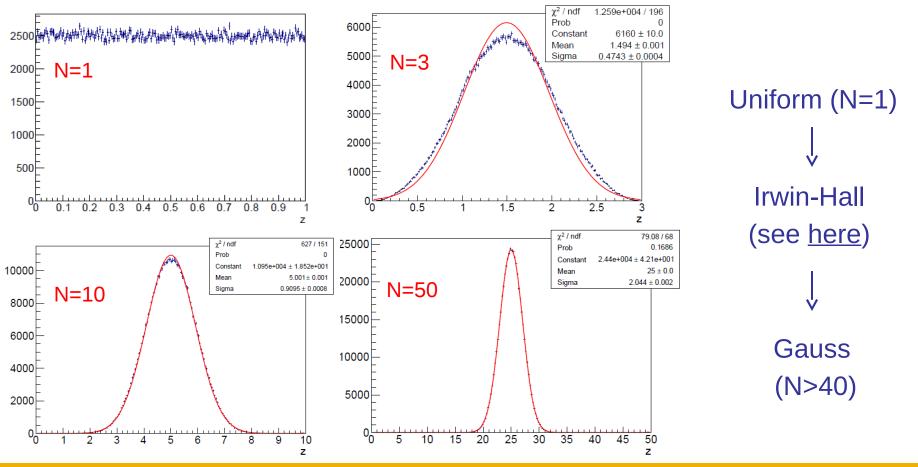
In general the distribution of this variable will be gaussian. The std deviation of the sample is associated to the std deviation of the Gauss distribution.

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

CLT at work

Simple illustration of CLT

- let's consider x: a random variable uniformly distributed in [0,1]
- and the distribution of N sums of x: $z = \sum_{i=1}^{N} x_i$



Multidimensional samples

Case where N measurements are performed of M different variables

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

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

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 $Ce_j = \lambda_j e_j$

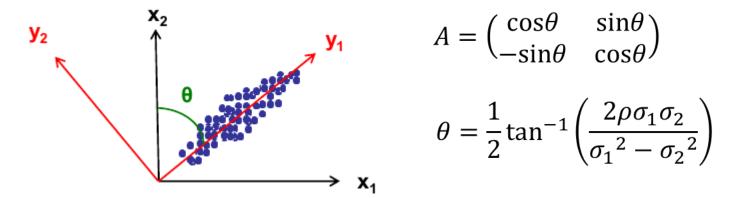
$$A^{T} = \begin{pmatrix} e_{1}^{(1)} & e_{1}^{(2)} & \cdots & e_{1}^{(N)} \\ & \vdots & \vdots & \\ & & & \\ e_{N}^{(1)} & e_{N}^{(2)} & \cdots & e_{N}^{(N)} \end{pmatrix} \text{ and } \mathsf{U} = \begin{pmatrix} \lambda_{1} & 0 & \cdots & 0 \\ 0 & \lambda_{2} & \cdots & 0 \\ \vdots & \vdots & \ddots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

 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)

Consider only the M<N dominant eigenvalues (=variance) terms in U \rightarrow Reduced covariance matrix C: M×M

Note: the decorrelation method is able to eliminate only **linear** correlations

Error propagation

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

- Each variable \mathbf{x}_i of mean $\mathbf{\mu}_i$ and variance $\mathbf{\sigma}_i^2$
- Perform 1st order Taylor expansion of *f* around mean value

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

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

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

Error propagation

Example:

x and y with correlation factor ρ

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

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

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

(matrix of derivatives)

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 ?



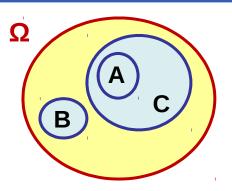




Probabilities

Sample space: Ω

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



Probability

• Frequentist: related to frequency of occurrence

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

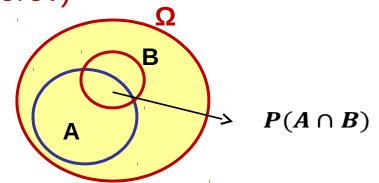
 Subjectivist (Bayesian): degree of belief that A is true Introduces concepts of prior and posterior probability
 P(A|data) \propto P(data|A) \times P(A)

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

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

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

$$\Omega \xrightarrow{A_1 \qquad A_2} \xrightarrow{A_3} \xrightarrow{A_5 \qquad A_6}$$

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

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.

stimates 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

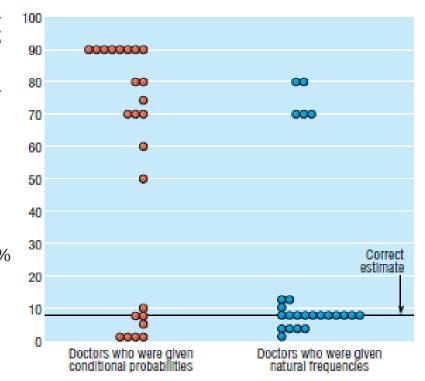
The probability that a woman has breast cancer is 0.8%. If she has breast cancer, the probability that a mammogram will show a positive result is 90%. If a woman does not have breast cancer the probability of a positive result is 7%. Take, for example, a woman who has a positive result. What is the probability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

$$P(C|+) = \frac{0.9 \times 8}{0.9 \times 8 + 0.07 \times 992} = 9.4\%$$



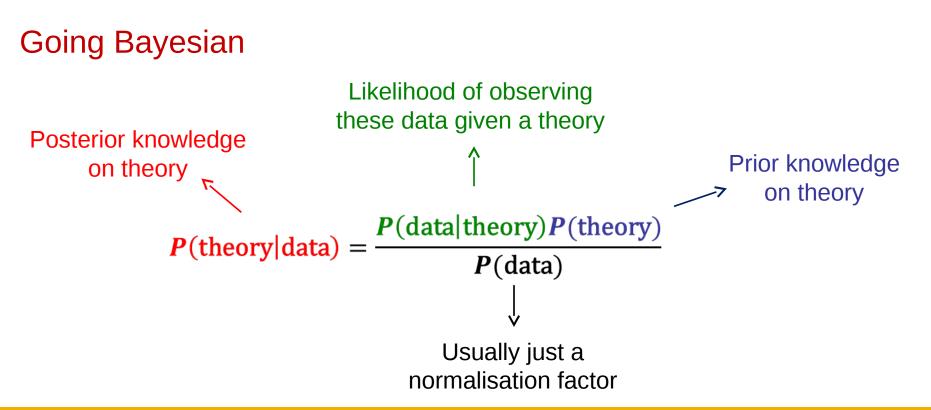
"Bad presentation of medical statistics such as the risks associated with a particular intervention can lead to patients making poor decisions on treatment"

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



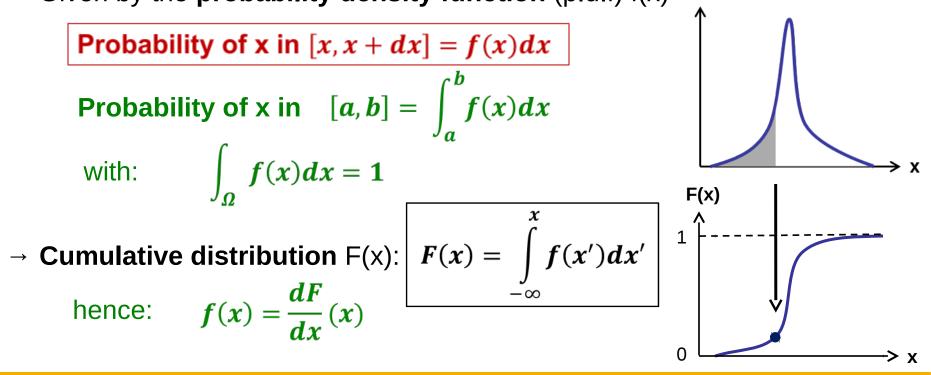
Probability distribution

Random variable X

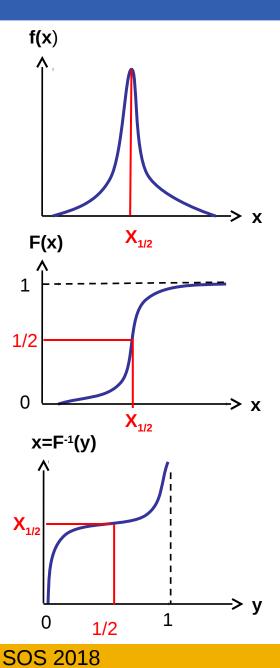
Discrete random variable: result (realizations) $x_i \in \Omega$ with probability $P(x_i)$

→ **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)}







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 : $x_{\alpha} = F^{-1}(\alpha)$

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, ...

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

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)

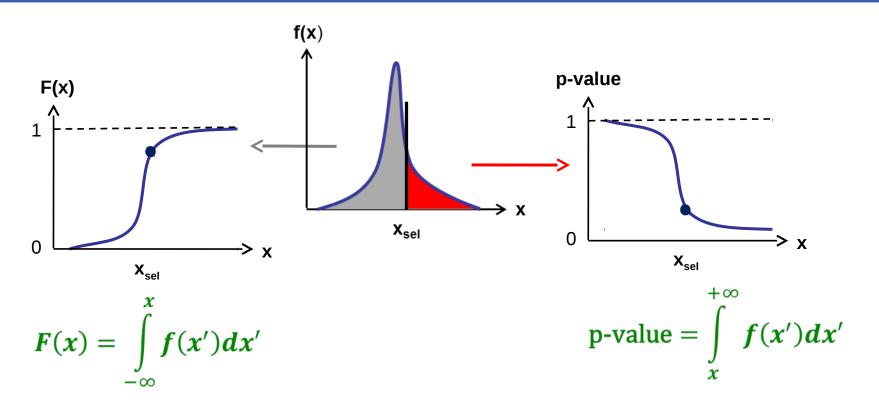
$$f(x;\mu,\sigma) = \frac{1}{\sqrt{2\pi}\sigma} e^{-\frac{1}{2}\left(\frac{x-\mu}{\sigma}\right)^2}$$

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

 \rightarrow Important for MC sample generation and hypothesis testing

(Silly) use case

Grading copies:



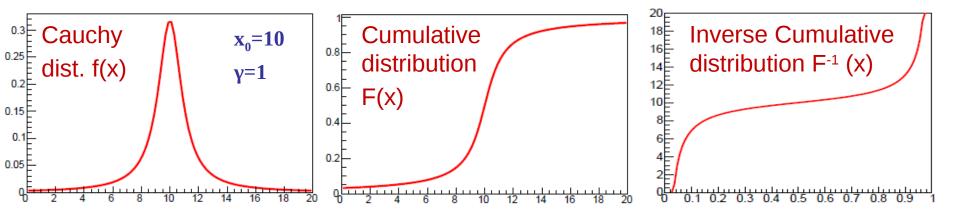
$$f(x) = \frac{1}{\pi \gamma \left[1 + \left(\frac{x - x_0}{\gamma}\right)^2\right]}$$

Try Cauchy distribution

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

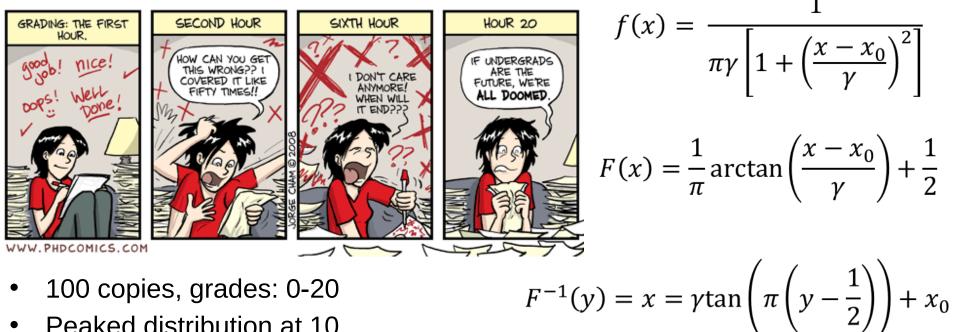
- 100 copies, grades: 0-20
- Peaked distribution at 10

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



(Silly) use case

Grading copies:

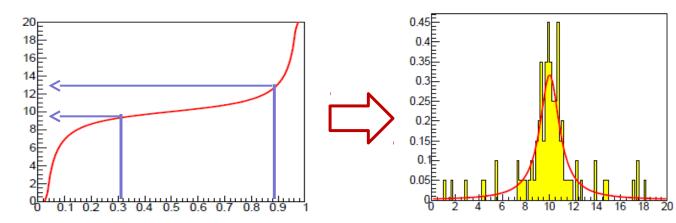


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Try Cauchy distribution

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

- 100 copies, grades: 0-20
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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

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

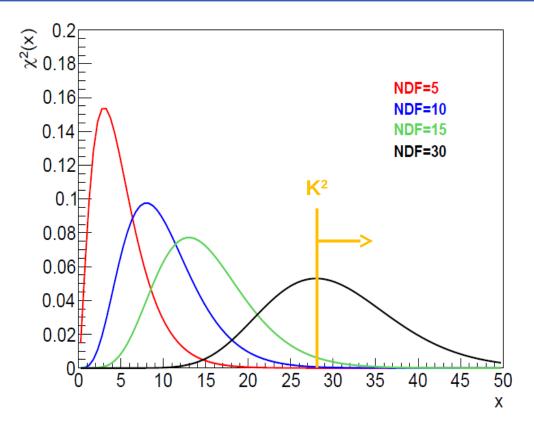
Cumulative distribution

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

Mean: k Variance: 2k

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

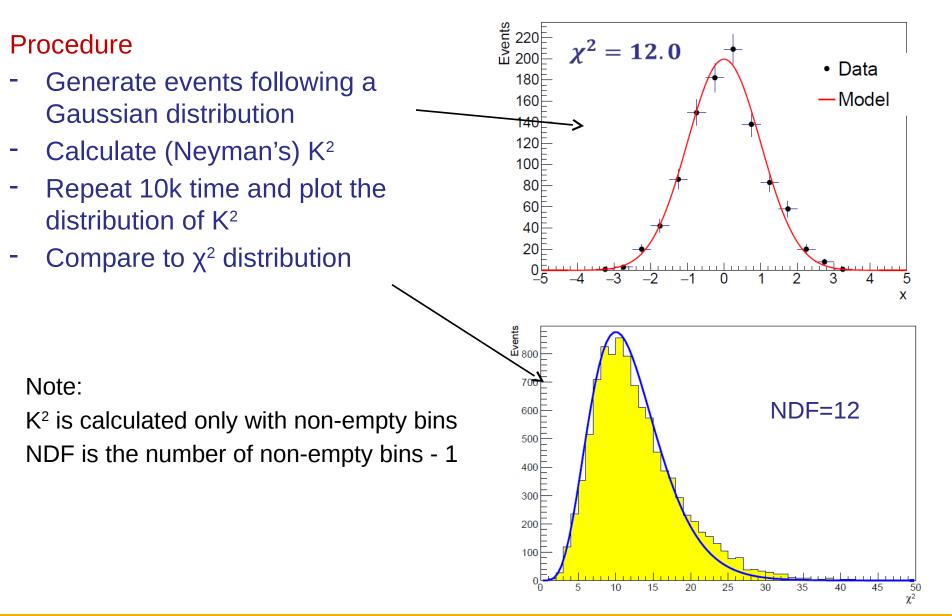
 $\Gamma(s) = \int_0^{+\infty} t^{s-1} e^{-t} dt$



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

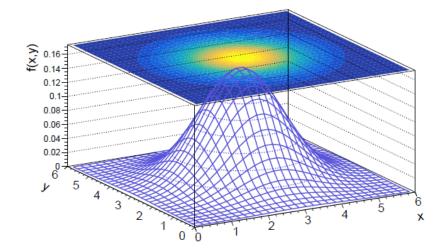
→ Vector of N measurements $\vec{x} = \{x_1, x_2, ..., x_N\}$

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

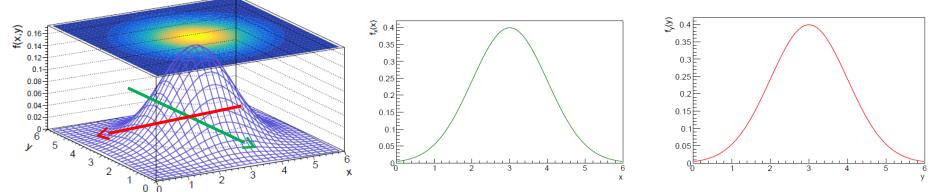


$$\iint_{\Omega} f(x,y) dx dy = 1$$

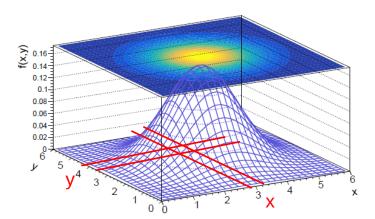
Marginal and conditional p.d.f

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

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

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

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

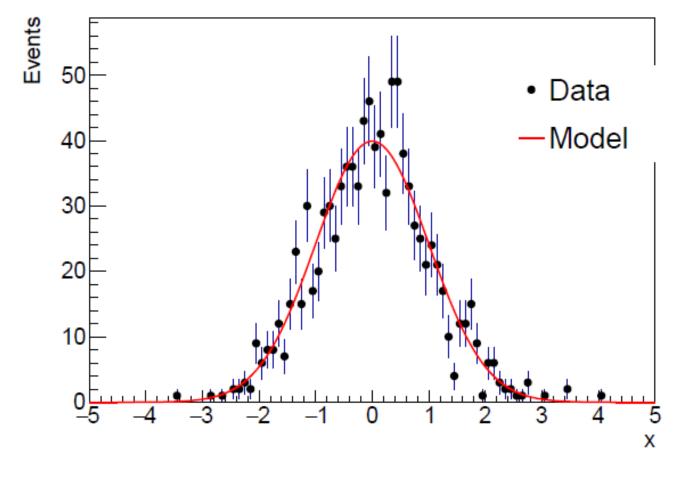
Independent variables: if x and y are independent $f(x, y) = f_y(y)f_x(x)$

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



What's "wrong" ?