



Basic Concepts of Statistics

Romain Madar (CNRS/IN2P3/LPC) School Of Statistics Carry-le-Rouet - 16/05/2022



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Goals of the lecture

- recap the basics needed for the SOS
- learn how to be critical with statistics (in science, but not only)
- focus on meaning and (mis)intuition rather than mathematical rigour

Statistics versus probability (according to Persi Diaconis)

The problems considered by probability and statistics are inverse to each other. In probability theory we consider some underlying process which has some randomness [...] and we figure out what happens. In statistics we observe something that has happened, and try to figure out what underlying process would explain those observations.

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Few personal tips for this lecture

keywords/concepts will be listed at the end of each section
 → make sure you know the ideas behind them!

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- keywords/concepts will be listed at the end of each section \rightarrow make sure you know the ideas behind them!
- statistics is almost like a language: you need practice to learn it!
 → compute/code as much as simple examples as you can by yourself!

Some references





Frederick James

Statistical Methods in Experimental Physics ^{2nd Edition}





- 1. Statistics
- 2. Probability
- 3. Statistical model
- 4. The two big schools
- 5. Parameter estimation and hypothesis testing

Statistics

Definitions:

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- sample = set of observations $S \equiv \{x_1, x_2, ..., x_n\}$

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 - arithmetic mean: $\overline{x} = \frac{1}{n} \sum x_i$
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• variance: $v_x = \overline{(x - \overline{x})^2}$; $\sigma_x \equiv \sqrt{v_x}$ - dispersion

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 - Skewness: $\gamma_x = \overline{\left(\frac{x-\overline{x}}{\sigma_x}\right)^3}$ asymmetry
 - Kurtosis: $\beta_x = \left(\frac{x-\overline{x}}{\sigma_x}\right)^4$ importance of tails

Sample caracterisation - illustrations



blue: x_i , red: mean. black: median, green: σ_x

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Skewness and Kurtosis (using probability functions)



Right plot: Kurtosis $\gamma = \infty$ (red), 2 (blue), 1, 1/2, 1/4, 1/8, and 1/16 (gray), 0 (black)

Sample caracterisation - comments

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Statistical moments (more on this later)

- Order-r moment: $m_r = \overline{\left(\frac{x-\overline{x}}{\sigma_x}\right)^r}$ (relates directly to the mean of x^r)
- probability theory: all truth moments \equiv exact underlying probability
- first moments \equiv "main" features of the sample

- single observation i = several numbers: $x_i \rightarrow (x_i^{(1)}, x_i^{(2)}, ..., x_i^{(p)})$
- e.g. biological dataset: person size, weight, age and genre

Previous description applies to each variable $x_i^{(j)}$ but one can now explore how variables behave wrt each other.

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Covariance and correlations between two variables *a* and *b*:

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; $\rho_{ab} \equiv \frac{\operatorname{cov}_{ab}}{\sigma_a \sigma_b}$

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- covariance (and correlation) are symetric fortunate
- covariance of x with itself is the variance
- $\rho_{a,b} \in [-1,1]$; 0 = uncorrelated (\neq indep!), (-)1 = (anti-)correlated

Covariance matrix or error matrix

- $C_{ij} = \rho_{ij} \times \sigma_i \sigma_j$ real and symmetric.
- ρ_{ij} is the correlation matrix symmetric with 1's on diagonal.

Why is this object so important?

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- x_1 and x_2 both have a large σ
- but, they are highly correlated
- most of the information is in y₁ (largest σ)
 → idea of dimension reduction
 - \rightarrow idea of pre-processing in ML

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Non-correlation *dosen't* imply independence (matter of vocabulary)

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(Never go to the hospital, people there die 10 times more than at home)

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Worldwide non-commercial space launches

correlates with

Sociology doctorates awarded (US)



tylervigen.co
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tylervigen.o

Part I

descriptive statistics - sample - mean - (co)variance - (de)correlation

Probability

Some definitions

Caution: what follows is not mathematically rigorous

Random variable and associated probability

- a random variable X describes an observable which is not certain
- all possible outcomes realisations of X form a set Ω
- a probability P_i is associated to each realisation i of Ω
- $\{P_i\}$ must satisfy $P_i \in [0,1]$ and $\sum P_i = 1$

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Simple concrete example: a flippin coin

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- $P_0 = 1/2$ and $P_1 = 1/2$
- $\rightarrow\,$ these notions can be defined and manipulated without any sample

Previously: sample mean \neq "true mean". What is the true mean?

$$\mu = \sum_{\Omega} P_i x_i \quad ; \quad \sigma^2 = \sum_{\Omega} P_i \times (x_i - \mu)^2 \quad ; \quad m_r = \sum_{\Omega} P_i \times \left(\frac{x_i - \mu}{\sigma}\right)^r$$

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E.g. of the flipping coin

•
$$\mu = 1/2$$
, $\sigma = 1/2$, $m_r = 1$ if r is even and 0 if r is odd

Bias theorem - math version

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Comments

- many ways to understand this fundamental equation
- in some case, each of these term has a clear meaning
- these two posts are quit interesting post 1 and post 2

Example: *hypothesis* = *fire* and *evidence* = *smoke*

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N.B.: P(evidence) is independent from the hypothesis, and is sometime impossible to compute. It is often seen as a "normalization factor" and dropped while comparing different hypothesis.

Everyday life questions are often bayesian

Few examples:

- I'm not feeling so well \rightarrow Am I sick ?
- There are clouds \rightarrow will it rain?
- I go out in a bar \rightarrow will I end up drunk?
- I attend to a school statistics \rightarrow will I learn something?

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Always the same thinking:

- 1. you observe a fact
- 2. you wonder the probability of something, given you this fact happened
- 3. you have (somtimes rough/wrong) prior, based on past knowledge
- 4. your brain applies Bias theorem, even you don't know it!

- There is a whole continuum of outcome (realization) for X
- Probability described by a density probability function (PDF), f(x):

$$P(x \in [x_1, x_2]) = \int_{x_1}^{x_2} f(x) \mathrm{d}x$$
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- knowing all moments \equiv knowing the full PDF
- moments are the Taylor expension coefficients: $m_r = (-i)^r \frac{d'\varphi_X}{dt'}\Big|_{t=0}$

Important PDF examples

Binomial law: efficiency, trigger rates, ...

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

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

Multidimensional PDF

How to describe several random variables simulataneously?

- X and Y are two random variables \rightarrow PDF is f_{XY} ,
- several questions can be asked about X, Y or both.



- Probability that $X \in [x, x + dx]$ and $Y \in [y + dy]$: $d^2P(x, y) = f_{XY}(x, y)dxdy$
- Probability that $X \in [x, x + dx]$ $dP(x) = \left(\int_{y} f_{XY}(x, y) dy\right) dx$ $\rightarrow \text{ this is the marginal PDF}$

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Independent variables $\rightarrow f_{XY}(x, y) = f_X(x) \times f_Y(y)$

• Why? Because marginal PDF is independent from Y behaviour

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• Why? Because marginal PDF is independent from Y behaviour $\rightarrow dP(x) = \left(\int_{y} f_{XY}(x, y) dy\right) dx = \underbrace{\left(\int_{y} f_{Y}(y) dy\right)}_{=1} f_{X}(x) dx$

Multidimensional normal distribution

$$f(\vec{x};\vec{\mu},\Sigma) = \frac{1}{\sqrt{(2\pi)^n \det \Sigma}} \exp\left(-\frac{1}{2} \left(\vec{x}-\vec{\mu}\right)^T \Sigma^{-1} \left(\vec{x}-\vec{\mu}\right)\right)$$

• $\vec{\mu}$ mean position of \vec{x} , Σ covariance matrix
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If *n* random variables $\{X_i\}$ are distributed according to the same PDF f_X with a defined mean μ_x and a std σ_x , then the random variable $Y = \frac{1}{n}(X_1 + ... + X_n)$ is following a normal distribution of mean μ_x and std σ_x/\sqrt{n} .

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For 2 variables $Y = X_1 + X_2$

- The PDF of Y is $f_Y(y) = \int f_{X_1}(x_1) \times f_{X_2}(y x_1) dx_1 \rightarrow \text{convolution}!$
- Caracteristic function: $\varphi_Y(t) = \varphi_{X_1}(t) \times \varphi_{X_2}(t) = \varphi_X(t)^2$ same PDF!
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Generalizing for sum of n variables:

- $\varphi_Y(t) = \varphi_x(t)^n \sim \left(1 \frac{t^2}{n}\right)^n \to e^{-t/2}$ for $n \to \infty$
- · going back to real space, a normal distribution is obtained

N.B. this reasonning doesn't explain why $\sigma_Y = \sigma_x / \sqrt{n}$, this needs to properly re-scale Y.

Central limit theorem – continued

One way to understand why it works



Central limit theorem – continued

One way to understand why it works

200

200



500



2.5 3.0 3.5 4.0

Proof

Proove that $\sigma_Y = \sigma_X / \sqrt{n}$ with the proper scalings to define Y.

Application

Proove, using the CLT, that a Poisson distribution $P(n; \lambda)$ tends to a normal distribution for large numbers.

Hint: $N = 1 + 1 + 1 \dots + 1$ N-times

Final observable is very often a combination of (random) variable.

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Comments:

- these equations are known as error propagation
- this procedure is not exact and relies on Taylor expansion
- only 1st and 2nd moments of \vec{X} are needed (or their estimators)

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Error propagation formula is not exact

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Part I: statistics

descriptive statistics - sample - mean - (co)variance - (de)correlation

Part II: probability

Bias theorem – prior – posterior – random variable – (marginal) PDF – moments – caracteristic function – (in)dependent variables – CLT – error propagation

- 1. Statistics
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Statistical model





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Why? because a measurement is always one realization of a random variable.



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Statistical model ingredients:

- (pseudo-)observations, written \vec{x} (or x)
- parameters we want: parameter(s) of interest, written $\vec{\mu}$ or μ (POI)
- parameters we don't care about: nuisance parameters, written $\vec{\theta}$ or θ



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A statistical model is also called likelihood function $\mathcal{L}(\vec{\mu}, \vec{\theta}; \vec{x})$. It can be seen as the probability that the physical model predicts the observable \vec{x} , given the parameters $(\vec{\mu}, \vec{\theta})$.

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Statistical model

$$\mathcal{L}(\sigma; N) = e^{-\sigma L\epsilon} \frac{(\sigma L\epsilon)^N}{N!}$$

Given a value of σ , what's the "probability" to observe N ?



Anticipation: frequentist "usage" of the likelihood

If we observed a value for N, what's the "probability" that $\sigma = X$?



Anticipation: bayesian "usage" of the likelihood

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Systematic uncertainties turn numbers into new random variables. They PDFs depends on parameters, we don't really care about: nuisances parameters. *Example* of systematic parametrization:

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- What is more relvant: more regions or more bins?
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- Why do we multiply terms?

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Systematic uncertainty estimation and treatment is not an exact science.

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Implications:

- arbitrariness (and a loooot of discussion that go with it)
- always check the robustness of the conclusion wrt to those
- that's the way it is, no choice! \rightarrow be *smartly* practical!

Part I: statistics

descriptive statistics - sample - mean - (co)variance - (de)correlation

Part II: probability

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Part III: statistical model

Likelihood – nuisance parameter – parameter of interest – systematic uncertainties

Overview



- 1. Statistics
- 2. Probability
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The two big schools

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Bayesian

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degree of belief

Frequentist

probability	frequency of occurence
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- *bayesian:* exploits the Bayes theorem to compute the posterior P(para|obs), using the prior P(para) and P(obs|para) the **likelihood**

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We toss a coin 113 times and we got 'tail' 68 times. Is the coin tricked?

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Statistical Model assuming N = 113 is large enough to apply CLT

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Let's try to analyze the same experiment with both frequentist and bayesian approaches



Toys with a normal coin

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Toys with a tricked coin 36.8% of pseudo-experiments using an tricked coin with p = 0.57 would lead to $N_{tail} \ge 68$



In the end, is the coin tricked?

Toys with a normal coin 14.1% of pseudo-experiments using an normal coin would lead to $N_{tail} \ge 68$

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- according to you, is p = 0.57 more probable than p = 0.50?
 → this question has no sense in frequentist

$$P(p|N_{tail}) = Prior(p) imes rac{P(N_{tail}|p)}{P(N_{tail})}$$

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Flat prior



$$p = 0.60$$

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 \rightarrow expect it depends on the choice of the prior \ldots



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Frequentists say "Yes, the coin is tricked!"

Certainty comes from the extremely low fraction of pseudo-experiments of a normal coin, that would lead the observed result.

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Handling many measurements in Bayesian

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Bayesians also say "Yes, the coin is tricked!"

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One thing I like from the two approaches

- probability intepretation from the frequentist
- ranking two theories using their probability, called Bias factors

Part I: statistics

descriptive statistics - sample - mean - (co)variance - (de)correlation

Part II: probability

Bias theorem – prior – posterior – random variable – (marginal) PDF – moments – caracteristic function – (in)dependent variables – CLT – error propagation

Part III: statistical model

Likelihood – nuisance parameter – parameter of interest – systematic uncertainties

Part IV: The two big school

Frequentist – occurence frequency – pseudo-data (toys) – bayesian – degree of belief

Overview



- 1. Statistics
- 2. Probability
- 3. Statistical model
- 4. The two big schools
- 5. Parameter estimation and hypothesis testing

Parameter estimation and hypothesis testing

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- Maximum likelihood (ML) and χ^2 estimators
- uncertainty: confidence interval, notion of coverage

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3. Coming back on nuisance parameters (i.e. uncertainties on the model)

Definition: random variable which gives a 'good' estimate of your parameter of interest ($\hat{\mu} = \frac{1}{N} \sum_{i} x_i$ as estimator of $\mathbb{E}[X]$). Estimator depends on observation $\hat{\mu}(x_1, ..., x_n)$ and is *not* constant. N_{meas} needed to assess its quality.

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Two important examples of estimators

- **1.** Maximum likelihood estimator (MLE): $\hat{\mu}$ which maximizes $\mathcal{L}(\mu; x)$
 - \rightarrow numerically easier to minimze $-2\ln\mathcal{L}(\mu;x)$ negative log likelihood (NLL)
- 2. χ^2 estimator: $\hat{\mu}$ which minimizes $\chi^2(\mu) \equiv \sum_i w_i (X_i^{pred}(\mu) x_i)^2$

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Question 1 for the audience:

In frequentist, we sayed that the parameters are fixed (once chosen), while here were are talking about $P(\hat{\mu})$ or $\mathbb{E}[\hat{\mu}]$... So in the end, is there in frequentist a probability associated to the parameter or not?

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Question 2 for the audience:

Why consistency and bias of an estimator are different?

Example: linear fit

Model $N^{pred}(p_0, p_1; t) = p_0 + p_1 t$

4 estimators (or "cost function") are used:

 $-2\log \mathcal{L}_{poisson}$

$$\chi^{2}(p_{0}, p_{1}) = \sum_{i} (N_{i}^{pred}(p_{0}, p_{1}) - N_{i})^{2}$$
$$\chi^{2}_{Pearson}(p_{0}, p_{1}) = \sum_{i} \left(\frac{N_{i}^{pred}(p_{0}, p_{1}) - N_{i}}{\sqrt{N_{i}^{pred}(p_{0}, p_{1})}}\right)^{2}$$

$$\chi^{2}_{Neyman}(p_{0}, p_{1}) = \sum_{i} \left(\frac{(N^{pred}_{i}(p_{0}, p_{1}) - N_{i})^{2}}{\sqrt{N_{i}}} \right)^{2}$$








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- Doing a fit is always possible. Is the result statisfying? \rightarrow goodness-of-fit is possible to evaluate since χ^2 PDF is known

The basics of goodness-of-fit



 $\chi^2_{min} = 6.7$ with 10 data points $(nDoF = 10) \rightarrow$ blue PDF tells us this is a good fit, even if not a point is on the line.

We can actually compute the fraction of pseudo-data that would lead to a higher χ^2 (*p*-value), to quantify this statement.

1. Perform a fit of an histogram in ROOT, with quite wide binning. Do you recover the true value? Does the result depends on the number of bins? How to solve it?

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2. Imagine you have one dataset, but you want to fit simultaneously two distributions of these events. How to write the χ^2 ?



Confidence interval and level $\mu \in [\mu_{\min}, \mu_{\max}] @ \alpha CL$

- \equiv the true value is in $[\mu_{min}, \mu_{max}]$ in α % of all possible realisations
- $\mu_{min} (\mu_{max})$ is the lower (upper) bound
- α is the confidence level
- μ_{min} and μ_{max} are random variables (as μ_{hat}): fluctuate with data

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n is called "number of σ " and $\alpha(n)$ is known for a normal PDF:

- $\alpha(1) = 68\%$
- α(1.64) = 90%
- $\alpha(1.95) = 95\%$
- α(2) = 95.4%
- α(3) = 99.7%
- α(5) = 99.99994%

Quality of a given confidence interval

- Cl \equiv random variable: consider the limit of ∞ number of meas.
- Coverage \equiv probability *P* that the true parameter *actually is* in C
- "Confidence level = what we target" while "coverage = what we get"

The 3 cases

- **1.** $P = \alpha$: perfect coverage \rightarrow ideal
- **2.** $P > \alpha$: over-coverage \rightarrow acceptable (conservative conclusions)
- **3.** $P < \alpha$: under-coverage \rightarrow dangerous (agressive conclusions)

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In practice: estimating coverage can be done using toys experiment (CPU-intensive for realistic models).

Example: binomial distribution, with parameter of interest *p*

$$P(k; N, p) = \binom{N}{k} p^{k} (1-p)^{N-k}$$

$$\hat{p} = \frac{k}{N}$$

$$p \in \left[\hat{p} - d\sqrt{\frac{\hat{p}(1-\hat{p})}{N}}; \hat{p} + d\sqrt{\frac{\hat{p}(1-\hat{p})}{N}}\right] \quad (Wald interval)$$

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Take away messages:

- notation $\mu = X_{-Z}^{+Y}$ (assuming 68% C.L.) is sometimes only indicative
- only object which contains the full information is likelihood
- OK to manipulate these approximate quanties just know what they are(n't)

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• Replace $\mathbb{E}[\mu]$ by the mode, or the median ...





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- frequentist pprox bayesien with flat prior (numbers are = but meaning is eq)
- questions: (1) why there is no coverage in bayesian?(2) Why the 3 properties of frequentist estimator are defined in baysien?

Frequentist approach imagine you measure energy response r_E of a detector using a dedicated data d_E

- this measure is described by a likelihood $\mathcal{L}_{energy}(r_E, d_E)$
- the parameter of interest will be better known with more data
- this unknown can be added to the stat model using the full likelihood

$$\mathcal{L}(\mu, r_E; data, d_E) = \mathcal{L}(\mu,; data) \mathcal{L}_{energy}(r_E, d_E)$$

- this is notion of auxiliary measurement.
- $\mathcal{L}_{energy}(r_E, d_E)$ is usally too complex to be implemented.
- One uses its approximation (Taylor Expension of order 2 of NLL around the min, leading to a gaussian likelihood)

Bayesian approach imagine you have a calculation with some approximations, to which an uncertainty is associated.

- this uncertainty is closer to a degree of beleif
- a prior $\pi(\theta)$ is required to quantify, were the true value of θ is more likely to be
- this unknown can be added to the stat model using the full likelihood

$$\mathcal{L}(\mu, heta; data) = \mathcal{L}(\mu, ; data) \pi(heta)$$

• this final likelihood is marginalized over θ :

$$\mathcal{L}_m(\mu; \textit{data}) = \int \mathcal{L}(\mu, heta; \textit{data}) \, \pi(heta) \mathrm{d} heta$$

• Interpretation: average all possible situations (defined by a θ value), accounting for the probability to actually have this value

Coming back to model uncertainties - III



Example of marginalization

Coming back to model uncertainties - III



Example of marginalization

What's the proper way to implement uncertainties?

- no absolute answer to this question ightarrow arbitrariness
- make your choice depending on the context (ease interpretation or calculation, or ...?)
- always check the robustness of your conclusion wrt these choices
Why it is relevant

Most emblematic question: is there a signal in my data?

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Formalism

- 2 hypothesis: H_1 =there is signal and H_0 : there is no signal
- \rightarrow test statistics $t \equiv$ random variable, discrimating H_1 from H_0

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Most naive approch: event count as test statistics t = N

- e.g. H_1 predicts $N_1 = 110$, while H_0 predicts $N_1 = 100$
- observation $N_{obs} = 112$: do I reject the signal hypothesis?
- Steps of test hypothesis
 - find distribution of t in both hypothesis $f(t|H_0)$ and $f(t|H_1)$
 - check where t_{obs} fall wrt to $f(t|H_0)$ and $f(t|H_1)$
 - conclude with a confidence level (p-value)





Quantitative agreement with an hypothsis: p-value

p-value = probability to observe what you observed in measurement or "more extreme" values

How to find exclusion limit



 \rightarrow Increase the signal until the signal hypothesis get rejected (at a given confidence level).



Egon Pearson



Jerzy Neyman

Pearson-Neyman Lemma (1933)

• the most powerful statistical test is Negative Log Likelihood ratio

$$NLL \equiv -2\log rac{\mathcal{L}(H_1|data)}{\mathcal{L}(H_0|data)}$$



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- \rightarrow this always turns any *n*-dim problem into a 1-dim problem *e.g.* imagine you have two event counts (N_1, N_2) , instead of one N



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- → this always turns any *n*-dim problem into a 1-dim problem *e.g.* imagine you have two event counts (N_1, N_2) , instead of one N In practice: hunders or thousands of event counts!

Part I: statistics

descriptive statistics - sample - mean - (co)variance - (de)correlation

Part II: probability

Bias theorem – prior – posterior – random variable – (marginal) PDF – moments – caracteristic function – (in)dependent variables – CLT – error propagation

Part III: statistical model

Likelihood – nuisance parameter – parameter of interest – systematic uncertainties

Part IV: The two big school

Frequentist – occurence frequency – pseudo-data (toys) – bayesian – degree of belief

Part VI: Parameter estimation & hypothesis testing

estimator and its properties – χ^2 – confidence/credibility level/interval – coverage – p-value – LLR

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1. Statistics \equiv link between measurement and conclusion

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Ernest Rutherford

"If your experiment needs a statistician, you need a better experiment"

Thanks for you attention !