

Probability and Statistics Basic concepts

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Kendall's Advanced theory of statistics, Hodder Arnold Pub.

volume 1: Distribution theory, A. Stuart et K. Ord volume 2a: Classical Inference and and the Linear Model, A. Stuart, K. Ord, S. Arnold volume 2b: Bayesian inference, A. O'Hagan, J. Forster

The Review of Particle Physics, K. Nakamura et al., J. Phys. G 37, 075021 (2010) (+Booklet) Data Analysis: A Bayesian Tutorial, D. Sivia and J. Skilling, Oxford Science Publication Statistical Data Analysis, Glen Cowan, Oxford Science Publication

Analyse statistique des données expérimentales, K. Protassov, EDP sciences
Probabilités, analyse des données et statistiques, G. Saporta, Technip
Analyse de données en sciences expérimentales, B. Clément, Dunod





First lecture: Probability theory - Sample and population



Characterization of the sample, the population and the sampling process





Physics

Second lecture: Statistical inference



Using the sample to estimate the characteristics of the population

- Random process ("measurement" or "experiment"): Process whose outcome cannot be predicted with certainty.
- Described by:

Universe: Ω = Set of all possible outcomes

Event: Logical condition on an outcome Either true or false An event splits the universe in 2 subsets



• An event \mathcal{A} will be identified by the subset **A** for which \mathcal{A} is true.



$$P : \{Events\} \longrightarrow [0:1]$$
$$A \longrightarrow P(A)$$

Properties:

$$P(\Omega) = 1$$

P(A or B) = P(A) + P(B) if (A and B) = Ø

Interpretation:

- Frequentist approach: if we repeat the random process a great number of times \mathcal{N} , and count the number of times the outcome satisfies event A, \mathcal{N}_A then the ratio:

$$\lim_{n \to +\infty} rac{n_{\mathrm{A}}}{n} = \mathrm{P}(\mathrm{A}) \,\,$$
 defines a probability

- **Bayesian interpretation:** A probability is a measure of the credibility associated to the event.

Logical relations





• Event "not A" associated with the complement of A:

$$P(\bar{A}) = 1 - P(A)$$
$$P(\emptyset) = 1 - P(\Omega) = 0$$

• Event "A and B" associated with the intersection of the subsets

• Event "A or B" associated with the union of the subsets

P(A or B) = P(A) + P(B) - P(A and B)

Event B known to be true → restriction of the universe to Ω' = B
 Definition of a new probability function on this universe, the conditional probability:

Conditional probability

P(A|B) = "probability of A given B"

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• The definition of the conditional probability leads to:

P(A and B) = P(A|B).P(B) = P(B|A).P(A)

Relation between P(A|B) and P(B|A), the **Bayes theorem**:

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

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Major role in Bayesian inference



• Two incompatible events cannot be true simultaneously: P(A and B) = 0

$$P(A \text{ or } B) = P(A) + P(B)$$

• Two events are independent, if the realization of one is not linked in any way to the realization of the other: P(A|B) = P(A) and P(B|A) = P(B)

$$P(A \text{ and } B) = P(A).P(B)$$



- When the outcome of the random process is a **number** (real or integer), we associate to the random process a random variable X.
- Each realization of the process leads to a particular result: X = x



x is a realization of X

• For a discrete variable:

Probability law: p(x) = P(X = x)

• For a real variable: P(X = x) = 0

Cumulative density function: F(x) = P(X < x)

$$d\mathbf{F} = \mathbf{F}(x + dx) - \mathbf{F}(x) = \mathbf{P}(X < x + dx) - \mathbf{P}(X < x)$$

= $\mathbf{P}(X < x \text{ or } x < X < x + dx) - \mathbf{P}(X < x)$
= $\mathbf{P}(X < x) + \mathbf{P}(x < X < x + dx) - \mathbf{P}(X < x)$
= $\mathbf{P}(x < X < x + dx) = f(x)dx$
Probability density function (pdf): $f(x) = \frac{d\mathbf{F}}{dx}$



Probability density function:



$$\int_{-\infty} f(x)dx = P(\Omega) = 1$$

Note - Discrete variables can also be described by a probability density function using Dirac distributions:

$$f(x) = \sum_{i} p(i)\delta(i-x)$$
 with
$$\sum_{i} p(i) = 1$$

Cumulative density function:



By construction:

$$F(-\infty) = P(\emptyset) = 0$$

$$F(+\infty) = P(\Omega) = 1$$

$$F(a) = \int_{-\infty}^{a} f(x) dx$$

$$< X < b) = F(b) - F(a) = \int_{a}^{b} f(x) dx$$

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P(a

- For any function g(x), the **expectation** of g is: $E[g(X)] = \int g(x)f(x)dx \quad \text{Mean value of } g$
- Moments μ_k are the expectation of X^k

Oth moment: $\mu_0 = 1$ (pdf normalization) 1st moment: $\mu_1 = \mu$ (mean) $X' = X - \mu_1$ is called a **central variable** 2nd central moment: $\mu'_2 = \sigma^2$ (variance)

• Characteristic function: $\phi(t) = E[e^{ixt}] = \int f(x)e^{ixt}dx = FT^{-1}[f]$

Taylor expansion
$$\phi(t) = \int \sum_k \frac{(itx)^k}{k!} f(x) dx = \sum_k \frac{(it)^k}{k!} \mu_k$$

$$-i^k \frac{d^k \phi}{dt^k}\Big|_{t=0}$$
 Pdf entirely defined
Characteristic function

Pdf entirely defined by its moments Characteristic function: usefull tool for demonstrations

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- A sample is obtained from a random drawing within a population, described by a probability density function.
- We're going to discuss how to characterize, independently from one another:

Sample PDF

- a **population**
- a **sample**
- To this end, it is useful to consider a sample as a finite set from which one can randomly draw elements, with equipropability.

We can then associate to this process a probability density: the **empirical density** or **sample density**

$$f_{\text{sample}}(x) = \frac{1}{n} \sum_{i} \delta(x-i)$$

This density will be useful to translate properties of distribution to a finite sample.



How to reduce a distribution / sample to a finite number of values ?

Measure of location:

Reducing the distribution to one central value



Measure of dispersion:

Spread of the distribution around the central value



Uncertainty / Error

• Frequency table / histogram (for a finite sample)



Standard deviation (σ) and variance ($v = \sigma^2$): Mean value of the squared deviation to the mean

$$v = \sigma^2 = \int (x - \mu)^2 f(x) dx$$

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

Koenig's theorem:

$$\sigma^{2} = \int x^{2} f(x) dx + \mu^{2} \int f(x) dx - 2\mu \int x f(x) dx = \overline{x^{2}} - \mu^{2} = \overline{x^{2}} - \overline{x}^{2}$$



• **Binomial distribution:** randomly choosing K objects within a finite set of n, with a fixed drawing probability of \mathcal{P}

Discrete distributions

Variable

Law

Mean

Variance





- Poisson distribution: limit of the binomial when $n \longrightarrow +\infty, \, p \longrightarrow 0, \, np = \lambda$ Counting events with fixed probability per time/space unit.

Variable

Parameters

Law

Mean

Variance







• Uniform distribution: equiprobability over a finite range [a, b]

Parameters

Law

Mean

Variance

:
$$a, b$$

: $f(x; a, b) = \frac{1}{b-a}$ if $a < x < b$
: $\mu = (a+b)/2$

:
$$v = \sigma^2 = (b - a)^2 / 12$$

Normal distribution: limit of many processes

Parameters : μ, σ Law : $f(x; \mu, \sigma) = \frac{1}{\sigma\sqrt{2\pi}}e^{-\frac{(x-\mu)^2}{2\sigma^2}}$

- Chi-square distribution: sum of the square of \boldsymbol{n} normal reduced variables

Variable

Parameters

Law

Mean









Convergence







• Random variables can be generalized to random vectors:

$$\vec{X} = (X_1, X_2, ..., X_n)$$

The probability density function becomes:

$$f(\vec{x})d\vec{x} = f(x_1, x_2, ..., x_n)dx_1dx_2...dx_n$$

= $P(x_1 < X_1 < x_1 + dx_1 \text{ and } x_2 < X_2 < x_2 + dx_2...$
...and $x_n < X_n < x_n + dx_n)$

and
$$P(a < X < b \text{ and } c < Y < d) = \int_{a}^{b} dx \int_{c}^{d} dy f(x, y)$$

• Marginal density: probability of only one of the component

$$f_X(x)dx = P(x < X < x + dx \text{ and } -\infty < Y < +\infty) = \int (f(x, y)dx)dy$$

$$f_X(x) = \int f(x, y)dy$$





- For a fixed value of $Y = y_0$: $f(x|y_0)dx =$ "Probability of x < X < x + dx knowing that $Y = y_0$ " is a conditional density for X. It is proportional to f(x, y)Therefore: $f(x|y) \propto f(x, y) \qquad \int f(x|y)dx = 1$ $f(x|y) = \frac{f(x, y)}{\int f(x, y)dx} = \frac{f(x, y)}{f_Y(y)}$
- The two random variables X and Y are **independent** if all events of the form x < X < x + dx are independent from y < Y < y + dy $f(x|y) = f_X(x)$ and $f(y|x) = f_Y(y)$ hence $f(x, y) = f_X(x) \cdot f_Y(y)$
- For probability density functions, Bayes' theorem becomes:

$$f(y|x) = \frac{f(x|y)f_Y(y)}{f_X(x)} = \frac{f(x|y)f_Y(y)}{\int f(x|y)f_Y(y)dy}$$



- A random vector (X, Y) can be treated as 2 separate variables marginal densities
- mean and standard deviation for each variable: $\mu_{X}, \mu_{Y}, \sigma_{X}, \sigma_{Y}$
- These quantities do not take into account correlations between the variables:







- Generalized measure of dispersion: Covariance of $X \operatorname{and} Y$



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• Covariance matrix for n variables X_i :

$$\Sigma_{ij} = \operatorname{Cov}(X_i, X_j) \longrightarrow \Sigma =$$

$$\begin{bmatrix} \sigma_1^2 & \rho_{12}\sigma_1\sigma_2 & \dots & \rho_{1n}\sigma_1\sigma_n \\ \rho_{12}\sigma_1\sigma_2 & \sigma_2^2 & \dots & \rho_{2n}\sigma_2\sigma_n \\ \vdots & \vdots & \ddots & \vdots \\ \rho_{1n}\sigma_1\sigma_n & \rho_{2n}\sigma_2\sigma_n & \dots & \sigma_n^2 \end{bmatrix}$$

- For uncorrelated variables Σ is diagonal
- Matrix real and symmetric: \sum can be diagonalized Definition of n new uncorrelated variables Y_i

$$\Sigma' = \begin{bmatrix} \sigma_1'^2 & 0 & \dots & 0 \\ 0 & \sigma_2'^2 & \dots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \dots & \sigma_n'^2 \end{bmatrix} = B^{-1} \Sigma B \text{ with } Y = BX$$

 $\sigma_i^{\,\,2}$ are the **eigenvalues** of Σ

 \boldsymbol{B} contains the orthonormal eigenvectors

- The \mathbf{Y}_i are the principal components. Sorted from the largest to the smallest σ' , they allow dimensional reduction





- Measure of location:
 - A point: $(\mu_{\mathrm{X}}, \mu_{\mathrm{Y}})$
 - A curve: line which is the closest to the points linear regression
- Minimizing the dispersion between the curve "y = ax + b " and the distribution

Regression

Let:
$$w(a,b) = \iint (y - ax - b)^2 f(x,y) dx dy \left(= \frac{1}{n} \sum_i (y_i - ax_i - b)^2 \right)$$

$$\begin{cases} \frac{\partial w}{\partial a} = 0 = \iint x(y - ax - b)f(x, y)dxdy\\ \frac{\partial w}{\partial b} = 0 = \iint (y - ax - b)f(x, y)dxdy\end{cases}$$

$$a(\sigma_{\rm X}^2 + \mu_{\rm X}^2) + b\mu_{\rm X} = \rho\sigma_{\rm X}\sigma_{\rm Y} + \mu_{\rm X}\mu_{\rm Y}$$

$$a\mu_{\rm X} + b = \mu_{\rm Y}$$

$$\begin{cases} a = \rho \frac{\sigma_{\rm Y}}{\sigma_{\rm X}} \\ b = \mu_{\rm Y} - \rho \frac{\sigma_{\rm Y}}{\sigma_{\rm X}} \mu_{\rm X} \end{cases}$$





• Multinomial distribution: randomly choosing $K_1, K_2, ..., K_S$ objects within a finite set of n, with a fixed drawing probability for each category $p_1, p_2, ..., p_S$ with $\sum K_i = n$ and $\sum p_i = 1$

Multidimensional PDFs

Note: Variables are not independent. The binomial corresponds to S=2 but has only one independent variable

Multinormal distribution:





- The sum of several random variable is a new random variable ${\rm S}$

$$\mathbf{S} = \sum_{i=1}^{N} \mathbf{X}_i$$

- Assuming the mean and variance of each variable exist:
 - Mean value of S :

$$\mu_{\mathbf{S}} = \int \left(\sum_{i=1}^{n} x_i\right) f(x_1, \dots, x_n) dx_1 \dots dx_n = \sum_{i=1}^{n} \int x_i f_{\mathbf{X}_i}(x_i) dx_i = \sum_{i=1}^{n} \mu_i$$

The mean is an additive quantity

• Variance of S:

$$\sigma_{\rm S}^2 = \int_n \left(\sum_{i=1}^n x_i - \mu_{{\rm X}_i} \right)^2 f(x_1, ..., x_n) dx_1 ... dx_n$$
$$= \sum_{i=1}^n \sigma_{{\rm X}_i}^2 + 2 \sum_i \sum_{j < i} \operatorname{Cov}({\rm X}_i, {\rm X}_j)$$

For **uncorrelated variables**, the variance is an additive quantity used for error combinations





- Probability density function of ${
 m S}$: $f_{
 m S}(s)$
- Using the characteristic function:

$$\phi_{\rm S}(t) = \int f_{\rm S}(s) e^{ist} ds = \int f_{\vec{\rm X}}(\vec{x}) e^{it\sum x_i} d\vec{x}$$

For independent variables:

$$\phi_{\mathbf{S}}(t) = \prod \int f_{\mathbf{X}_k}(x_k) e^{itx_k} dx_k = \prod \phi_{\mathbf{X}_i}(t)$$

The characteristic function factorizes.

• The PDF is the **Fourier transform** of the characteristic function, therefore:

$$f_{\mathrm{S}} = f_{\mathrm{X}_1} * f_{\mathrm{X}_2} * \dots * f_{\mathrm{X}_n}$$

The PDF of the sum of random variables is the convolution of the individual PDFs



Weak law of large numbers

Sample of size n = realization of n independent variables with the same distribution (mean μ , variance σ^2)

The sample mean is a realization of $M = \frac{S}{-} = \frac{1}{-}\sum X_i$

• Mean value of M: $\mu_M = \mu$

• Variance of
$$M$$
: $\sigma_M^2 = \sigma^2/n$

Central limit theorem

n independent random variables of mean μ_i and variance σ_i^2 Sum of the reduced variables: $C = \frac{1}{2} \sum \frac{X_i - \mu_i}{2}$

Sum of the reduced variables:
$$C = \frac{1}{\sqrt{n}} \sum \frac{m_i - \mu_i}{\sigma_i}$$

The PDF of C converges to a reduced normal distribution:

$$f_C(c) \xrightarrow[n \to +\infty]{} \frac{1}{\sqrt{2\pi}} e^{-\frac{c^2}{2}}$$

The sum of many random fluctuations is normally distributed

Central limit theorem





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- Any measure (or combination of measures) is a realization of a random variable.
 - Measured value: heta
 - True value: $heta_0$
- The uncertainty quantifies the difference between heta and $heta_0$:

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Measure of dispersion
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Postulate: $\Delta \theta = \alpha \sigma_{\theta}$ \longrightarrow Absolute error always positive

- Usually one differentiates:
 - Statistical errors: due to the measurement PDF
 - Systematic errors or bias: fixed but unknown deviation (equipment, assumptions, ...)
 Systematic errors can be seen as statistical error in a set of similar experiments



$$\begin{array}{l} \Delta_O &= \alpha \sigma_O \\ \Delta_S &= \alpha \sigma_S \\ \Delta_P &= \alpha \sigma_P \end{array} \right\} \Delta_{\text{tot}}^2 = (\alpha \sigma_{\text{tot}})^2 = \alpha^2 (\sigma_O^2 + \sigma_S^2 + \sigma_P^2) = \Delta_O^2 + \Delta_S^2 + \Delta_P^2 \\ \end{array}$$

- Choice for α :

Many sources of error — central limit theorem — normal distribution

- $\alpha=1\,$ gives (approximately) a 68% confidence interval
- $\alpha = 2$ gives a 95% confidence interval

Error propagation



• Measure: $x \pm \Delta x$

• Compute: $f(x) \longrightarrow \Delta f$?



Assuming small errors and using the Taylor expansion:







- Estimating a parameter θ from a finite sample $\{x_i\}$
- Statistic: a function $S = f(\{x_i\})$

Any statistic can be considered as an **estimator** of θ To be a good estimator it needs to satisfy:

- **Consistency:** limit of the estimator for an infinite sample
- Bias: difference between the estimator and the true value
- Efficiency: speed of convergence
- Robustness: sensitivity to statistical fluctuations
- A good estimator should at least be consistent and asymptotically unbiased
- Efficient / Unbiased / Robust often contradict each others



Need to make a choice for a given situation



 As the sample is a set of realizations of random variables (or one vector variable), so is the estimator:

 $\hat{ heta}$ is a realization of $\hat{\Theta}$

It has a mean, a variance, ..., and a probability density function

Bias: characterize the mean value of the estimator $\longrightarrow b(\hat{\theta}) = E[\hat{\Theta} - \theta_0] = \mu_{\hat{\Theta}} - \theta_0$ Unbiased estimator: $b(\hat{\theta}) = 0$ Asymptotically unbiased: $b(\hat{\theta}) \xrightarrow[n \to +\infty]{} 0$ • Consistency: formally $P(|\hat{\theta} - \theta| < \epsilon) \xrightarrow[n \to +\infty]{} 1, \forall \epsilon$ In practice, if the estimator is asymptotically unbiased $\int \sigma_{\hat{\Theta}} \frac{\sigma_{\hat{\Theta}}}{n \to +\infty}$ **Biased** Asymptotically unbiased Unbiased

• For any unbiased estimator of θ , the variance cannot exceed (Cramer-Rao bound):

Efficiency

$$\sigma_{\hat{\Theta}}^{2} \geq \frac{1}{E\left[\left(\frac{\partial \ln \mathcal{L}}{\partial \theta}\right)^{2}\right]} \left(= \frac{-1}{E\left[\frac{\partial^{2} \ln \mathcal{L}}{\partial \theta^{2}}\right]} \right)$$

• The efficiency of a convergent estimator is given by its variance.

An efficient estimator reaches the Cramer-Rao bound (at least asymptotically)

- Minimal variance estimator
- The minimal variance estimator will often be biased, asymptotically unbiased



- Sample mean is a good estimator of the population mean
 - → weak law of large numbers: convergent, unbiased

$$\hat{\mu} = \frac{1}{n} \sum x_i$$
 $\mu_{\hat{\mu}} = E[\hat{\mu}] = \mu$ $\sigma_{\hat{\mu}}^2 = E[(\hat{\mu} - \mu)^2] = \frac{\sigma^2}{n}$

• Sample variance as an estimator of the population variance:

$$\hat{s}^{2} = \frac{1}{n} \sum_{i} (x_{i} - \hat{\mu})^{2} = \left(\frac{1}{n} \sum_{i} (x_{i} - \mu)^{2}\right) - (\hat{\mu} - \mu)^{2}$$

$$E[\hat{s}^{2}] = \left(\frac{1}{n} \sum_{i} \sigma^{2}\right) - \sigma_{\hat{\mu}}^{2} = \sigma^{2} - \frac{\sigma^{2}}{n} = \frac{n - 1}{n} \sigma^{2} \text{ biased, asymptotically unbiased}$$

$$\Rightarrow \text{ unbiased variance estimator:} \qquad \hat{\sigma}^{2} = \frac{1}{n - 1} \sum_{i} (x_{i} - \hat{\mu})^{2}$$

Variance of the estimator (convergence): $\sigma_{\hat{\sigma}^2}^2 = \frac{\sigma^4}{n-1} \left(\frac{n-1}{n} \gamma_2 + 2 \right) \longrightarrow \frac{2\sigma^4}{n}$



Uncertainty **Estimator standard deviation**

Errors on estimators

- Use an estimator of standard deviation: $\hat{\sigma}=\sqrt{\hat{\sigma}^2}$ (biased !)





 Central-Limit theorem — empirical estimators of mean and variance are normally distributed for large enough samples

 $\hat{\mu}\pm\Delta\hat{\mu}$, $\hat{\sigma}\pm\Delta\hat{\sigma}$ define 68% confidence intervals







For a **sample**: n independent realizations of the same variable X

$$\mathcal{L}(\theta) = \prod_{i} k(x_i, \theta) = \prod_{i} f(x_i; \theta)$$



• Let a sample of measurements: $\{x_i\}$

The analytical form of the density is known and depends on several unknown parameters $\boldsymbol{\theta}$

For example: Event counting follows a Poisson distribution with a parameter $\lambda_i(\theta)$ depending on the physics.

$$\mathcal{L}(\theta) = \prod_{i} \frac{e^{\lambda_i(\theta)} \lambda_i(\theta)^{x_i}}{x_i!}$$

• An estimator of the parameters θ is given by the position of the maximum of the likelihood function

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Parameter values which maximize the probability to get the observed results

$$\frac{\partial \mathcal{L}}{\partial \theta}\Big|_{\theta=\hat{\theta}} = 0$$

Note: system of equations for several parameters Note: minimizing $-ln\mathcal{L}$ often simplify the expression



 Mostly asymptotic properties: valid for large samples, often assumed in any case for lack of better information

Asymptotically unbiased

Asymptotically **efficient** (reaches the Cramer-Rao bound)

Asymptotically normally distributed

Multinormal law with covariance given by a generalization of the CR bound:

$$f(\hat{\vec{\theta}};\vec{\theta},\Sigma) = \frac{1}{\sqrt{2\pi|\Sigma|}} e^{-\frac{1}{2}(\hat{\vec{\theta}}-\vec{\theta})^{\mathrm{T}}\Sigma^{-1}(\hat{\vec{\theta}}-\vec{\theta})} \qquad \Sigma_{ij}^{-1} = -\mathrm{E}\left[\frac{\partial\mathrm{ln}\mathcal{L}}{\partial\theta_{i}}\frac{\partial\mathrm{ln}\mathcal{L}}{\partial\theta_{j}}\right]$$

• Goodness of fit: The value of $-2\ln \mathcal{L}(\hat{\theta})$ is Chi-2 distributed with

ndf = sample size - number of parameters

p - value =
$$\int_{-2\ln\mathcal{L}(\hat{\theta})}^{+\infty} f_{\chi^2}(x; \mathrm{ndf}) dx$$

Probability of getting a worse agreement





$$f(\hat{\vec{\theta}};\vec{\theta},\Sigma) = \frac{1}{\sqrt{2\pi|\Sigma|}} e^{-\frac{1}{2}(\hat{\vec{\theta}}-\vec{\theta})^{\mathrm{T}}\Sigma^{-1}(\hat{\vec{\theta}}-\vec{\theta})}$$

$$\Sigma_{ij}^{-1} = -\mathbf{E} \left[\frac{\partial \ln \mathcal{L}}{\partial \theta_i} \frac{\partial \ln \mathcal{L}}{\partial \theta_j} \right]$$

- Errors on the parameters given by the covariance matrix
- For one parameter, 68% confidence interval: $\Delta \theta = \hat{\sigma}_{\hat{\theta}} = \sqrt{\frac{-1}{\frac{\partial^2 \ln \mathcal{L}}{\partial \theta^2}}}$

only one realization of the estimator: empirical mean of 1 value

• More generally:

$$\Delta \ln \mathcal{L} = \ln \mathcal{L}(\hat{\theta}) - \ln \mathcal{L}(\theta) = \frac{1}{2} \sum_{i,j} \sum_{i,j} \sum_{i,j} \sum_{i,j} (\theta_i - \hat{\theta_i})(\theta_j - \hat{\theta_j}) + O(\theta^3)$$

Confidence contours are defined by the equation:

$$\Delta \ln \mathcal{L} = \beta(n_{\theta}, \alpha)$$
 with $\alpha = \int_{0}^{2\beta} f_{\chi^{2}}(x; n_{\theta}) dx$

Values of β for different number parameters n_{θ} and confidence levels α

$\begin{array}{c} n_{\theta} \rightarrow \\ \alpha \downarrow \end{array}$	1	2	3
68.3	0.5	1.15	1.76
95.4	2	3.09	4.01
99.7	4.5	5.92	7.08

Least squares



• Set of measurements (x_i, y_i) with uncertainties on y_i

Theoretical law given by: $y = f(x, \theta)$

Naive approach: use regression

$$w(\theta) = \sum_{i} (y_i - f(x_i, \theta))^2 \qquad \frac{\partial w}{\partial \theta_i} = 0$$

Reweight each term by its associated error:

$$K^{2}(\theta) = \sum_{i} \left(\frac{y_{i} - f(x_{i}, \theta)}{\Delta y_{i}} \right)^{2} \qquad \frac{\partial K^{2}}{\partial \theta_{i}} = 0$$



- Maximum likelihood assumes that each y_i is normally distributed with a mean equal to $f(x_i, \theta)$ and a standard deviation given by Δy_i
- The likelihood is then $\mathcal{L}(\theta) = \prod_{i} \frac{1}{\sqrt{2\pi}\Delta y_i} e^{-\frac{1}{2}\left(\frac{y_i f(x_i, \theta)}{\Delta y_i}\right)^2}$

 $\frac{\partial \mathcal{L}}{\partial \theta} = 0 \Leftrightarrow -2 \frac{\partial \ln \mathcal{L}}{\partial \theta} = \frac{\partial K^2}{\partial \theta} = 0$ Least squares or Chi-2 fit is the maximum likelihood estimator for Gaussian errors

• Generic case with correlations: $K^2(\vec{\theta}) = \frac{1}{2}(\vec{y} - \vec{f}(x, \vec{\theta}))^T \Sigma^{-1}(\vec{y} - \vec{f}(x, \vec{\theta}))$

Example: fitting a line





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Example: fitting a line

$$\Delta \hat{a} = \sigma_a = \sqrt{\frac{\mathbf{B}}{\mathbf{AB} - \mathbf{C}^2}}$$
, $\Delta \hat{b} = \sigma_b = \sqrt{\frac{\mathbf{A}}{\mathbf{AB} - \mathbf{C}^2}}$

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 $\frac{\partial^2 K^2}{\partial a \partial b} = 2\mathbf{C} = 2\Sigma_{12}^{-1}$









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- Directly estimating the probability density function
 - Likelihood ratio discriminant
 - Separating power of variables
 - Data / Monte Carlo agreement

...

- Frequency table: For a sample $\{x_i\}, i = 1...n$
 - 1. Define successive invervals (bins) $C_k = [a_k, a_{k+1}]$
 - 2. Count the number of events n_k in C_k
- Histogram: Graphical representation of the frequency table $h(x) = n_k$ if $x \in C_k$

Histogram



Bin	Number of N/Z	Frequency	Bin	Number of N/Z	Frequency
< 1.30	0	0	1.45 - 1.48	26	0.2363
1.30 - 1.33	2	0.0182	1.48 - 1.51	19	0.1727
1.33 - 1.36	2	0.0182	1.51 - 1.54	12	0.1091
1.36 - 1.39	9	0.0818	1.54 - 1.57	2	0.0182
1.39 - 1.42	13	0.1182	1.57 - 1.60	3	0.0273
1.42 - 1.45	22	0.2	≥ 1.60	0	0

N/Z for stable heavy nuclei

1.321, 1.357, 1.392, 1.410, 1.428, 1.446, 1.464, 1.421, 1.438, 1.344, 1.379, 1.413, 1.448, 1.389, 1.366, 1.383, 1.400, 1.416, 1.433, 1.466, 1.500, 1.322, 1.370, 1.387, 1.403, 1.419, 1.451, 1.483, 1.396, 1.428, 1.375, 1.406, 1.421, 1.437, 1.453, 1.468, 1.500, 1.446, 1.363, 1.393, 1.424, 1.439, 1.454, 1.469, 1.484, 1.462, 1.382, 1.411, 1.441, 1.455, 1.470, 1.500, 1.449, 1.400, 1.428, 1.442, 1.457, 1.471, 1.485, 1.514, 1.464, 1.478, 1.416, 1.444, 1.458, 1.472, 1.486, 1.500, 1.465, 1.479, 1.432, 1.459, 1.472, 1.486, 1.513, 1.466, 1.493, 1.421, 1.447, 1.460, 1.473, 1.486, 1.500, 1.526, 1.480, 1.506, 1.435, 1.461, 1.487, 1.500, 1.512, 1.538, 1.493, 1.450, 1.475, 1.500, 1.512, 1.525, 1.550, 1.506, 1.530, 1.487, 1.512, 1.524, 1.536, 1.518, 1.577, 1.554, 1.586, 1.586





• Statistical description: n_k are multinomial random variables

Parameters:
$$n = \sum_{k} n_k$$
 $p_k = P(x \in C_k) = \int_{C_k} f_X(x) dx$
 $\mu_{n_k} = np_k$ $\sigma_{n_k}^2 = np_k (1 - p_k) \approx \mu_{n_k}$ $Cov(n_k, n_r) = -np_k p_r \approx 0$
 $p_k \ll 1$

For a large sample:

For small classes (width δ):

^

$$\lim_{n \to +\infty} \frac{n_k}{n} = \frac{\mu_k}{n} = p_k \qquad p_k = \int_{C_k} f_{\mathbf{X}}(x) dx \approx \delta f(x_c) \Rightarrow \lim_{\delta \to 0} \frac{p_k}{\delta} = f(x)$$

Finally:
$$f(x) = \lim_{\substack{n \to +\infty \\ \delta \to 0}} \frac{1}{n\delta} h(x)$$

- The histogram is an estimator of the probability density function
- Each bin can be described by a Poisson density The 1σ error on n_k is then: $\Delta n_k=\sqrt{\hat\sigma_{n_k}^2}=\sqrt{\hat\mu_{n_k}}=\sqrt{n_k}$

• For a random variable, a confidence interval with confidence level α , is any interval [a, b] such that:

Confidence interval

$$P(X \in [a, b]) = \int_{a}^{b} f_{X}(x)dx = \alpha$$

Probability of finding a realization inside the interval

- Generalization of the concept of uncertainty: interval that contains the true value with a given probability
- For **Bayesians**: the posterior density is the probability density of the true value.



It can be used to estimate an interval:
$$P(\theta \in [a, b]) = \alpha$$

- No such thing for a Frequentist: the interval itself becomes the random variable [a,b] is a realization of $[{\rm A,B}]$

 $P(A < \theta \text{ and } B > \theta) = \alpha$ independently of θ

Confidence interval





• Mean centered, probability symetric interval: [a,b]

$$\int_{a}^{\mu} f(x)dx = \int_{\mu}^{b} f(x)dx = \frac{\alpha}{2}$$



• Mean centered, symetric interval: $[\mu - a, \mu + a]$

$$\int_{\mu-a}^{\mu+a} f(x)dx = \alpha$$



• Highest probability density (HDP) interval: [a, b] $\int_{a}^{b} f(x) dx = \alpha$

$$f(x) > f(y)$$
 for $x \in [a, b]$ and $y \notin [a, b]$



- To build a frequentist interval for an estimator $\hat{\theta}$ of θ :
 - 1. Make pseudo-experiments for several values of θ and compute the estimator $\hat{\theta}$ for each (Monte Carlo sampling of the estimator PDF)
 - 2. For each θ , determine $\Xi(\theta)$ and $\Omega(\theta)$ such that: $\hat{\theta} < \Xi(\theta)$ for a fraction $(1 - \alpha)/2$ of the pseudo-experiments $\hat{\theta} > \Omega(\theta)$ for a fraction $(1 - \alpha)/2$ of the pseudo-experiments

These 2 curves are the confidence belt for a confidence level α

3. Inverse these functions. The interval $[\Omega^{-1}(\hat{\theta}), \Xi^{-1}(\hat{\theta})]$ satisfies:



$$P\left(\Omega^{-1}(\hat{\theta}) < \theta < \Xi^{-1}(\hat{\theta})\right) = 1 - P\left(\Xi^{-1}(\hat{\theta}) < \theta\right) - P\left(\Omega^{-1}(\hat{\theta}) > \theta\right)$$
$$= 1 - P\left(\hat{\theta} < \Xi(\theta)\right) - P\left(\hat{\theta} > \Omega(\theta)\right) = \alpha$$

Confidence belt for a Poisson parameter λ estimated with the empirical mean of 3 realizations (68% CL)



- The variance of the estimator only measures the statistical uncertainty.
- Often, we will have to deal with parameters whose value is known with limit precision.



• The likelihood function becomes:

$$\mathcal{L}(heta,
u)$$
 with $u =
u_0 \pm \Delta
u$ or $u_0^{+\Delta
u_+}_{-\Delta
u_-}$

The known parameters \mathcal{V} are **nuisance parameters**



- In **Bayesian statistics**, nuisance parameters are dealt with by assigning them a prior $\pi(\nu)$.
- Usually a multinormal law is used with mean ν_0 and covariance matrix estimated from $\Delta\nu_0$ (+ correlation if needed)

$$f(\theta,\nu|x) = \frac{f(x|\theta,\nu)\pi(\theta)\pi(\nu)}{\iint f(x|\theta,\nu)\pi(\theta)\pi(\nu)d\theta d\nu}$$

• The final posterior distribution is obtained by marginalization over the nuisance parameters:

$$f(\theta|x) = \int f(\theta, \nu|x) d\nu = \frac{\int f(x|\theta, \nu) \pi(\theta) \pi(\nu) d\nu}{\iint f(x|\theta, \nu) \pi(\theta) \pi(\nu) d\theta d\nu}$$



- No true frequentist way to add systematic effects. Popular method of the day: profiling
- Deal with nuisance parameters as realization of random variables:

 $\longrightarrow \text{ extend the likelihood: } \mathcal{L}(\theta,\nu) \longrightarrow \mathcal{L}'(\theta,\nu) \mathcal{G}(\nu)$

- $\mathcal{G}(\nu)$ is the likelihood of the new parameters (identical to prior)
- For each value of $\theta,$ maximize the likelihood with respect to nuisance: profile likelihood $\mathrm{PL}(\theta)$
- $\mathrm{PL}(\theta)$ has the same statistical asymptotical properties than the regular likelihood





- Statistical tests aim at:
 - Checking the compatibility of a dataset $\{x_i\}$ with a given distribution
 - Checking the **compatibility of two datasets** $\{x_i\}$, $\{y_i\}$: are they issued from the same distribution ?
 - Comparing different hypothesis: background VS signal + background

- In every case:
 - Build a statistic that quantifies the agreement with the hypothesis
 - Convert it into a probability of compatibility/incompatibility: p-value



- Test for binned data: use the Poisson limit of the histogram
 - Sort the sample into k bins C_i : n_i
 - Compute the probability of this class: $p_i = \int_{C} f(x) dx$
 - For each bin, the test statistics compares the deviation of the observation from the expected mean to the theoretical standard deviation.



- χ^2 follows (asymptotically) a Chi-2 law with k-1 degrees of freedom (one constraint $\sum n_i = n$)
- **p-value**: probability of doing worse: $p value = \int_{\chi^2}^{+\infty} f_{\chi^2}(x; k-1) dx$ For a "good" agreement: $\chi^2/(k-1) \sim 1$ More precisely: $\chi^2 \in (k-1) \pm \sqrt{2(k-1)}$ (1 σ interval ~ 68% CL)



- · Test for unbinned data: compare the sample cumulative density function to the tested one
- Sample PDF (ordered sample)

$$f_{\rm S}(x) = \frac{1}{n} \sum_{i} \delta(x-i) \longrightarrow F_{\rm S}(x) = \begin{cases} 0 & x < x_0 \\ \frac{k}{n} & x_k \le x < x_{k+1} \\ 1 & x > x_n \end{cases}$$

• The Kolmogorov statistic is the largest deviation:

$$D_n = \sup_x |F_{\rm S}(x) - F(x)|$$

• The test distribution has been computed by Kolmogorov:

$$P(D_n > \beta \sqrt{n}) = 2 \sum_r (-1)^{r-1} e^{-2r^2 z^2}$$

 $[0,\beta]$ defines a confidence interval for D_n $\beta=0.9584/\sqrt{n}~~{\rm for}~68.3\%~{\rm CL}~~\beta=1.3754/\sqrt{n}~~{\rm for}~95.4\%~{\rm CL}$





- Test compatibility with an exponential law: $f(x)=\lambda e^{-\lambda x},\,\,\lambda=0.4$

0.008, 0.036, 0.112, 0.115, 0.133, 0.178, 0.189, 0.238, 0.274, 0.323, 0.364, 0.386, 0.406, 0.409, 0.418, 0.421, 0.423, 0.455, 0.459, 0.496, 0.519, 0.522, 0.534, 0.582, 0.606, 0.624, 0.649, 0.687, 0.689, 0.764, 0.768, 0.774, 0.825, 0.843, 0.921, 0.987, 0.992, 1.003, 1.004, 1.015, 1.034, 1.064, 1.112, 1.159, 1.163, 1.208, 1.253, 1.287, 1.317, 1.320, 1.333, 1.412, 1.421, 1.438, 1.574, 1.719, 1.769, 1.830, 1.853, 1.930, 2.041, 2.053, 2.119, 2.146, 2.167, 2.237, 2.243, 2.249, 2.318, 2.325, 2.349, 2.372, 2.465, 2.497, 2.553, 2.562, 2.616, 2.739, 2.851, 3.029, 3.327, 3.335, 3.390, 3.447, 3.473, 3.568, 3.627, 3.718, 3.720, 3.814, 3.854, 3.929, 4.038, 4.065, 4.089, 4.177, 4.357, 4.403, 4.514, 4.771, 4.809, 4.827, 5.086, 5.191, 5.928, 5.952, 5.968, 6.222, 6.556, 6.670, 7.673, 8.071, 8.165, 8.181, 8.383, 8.557, 8.606, 9.032, 10.482, 14.174



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