Statistics for HEP

Part 1: Probability and Statistics

Invited lectures, 12th Course on Physics of the LHC
(LIP, Lisboa, Portugal)

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If you are reading this as a web page: have fun! If you are reading this as a PDF: please visit

https://www.hep.uniovi.es/vischia/persistent/2024-03-20-22_StatisticsAtCoursePhysicsLHC_vischia_part1.html

to get the version with working animations

Lecture 1

Probability and statistics

Practicalities

- Significantly restructured with respect to the past years
  - Lecture 1: Probability and Statistics (minus hypothesis testing)
  - Lecture 2: Machine Learning (and hypothesis testing)
- More detailed material in my twenty-hours intensive course
  - It may be useful if you tried out the exercises, at your pace!
- Many references here and there, and in the last slide
  - Try to read some of the referenced papers!
  - Unreferenced stuff copyrighted P. Vischia for inclusion in my (finally) upcoming textbook

Statistics answers questions

The quality of the answer depends on the quality of the question

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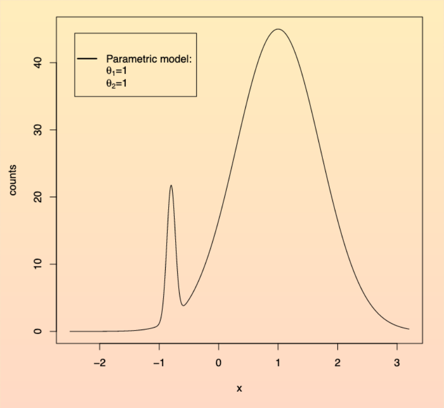
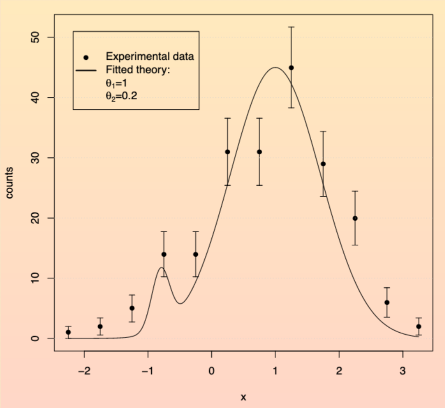
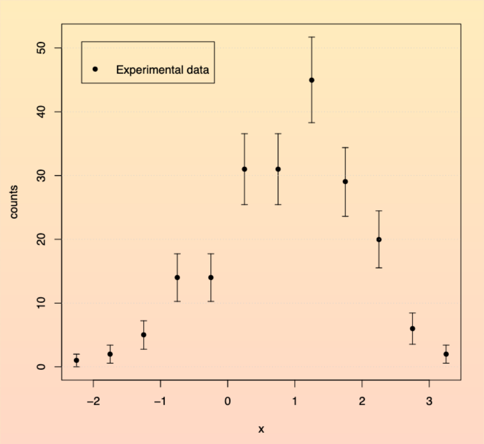
Image by ``The Tiger Lillies''

...in a mathematical way

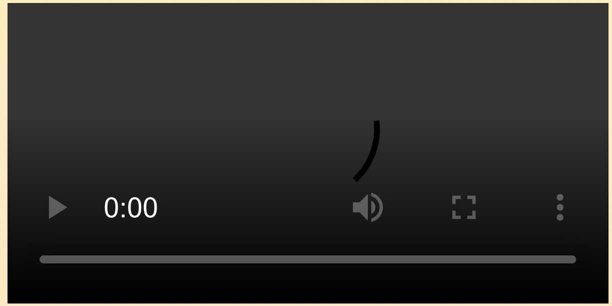
- Theory
  - Approximations
  - Free parameters
- Statistics
  - Estimate parameters
  - Quantify uncertainty
  - Test theories
- Experiment
  - Random fluctuations
  - Mismeasurements (detector effects, etc)







Why does Statistics work?



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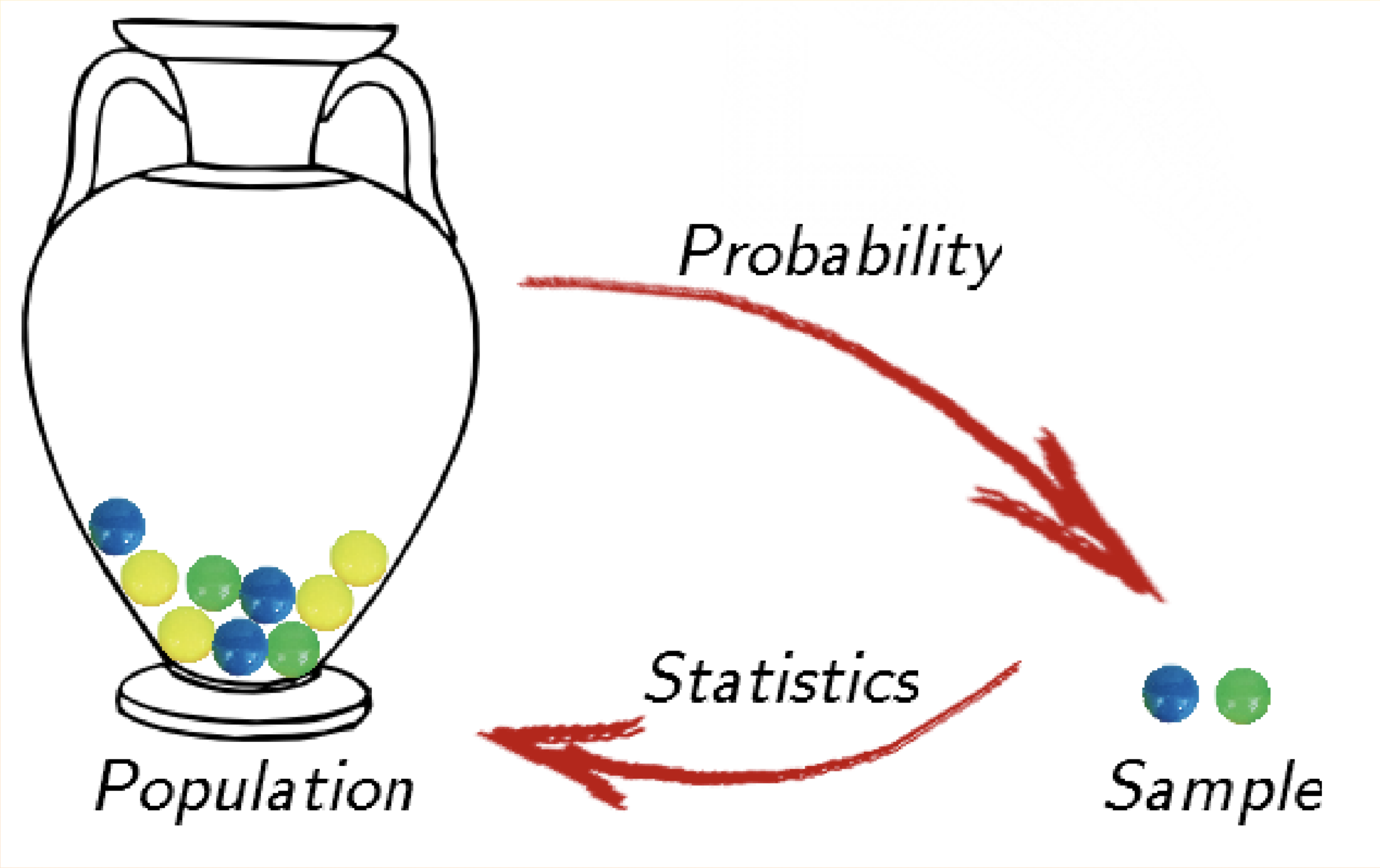
Thomas Garrity, video from YouTube

Probability and Statistics



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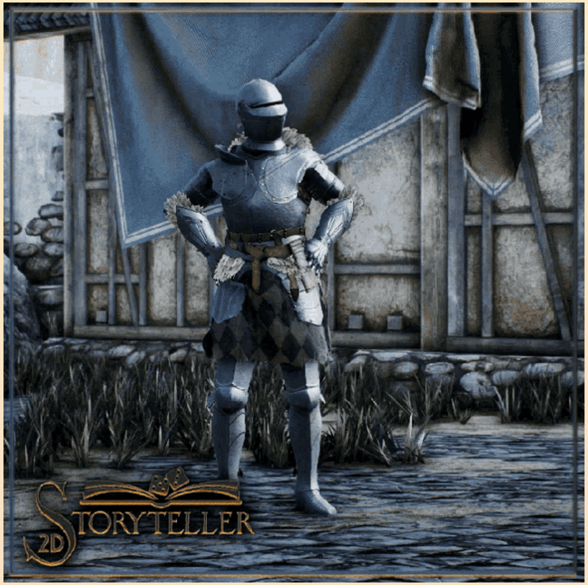
Picture by Rob Hall

Random Experiments

- A well-defined procedure that produces an observable outcome x that is not perfectly known

- S is the set of all possible outcomes
- S must be simple enough that we can tell whether $x \in S$ or not
- If we obtain the outcome x, then we say the event defined by $x \in S$ has occurred



- Repetitions of the experiment must happen under uniform conditions

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GIF from Tenor.com

Axiomatic definition of probability (Kolmogorov)

- $(\Omega, \mathcal{F}, P)$: measure space
  - a set Ω with associated field (σ-algebra) $\mathcal{F}$ and measure P
  - Define a random event $A \in \mathcal{F}$ (A is a subset of Ω)

then:

1. The probability of A is a real number $P(A) \geq 0$
2. If $A \cap B = \emptyset$, then $P(A+B) = P(A) + P(B)$
3. $P(\Omega) = 1$ (probability measures are finite)

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Image from Wikipedia, I think

Axiomatic definition for propositions (Cox and Jaynes)

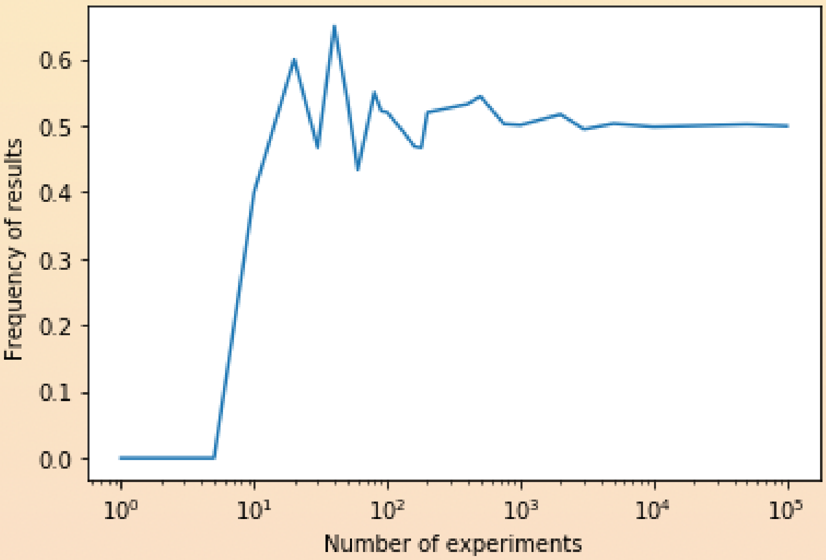
- Cox, 1946: start from reasonable premises about propositions
  - $A|B$ is the plausibility of the proposition A given a related proposition B
  - $\sim A$ the proposition $not - A$, i.e. answering "no" to "is A wholly true?"
  - $F(x,y)$ is a function of two variables
  - $S(x)$ a function of one variable
- Two postulates concerning propositions
  - $C \cdot B|A = F(C|B \cdot A, B|A)$
  - $\sim V|A = S(B|A)$, i.e. $(B|A)^m + (\sim B|A)^m = 1$
- Jaynes demonstrated that these axioms are formally equivalent to the Kolmogorov ones
  - Continuity as infinite states of knowledge rather than infinite subsets

Frequentist realization

- Repeat an experiment N times, obtain n times the outcome X
- Probability as empirical limit

$$P(X) = \lim_{N \to \infty} \frac{n}{N}$$

Hand	Distinct Hands	Frequency	Probability	Cumulative probability	Odds	Mathematical expression of absolute frequency
Royal flush	1	4	0.000154%	0.000154%	649,739 : 1	$\binom{4}{1}$
Straight flush (excluding royal flush)	9	36	0.00139%	0.0014%	72,192 : 1	$\binom{10}{1}\binom{4}{1} - \binom{4}{1}$
Four of a kind	156	624	0.0240%	0.0256%	4,164 : 1	$\binom{13}{1}\binom{12}{1}\binom{4}{1}$
Full house	156	3,744	0.1441%	0.17%	693 : 1	$\binom{13}{1}\binom{4}{3}\binom{12}{1}\binom{4}{2}$
Flush (excluding royal flush and straight flush)	1,277	5,108	0.1965%	0.367%	508 : 1	$\binom{13}{5}\binom{4}{1} - \binom{10}{1}\binom{4}{1}$
Straight (excluding royal flush and straight flush)	10	10,200	0.3925%	0.76%	254 : 1	$\binom{10}{1}\binom{4}{1}^5 - \binom{10}{1}\binom{4}{1}$
Three of a kind	858	54,912	2.1128%	2.87%	46.3 : 1	$\binom{13}{1}\binom{4}{3}\binom{12}{2}\binom{4}{1}^2$
Two pair	858	123,552	4.7539%	7.62%	20.0 : 1	$\binom{13}{2}\binom{4}{2}^2\binom{11}{1}\binom{4}{1}$
One pair	2,860	1,098,240	42.2569%	49.9%	1.37 : 1	$\binom{13}{1}\binom{4}{2}\binom{12}{3}\binom{4}{1}^3$
No pair / High card	1,277	1,302,540	50.1177%	100%	0.995 : 1	$\left[\binom{13}{5} - 10\right]\left[\binom{4}{1}^5 - 4\right]$
Total	7,462	2,598,960	100%	—	0 : 1	$\binom{52}{5}$



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Left: lost the reference, if you have info please let me know!. Right: P. Vischia

Subjective ("Bayesian") realization

- $P(X)$ is the subjective degree of belief in the outcome of a random experiment (in X being true)
  - Update your degree of belief after an experiment
- De Finetti: operative definition, based on the concept of coherent bet
  - Assume that if you bet on X, you win a fixed amount of money if X happens, and nothing (0) if X does not happen

$$P(X) := \frac{\text{The largest amount you are willing to bet}}{\text{The amount you stand to win}}$$

- Coherence is when the bet is fair, i.e. it doesn't guarantee an average profit/loss

Dutch book

Book	Odds	Probability	Bet	Payout
Trump elected	Even (1 to 1)	$1/(1+1) = 0.5$	20	$20+20=40$
Clinton elected	3 to 1	$1/(1+3) = 0.25$	10	$10+30=40$
All outcomes	---	$0.5+0.25=0.75$	30	40

Game Theory

- Outcomes are 1s and 0s
- $P(A)$ = $\{\text{stake Skeptic needs to get 1 if A happens, 0 otherwise}\}$
- Forecaster offers bets (bookie, statistical model)
- Skeptic chooses bet
- Reality announces outcomes

Skeptic announces $\mathcal{K}_0 \in \mathbb{R}$.
FOR $n = 1, 2, \ldots$:
  Forecaster announces $p_n \in [0, 1]$.
  Skeptic announces $L_n \in \mathbb{R}$.
  Reality announces $y_n \in \{0, 1\}$.
  $\mathcal{K}_n := \mathcal{K}_{n-1} + L_n(y_n - p_n)$.

$$\mathbb{P}\left(\frac{\sum_{i=1}^{n}(y_i - p_i)}{n} \to 0\right) = 1$$

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Figure by Glenn Shafer

Random variables...

- Numeric label for each element in the space of possible outcomes
  - In Physics, we usually assume Nature is continuous, and discreteness comes from our experimental limitations
- Work with probability density functions (p.d.f.s) normalized with respect to the interval

$$f(X) := \lim_{\Delta X \to 0} \frac{P(X)}{\Delta X}$$

$$P(a < X < b) := \int_a^b f(X) dX$$

... in many dimensions

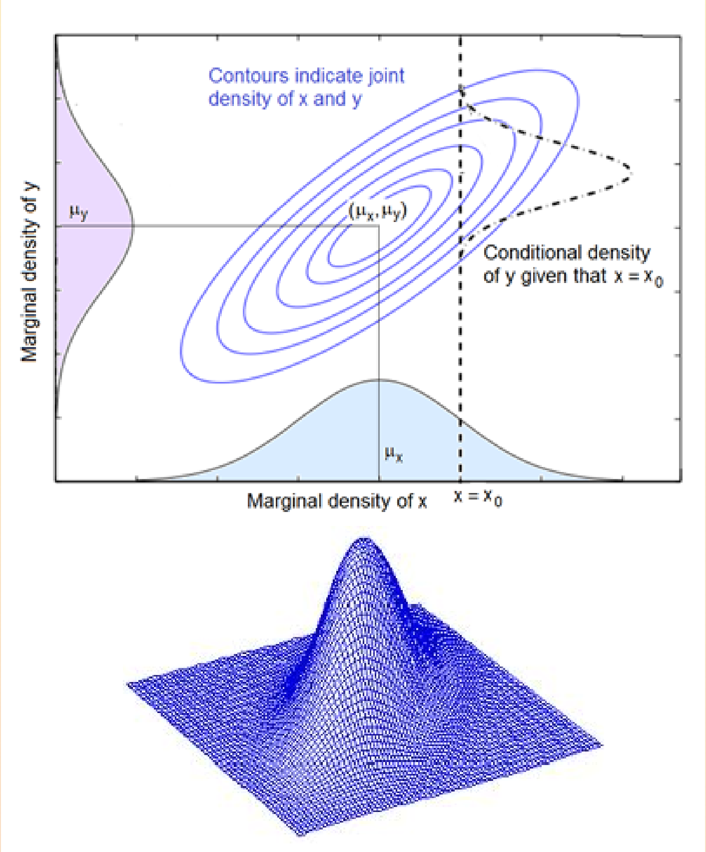
- Joint pdf for many variables: $f(X, Y, ...)$

- Marginal pdf
  integrate over the uninteresting variables

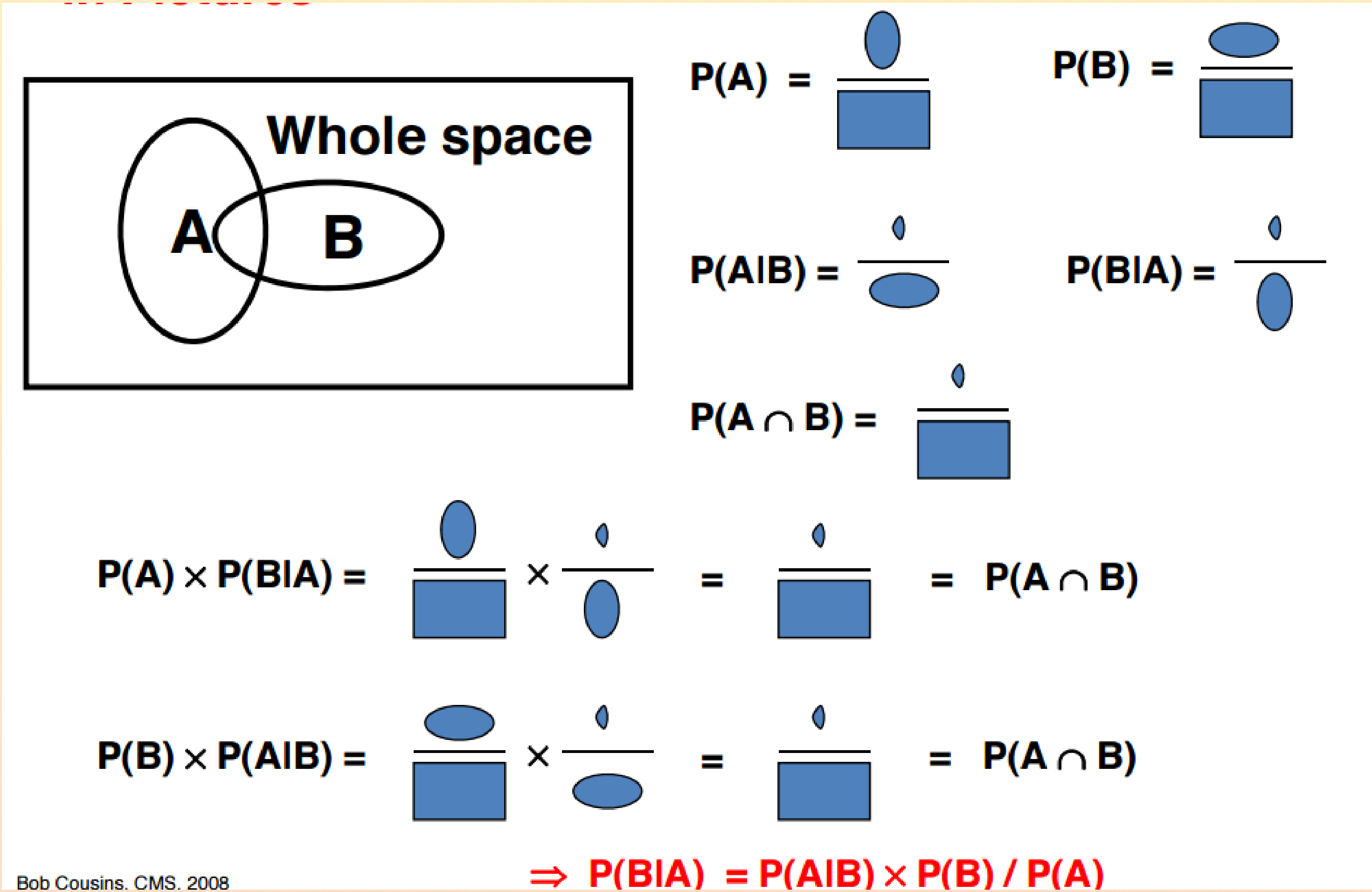
$$f_X(X) := \int f(X, Y) dY$$

- Conditional pdf
  fix the value of the uninteresting variables

$$f(X|Y) := \frac{f(X,Y)}{f_Y(Y)}$$



Bayes Theorem



- Venn diagrams were also the basis of Kolmogorov approach (Jaynes, 2003)

Diagram by Cousins, 2008 and 2018

Independence

- Two events A and B are independent if $P(AB) = P(A)P(B)$
  - Can be assumed (e.g. assume that coin tosses are independent)
  - Can be derived (verifying that equality holds)
  - E.g. if $A = \{2, 4, 6\}$, $B = \{1, 2, 3, 4\}$, we have $P(AB) = 1/3 = P(A)P(B)$
- Two disjoint outcomes with positive probability cannot be independent

$$P(AB) = P(\emptyset) = 0 \neq P(A)P(B) > 0$$

Law of Total Probability

- Bayes theorem is valid for any probability measure

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

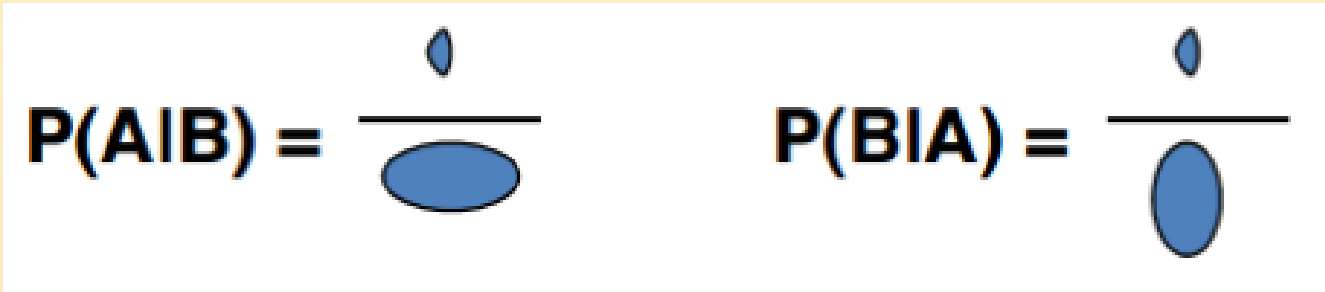
- Useful decomposition by partitioning S in disjoint sets A_i
  - $\cap A_i A_j = 0 \qquad \forall i, j$
  - $\cup_i A_i = S$

$$P(B) = \sum_i P(B \cap A_i) = \sum_i P(B|A_i)P(A_i)$$

- The Bayes theorem becomes

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

A Word of Advice



$$P(A|B) \neq P(B|A)$$

- $P(have\,TOEFL|speak\;English)$ is very small, say $<< 1\%$
- $P(speak\;English|have\,TOEFL)$, is (hopefully) $\sim 100\%$

Another Word of Advice

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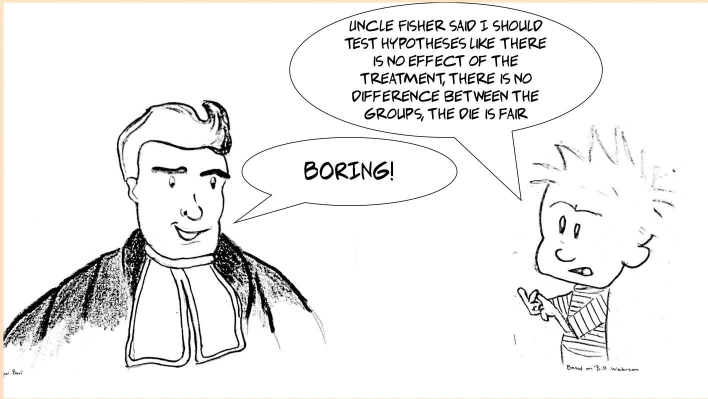
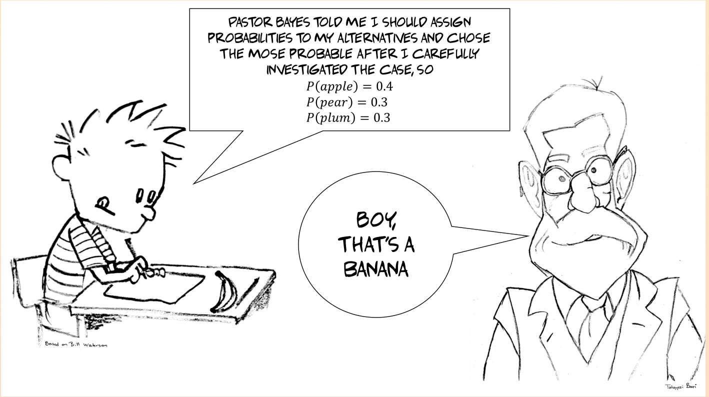
Image from r/dataisugly

P(outcome), P(hypothesis)

- Frequentist probability (Fisher) always refers to outcomes in repeated experiments
  - $P(hypothesis)$ is undefined
  - Criticism: statistical procedures rely on complicated constructions (pseudodata from hypotetical experiments)
- Bayesian probability assigns probabilities also to hypotheses
  - Statistical procedures intrinsically simpler
  - Criticism: subjectivity





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Images by Tolqyesi Bori

Intrinsically different statements

- The probability for the hypothesis to be true, given the observed data I collected, is 80%
- The probability that, when sampling many times from the hypothesis, I would obtain pseudodata similar to the data I have observed is 80%

Some history

- Bayes' 1763 (posthumous) article explains the theorem in a game of pool
- A full system for subjective probabilities was (likely independently) developed and used by Laplace
- Laplace in a sense is the actual father of Bayesian statistics

Stigler (1996) and McGrayne (2011)

The Obligatory COVID-19 slide

- Mortal disease
  - D: the patient is diseased (sick)
  - H: the patient is healthy
- Diagnostic test
  - $+$: the patient flags positive to the disease
  - $-$: the patient flags negative to the disease
- A very good test
  - $P(+|D) = 0.99$
  - $P(+|H) = 0.01$
- You take the test and you flag positive: do you have the disease?

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$$P(D|+) = \frac{P(+|D)P(D)}{P(+)} = \frac{P(+|D)P(D)}{P(+|D)P(D)+P(+|H)P(H)}$$

- We need the incidence of the disease in the population, $P(D)$!
  - $P(D) = 0.001$ (very rare disease): then $P(D|+) = 0.0902$, which is fairly small
  - $P(D) = 0.01$ (only a factor 10 more likely): then $P(D|+) = 0.50$, which is pretty high
  - $P(D) = 0.1$: then $P(D|+) = 0.92$, almost certainty!

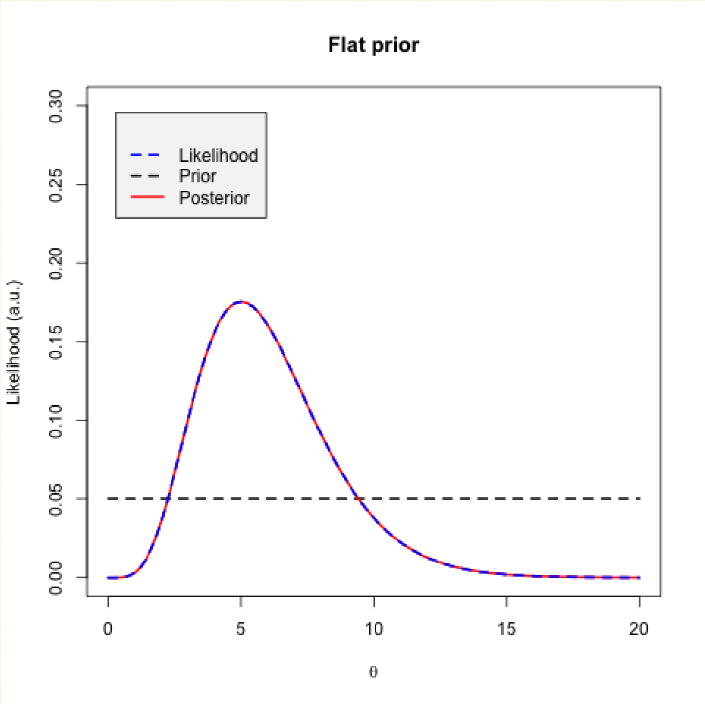
Naming Bayes

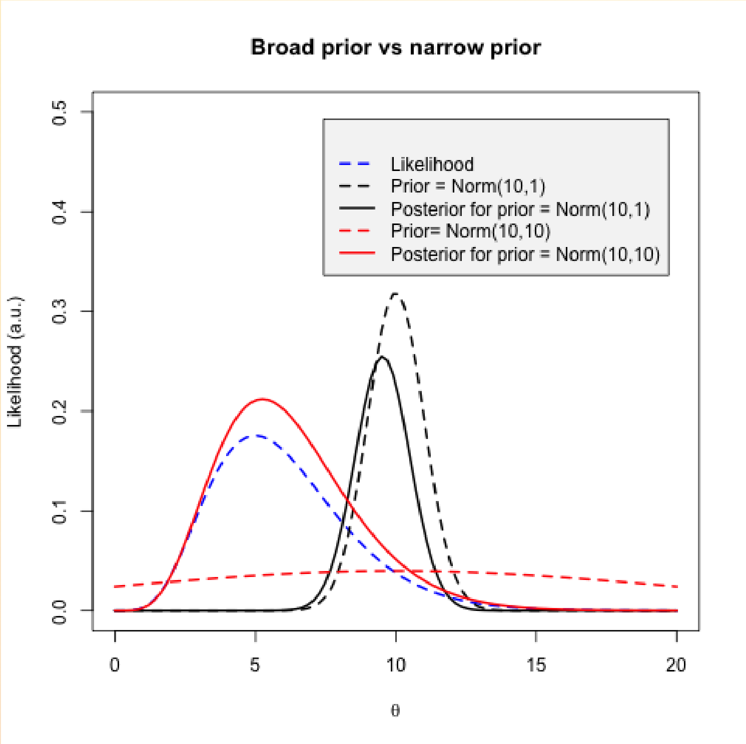
$$P(H|\vec{X}) := \frac{P(\vec{X}|H)\pi(H)}{P(\vec{X})}$$

- $\vec{X}$, the vector of observed data
- $P(\vec{X}|H)$, the likelihood function, encoding the result of the experiment
- $\pi(H)$, the probability we assign to H before the experiment
- $P(\vec{X})$, the probability of the data
  - usually expressed using the law of total probability
    $$\sum_i P(\vec{X}|H_i) = 1$$
  - often omitted when normalization is not important, i.e. searching for mode rather than integral
    $$P(H|\vec{X}) \propto P(\vec{X}|H)\pi(H)$$
- $P(H|\vec{X})$, the posterior probability, after the experiment
  - For a parametric $H(\theta)$, often written $P(\theta)$

Prior, Likelihood, and Posterior

- Likelihood is always the same: usually it is the frequentist answer





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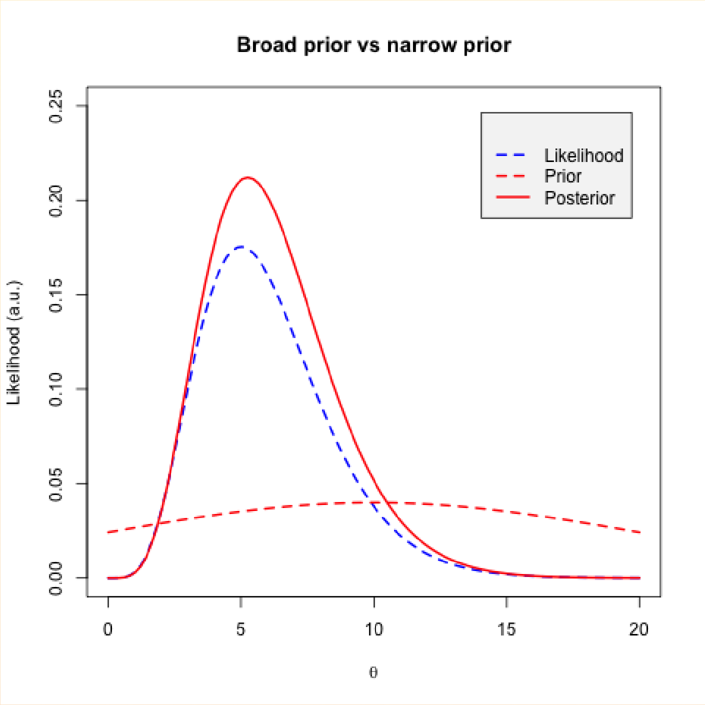
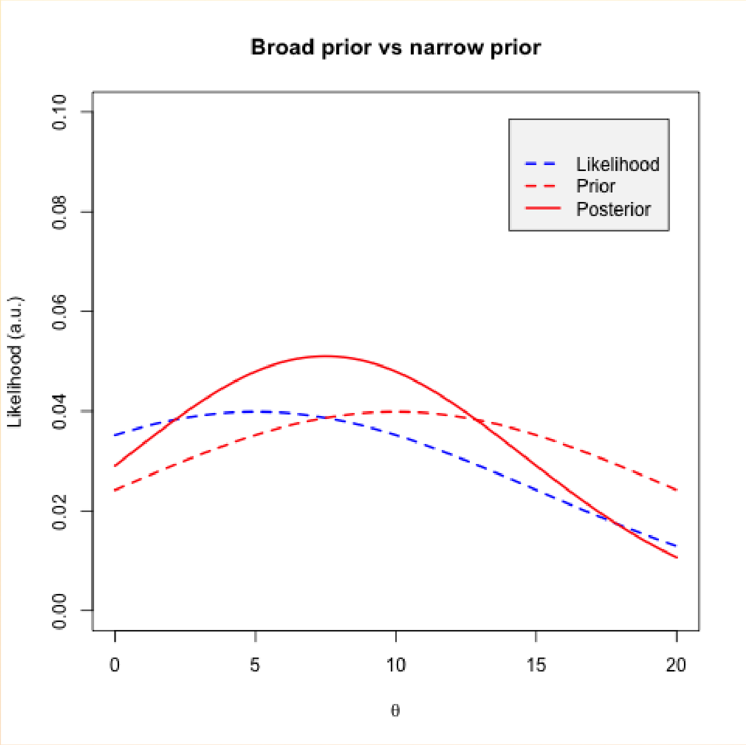
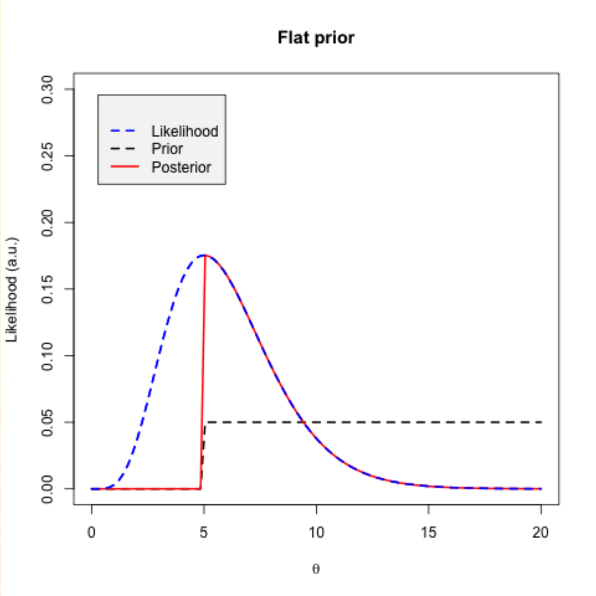




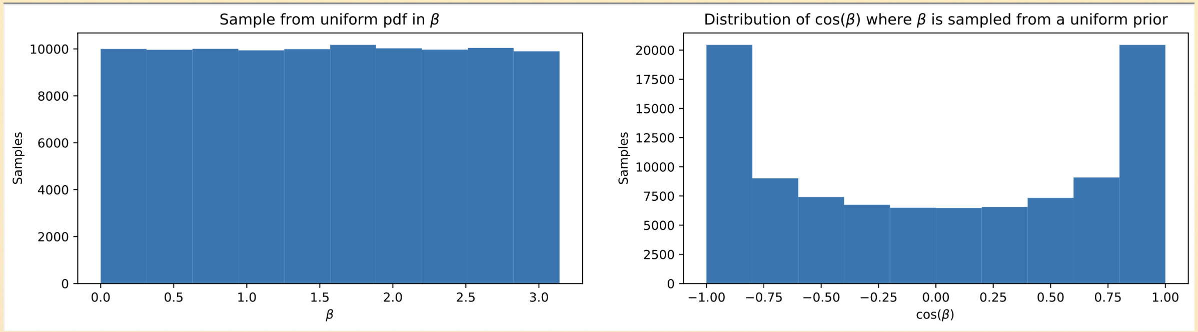
Priors to represent boundaries

- Can encode physical boundaries in the model
  - positivity of the mass of a particle
  - cross section is positive definite
- Strong assumptions on the model can hide weaknesses or anomalies
  - a transition probability such as V_{tb} is defined in $[0, 1]$ only if you assume the standard model



Representing ignorance

- Ignorance depends on the parameterization



- Elicitation of expert opinion

- *Jeffreys priors*
    - *Compute* information *on the parameter*
    - *Find a parameterization that keeps it constant*

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Figure on expert elicitation from Mikkola (2021)

Information (Fisher)

- Information should increase with the number of observations
  - 2x data, 2x information (if data are independent)
- Information should be conditional on the hypothesis we are studying
  - $I = I(\theta)$, irrelevant data should carry zero information on θ
- Information should be related to precision
  - Larger information should lead to better precision
- Formal equivalence with other definitions (e.g. Shannon)

The Likelihood Principle

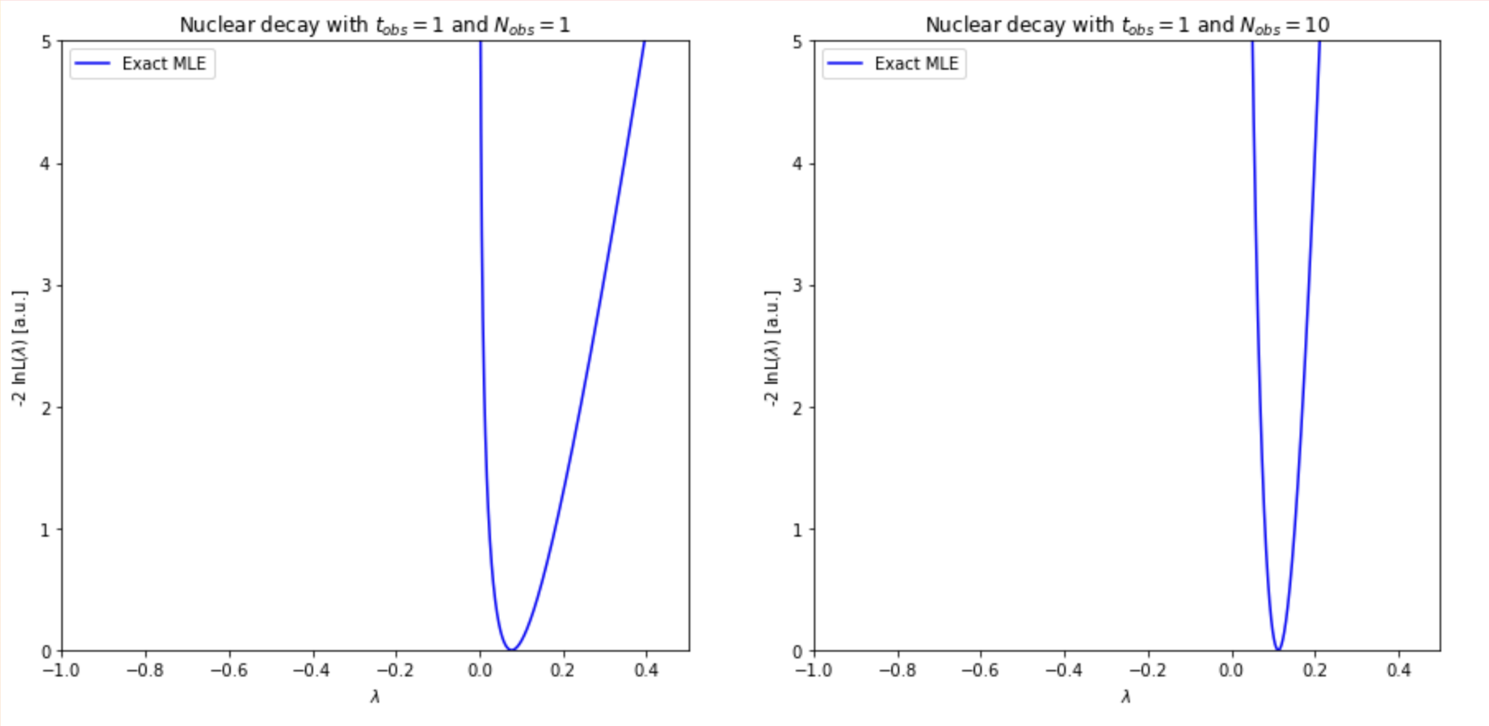
- Data sample $\vec{x}_{obs}$

$$\mathcal{L}(\vec{x};\theta) = P(\vec{x}|\theta)|_{\vec{x}obs}$$

- The likelihood function $L(\vec{x};\theta)$ contains all the information available in the data sample relevant for the estimation of θ
    - Automatically satisfied by Bayesian statistics: $P(\theta|\vec{x}) \propto L(\vec{x};\theta) \times \pi(\theta)$
    - Frequentist typically make inference in terms of hypothetical data (likelihood not the only source of information)
- Does randomness arise from our imperfect knowledge or is it an intrinsic property of Nature?

Likelihood and Fisher Information

- Define Fisher information via the curvature of the likelihood function, $\frac{\partial^2 \mathcal{L}(X;\theta)}{\partial\theta^2}$
  - Larger when there are more data
  - Conditional on the parameter studied
  - Larger when the spread is smaller (larger precision)



More formally...

- Score: $S(X;\theta) = \frac{\partial}{\partial\theta} lnL(X;\theta)$
- Fisher information as variance of the score

$$I(\theta) = E\left[\left(\frac{\partial}{\partial\theta} lnL(X;\theta)\right)^2 |\theta_{true}\right] = \int \left(\frac{\partial}{\partial\theta} lnf(x|\theta)\right)^2 f(x|\theta)dx \geq 0$$

- Under some regularity conditions (twice differentiability, differentiability of integral, support indep. on θ)

$$I(\theta) = -E\left[\left(\frac{\partial^2}{\partial\theta^2} lnL(X;\theta)\right)^2 |\theta_{true}\right]$$

Jeffreys Priors and Information

- Reparameterization: $\theta \to \theta'(\theta)$, when $\pi(\theta') := E\left[\left(\frac{\partial lnN}{\partial\theta'}\right)^2\right]$

$$\pi(\theta) = \pi(\theta')\left|\frac{d\theta'}{d\theta}\right| \propto \sqrt{E\left[\left(\frac{\partial lnN}{\partial\theta'}\right)^2\right]\left|\frac{\partial\theta'}{\partial\theta}\right|} = \sqrt{E\left[\left(\frac{\partial lnL}{\partial\theta'}\frac{\partial\theta'}{\partial\theta}\right)^2\right]}$$

$$= \sqrt{E\left[\left(\frac{\partial lnL}{\partial\theta}\right)^2\right]} = \sqrt{I(\theta)}$$

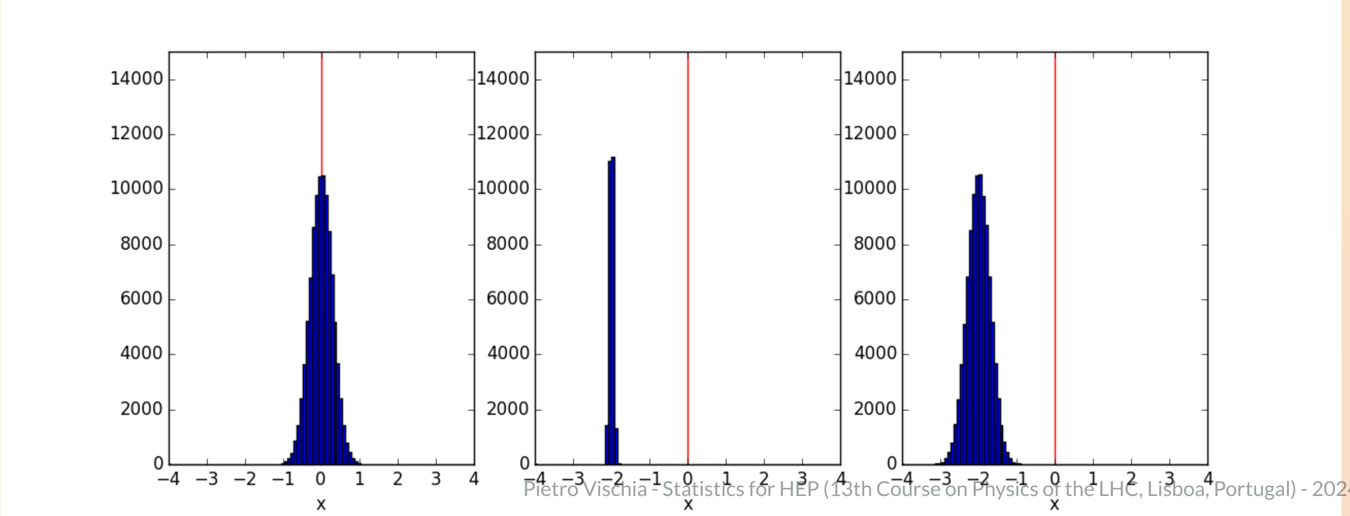
- To keep information constant, define prior via the information
  - Location parameters: uniform prior
  - Scale parameters: prior $\propto \frac{1}{\theta}$
  - Poisson processes: prior $\propto \frac{1}{\sqrt{\theta}}$
- The authors of STAN maintain a nice set of recommendations on priors

Location and Dispersion

- Draw inference on a population using a sample of experiment outcomes
  - Location ("where are most values concentrated at?")
  - Dispersion ("how spread are the values around the center?")

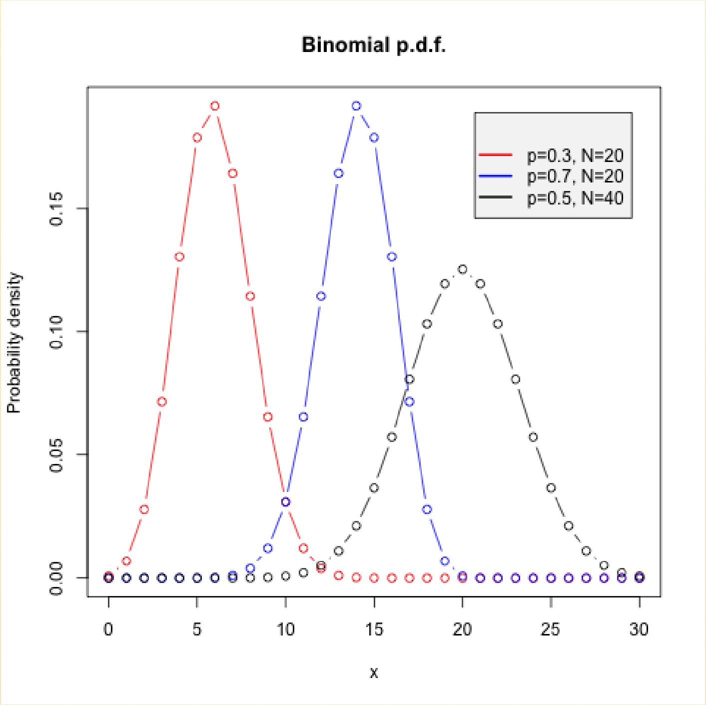
- Types of uncertainty
  - Error: deviation from the true value (bias)
  - Uncertainty: spread of the sampling distribution

- Sources of uncertainty
  - Random ("statistical"): randomness manifests as distribution spread
  - Systematic: wrong measurement manifests as bias



Binomial Distribution

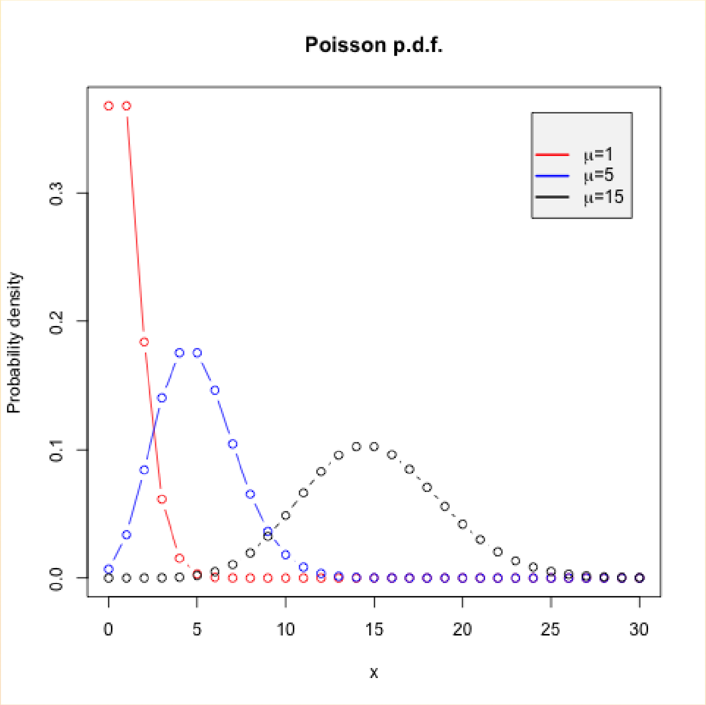
- Discrete variable: r, positive integer $\leq N$
- Parameters:
  - N, positive integer
  - $p, 0 \leq p \leq 1$
- Probability function: $P(r) = \binom{N}{r} p^r (1-p)^{N-r}, r = 0, 1, ..., N$
- $E(r) = Np, V(r) = Np(1-p)$
- Usage: probability of finding exactly r successes in N trials



- The distribution of the number of events in a single bin of a histogram is binomial (if the bin contents are independent)

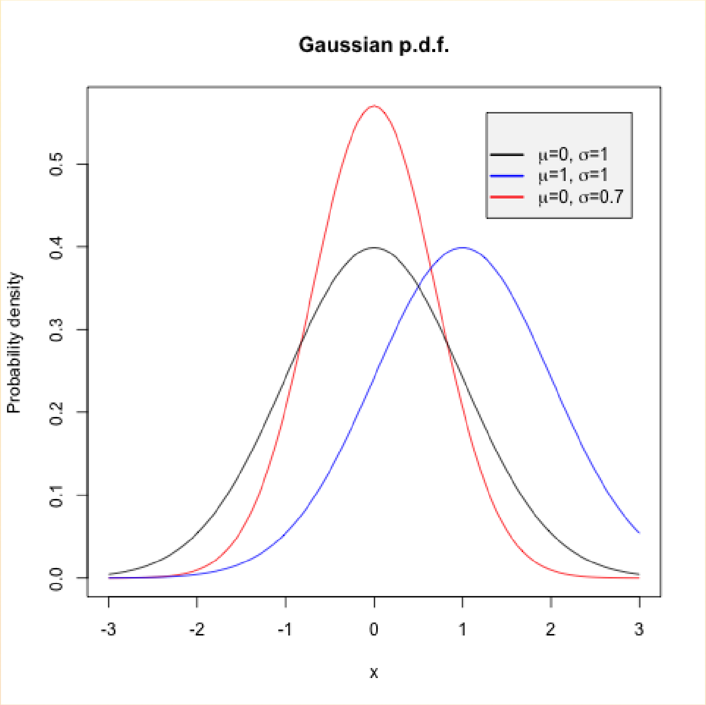
Poisson Distribution

- Discrete variable: r, positive integer
- Parameter: μ, positive real number
- Probability function: $P(r) = \frac{\mu^r e^{-\mu}}{r!}$
- $E(r) = \mu, V(r) = \mu$
- Usage: probability of finding exactly r events in a given amount of time, if events occur at a constant rate.



Gaussian ("Normal") Distribution

- Variable: X, real number
- Parameters:
  - μ, real number
  - σ, positive real number
- Probability function: $f(X) = N(\mu, \sigma^2) = \frac{1}{\sigma\sqrt{2\pi}} exp\Big[- \frac{1}{2}\frac{(X-\mu)^2}{\sigma^2}\Big]$
- $E(X) = \mu$, $V(X) = \sigma^2$
- Usage: describes the distribution of independent random variables. It is also the high-something limit for many other distributions



χ^2 distribution

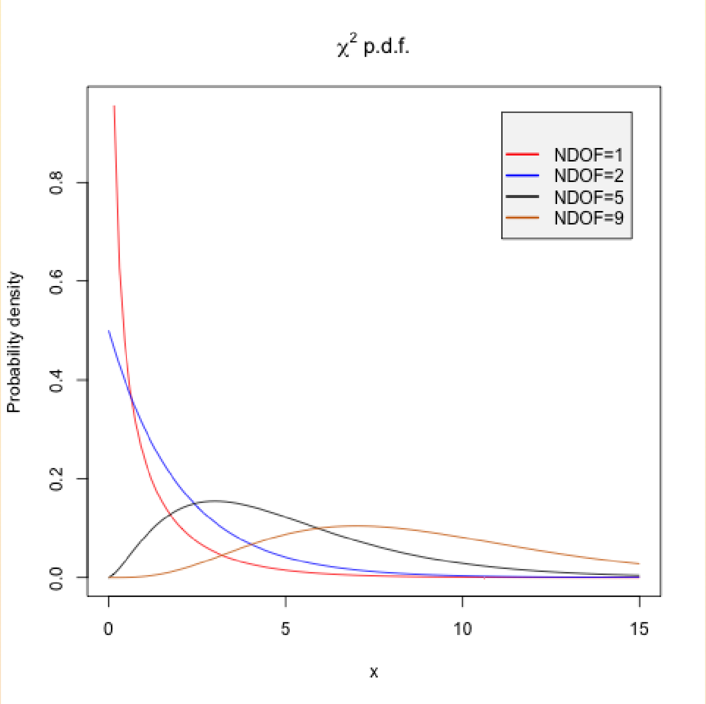
- Parameter: integer $N > 0$ {\em degrees of freedom}
- Continuous variable $X \in \mathcal{R}$
- p.d.f., expected value, variance

$$f(X) = \frac{\frac{1}{2}\left(\frac{X}{2}\right)^{\frac{N}{2}-1} e^{-\frac{X}{2}}}{\Gamma\left(\frac{N}{2}\right)}$$

$$E[r] = N$$

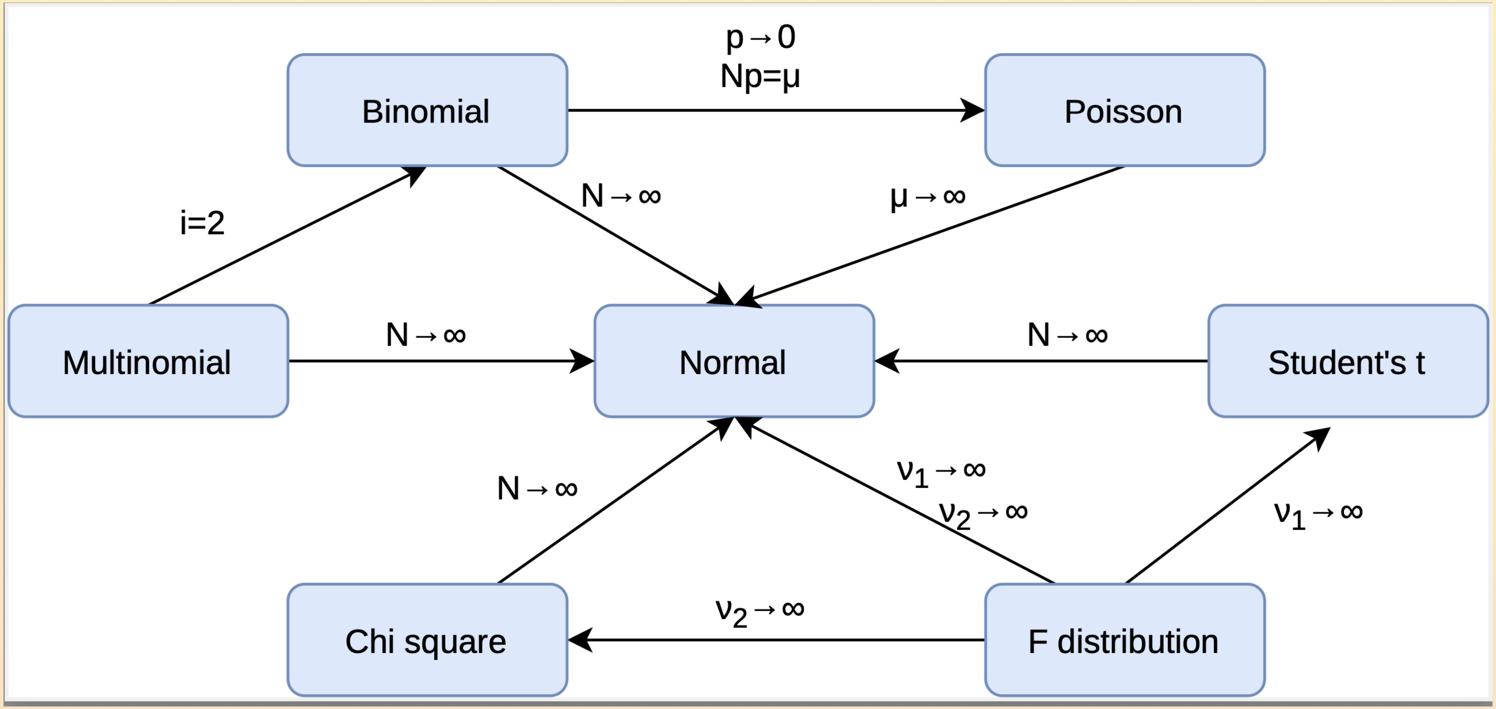
$$V(r) = 2N$$

- It describes the distribution of the sum of the squares of a random variable, $\sum_{i=1}^{N} X_i^2$



- Reminder: $\Gamma() := \frac{N!}{r!(N-r)!}$

Asymptotically



Estimate location and dispersion

- Expected value: $E[X] := \int_\Omega X f(X) dX$ (or $E[X] := \sum_i X_i P(X_i)$ in the discrete case)
    - Extended to generic functions of a random variable: $E[g] := \int_\Omega g(X) f(X) dX$
- Mean of X is $\mu := E[X]$
- Variance of X is $\sigma_X^2 := V(X) := E[(X - \mu)^2] = E[X^2] - (E[X])^2 = E[X^2] - \mu^2$
- Extension to more variables is trivial, and gives rise to the concept of
- Covariance (or error matrix) of two variables: $V_{XY} = E\big[(X - \mu_X)(Y - \mu_Y)\big] = E[XY] - \mu_X \mu_Y = \int XY f(X,Y) dX dY - \mu_X \mu_Y$
    - Symmetric, and $V_{XX} = \sigma_X^2$
    - Correlation coefficient $\rho_{XY} = \frac{V_{XY}}{\sigma_X \sigma_Y}$

Yes...

- ρ_{XY} is related to the angle in a linear regression of X on Y (or viceversa)

From: Glen Cowan, Statistical Data Analysis (OUP 1998)

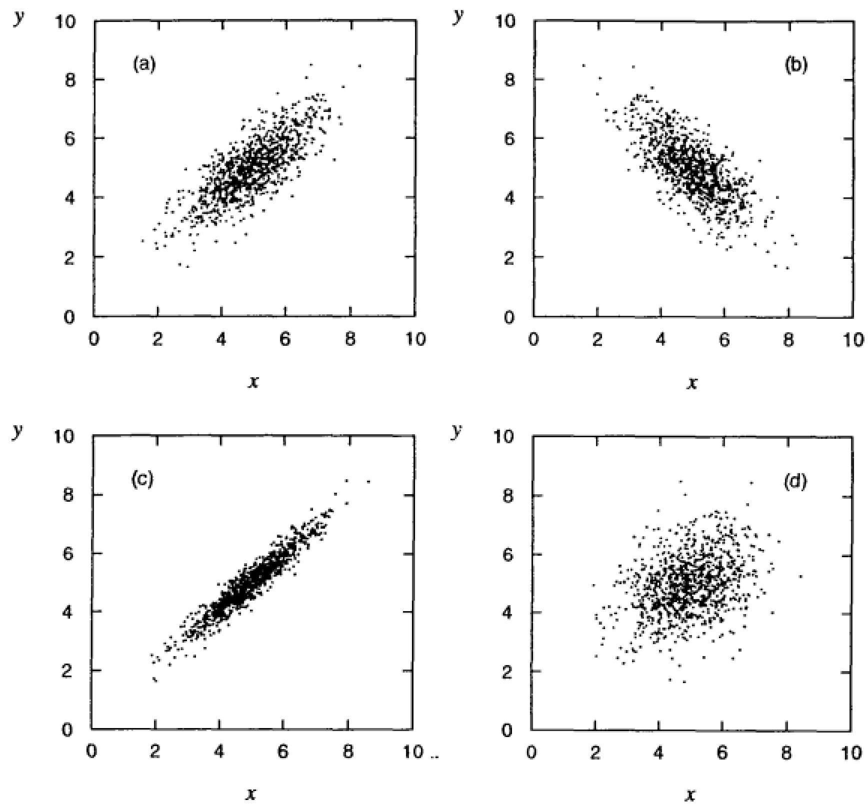
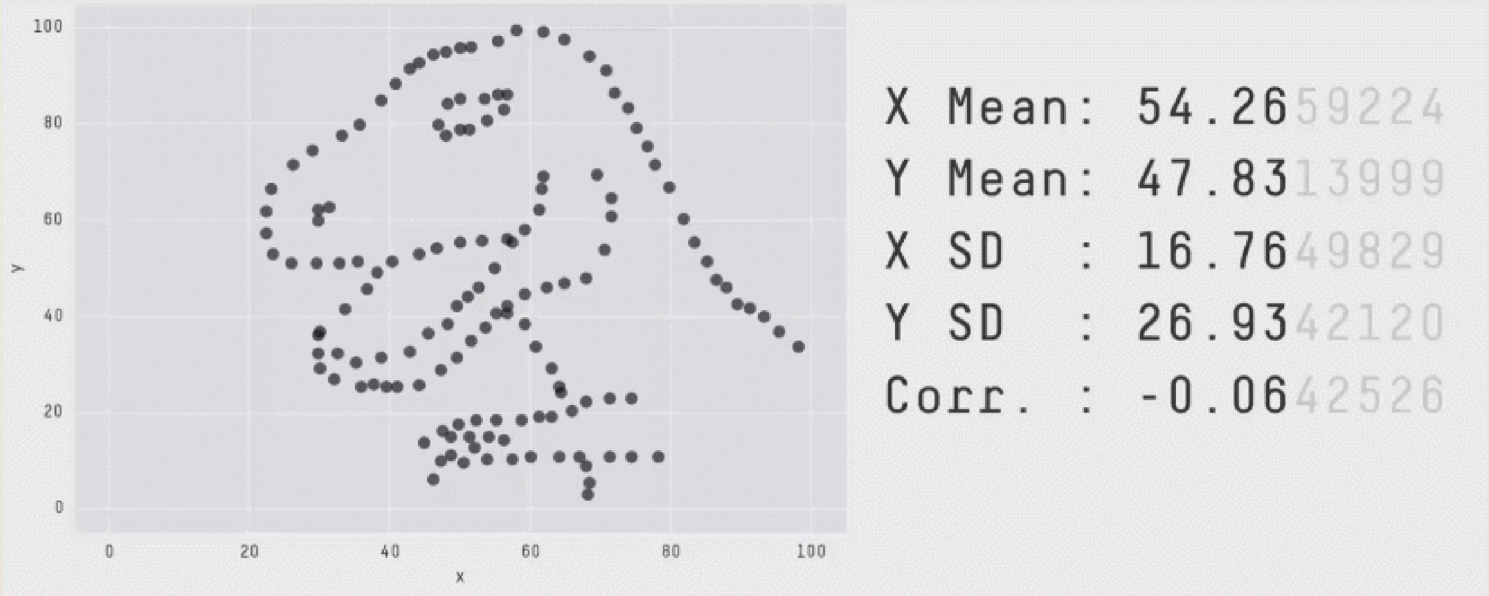


Fig. 1.9 Scatter plots of random variables x and y with (a) a positive correlation, $\rho = 0.75$, (b) a negative correlation, $\rho = -0.75$, (c) $\rho = 0.95$, and (d) $\rho = 0.25$. For all four cases the standard deviations of x and y are $\sigma_x = \sigma_y = 1$.

... but:

- Several nonlinear correlations may yield the same ρ_{XY} (and other summary statistics)



Linear correlation is weak

- X and Y are independent if the occurrence of one does not affect the probability of occurrence of the other
  - X, Y independent $\implies \rho_{XY} = 0$
  - $\rho_{XY} = 0 \not\Rightarrow X, Y$ independent

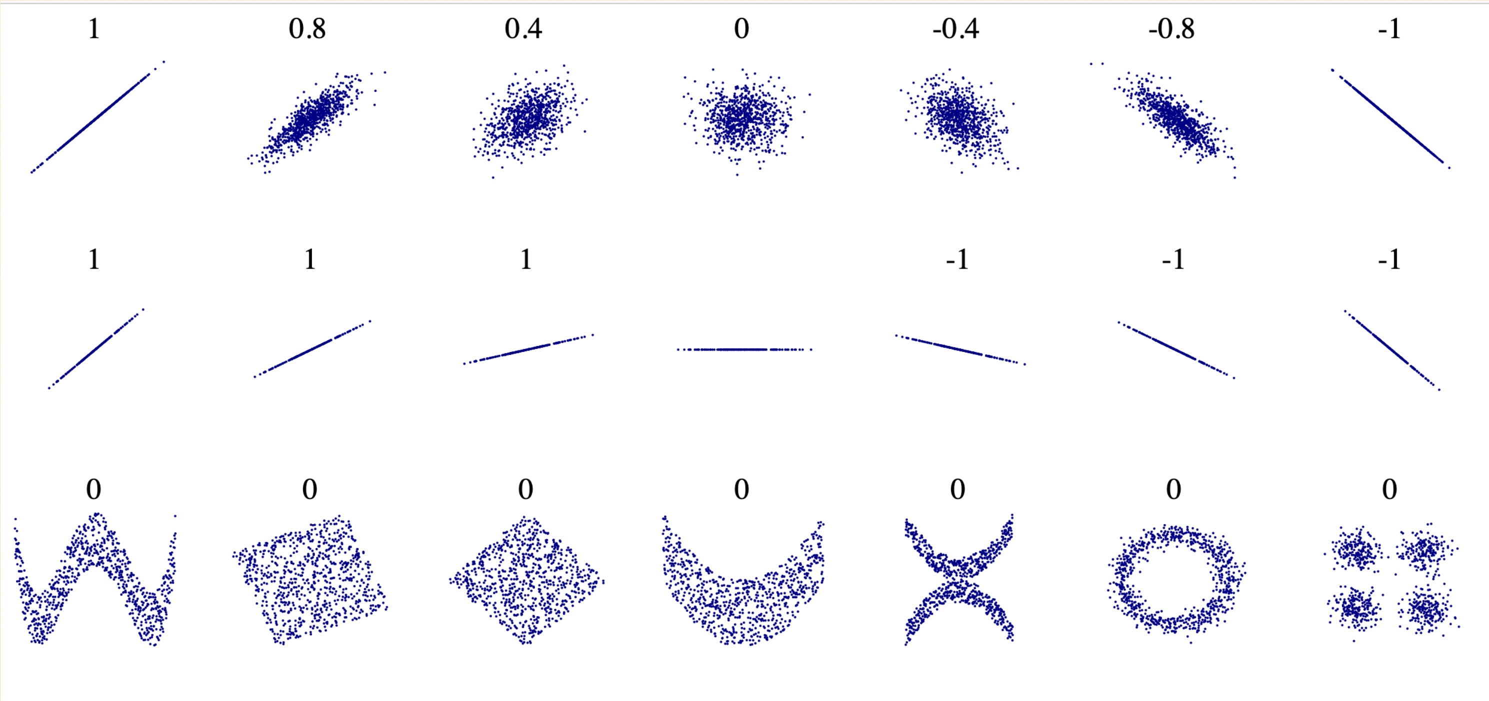


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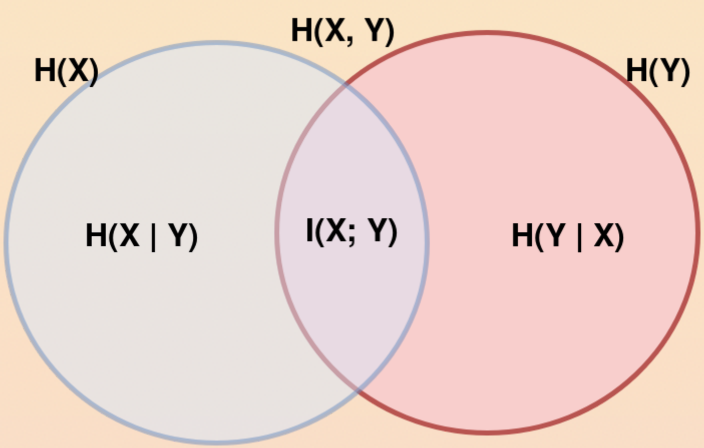
Figure by Denis Boigelot

Mutual information

$$I(X;Y) = \sum_{y\in Y} \sum_{x\in X} p(x,y) log\left(\frac{p(x,y)}{p_1(x)p_2(y)}\right)$$

- General notion of correlation linked to the information that X and Y share
  - Symmetric: $I(X;Y) = I(Y;X)$
  - $I(X;Y) = 0$ if and only if X and Y are totally independent

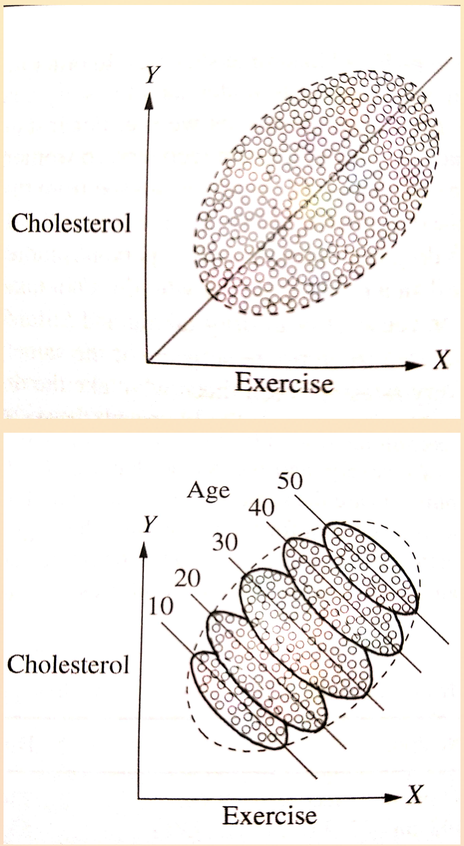


- Related to entropy

$$\begin{aligned} I(X;Y) &= H(X) - H(X|Y) \\ &= H(Y) - H(Y|X) \\ &= H(X) + H(Y) - H(X,Y) \end{aligned}$$

Causal inference

- Disentangle with interventions on Directed Acyclic Graphs



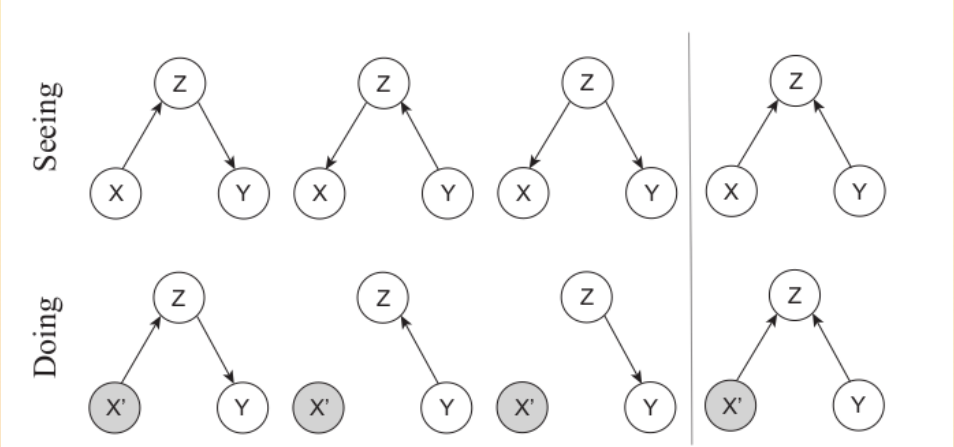


Figure 6. Seeing: DAGs are used to encode conditional independencies. The first three DAGs encode the same associations. *Doing*: DAGs are causal. All of them encode distinct causal assumptions.

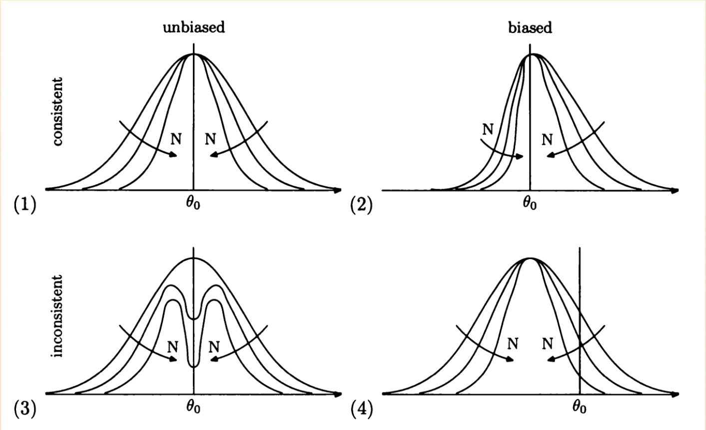
—

Left: From Pearl and Glymour (2106). Right: Dablander (2019)

Estimators

- $x = (x_1, ..., x_N)$ of N statistically independent observations $x_i \sim f(x)$
  - Determine some parameter θ of $f(x)$
  - x, θ in general are vectors
- Estimator is a function of the observed data that returns numerical values $\hat{\theta}$ for the vector θ.

- (Asymptotic) Consistency: $\lim_{N\to\infty} \hat{\theta} = \theta_{true}$
- Unbiasedness: the bias is zero
  - Bias: $b := E[\hat{\theta}] - \theta_{true}$
  - If bias known: $\hat{\theta}' = \hat{\theta} - b$, so $b' = 0$
- Efficiency: smallest possible $V[\hat{\theta}]$



- Robustness: insensitivity from small deviations from the underlying p.d.f.

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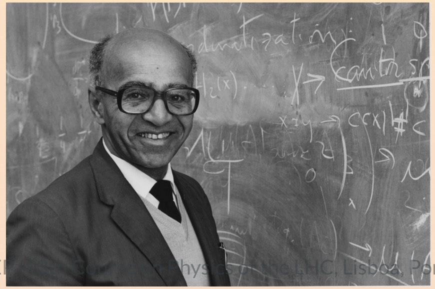
Image from James, 2nd ed.

Sufficient statistic

- Test statistic: a function of the data (a quantity derived from the data sample)
- $X \sim f(X|\theta)$, then $T(X)$ is sufficient for θ if $f(X|T)$ is independent of θ
- T carries as much information about θ as the original data X
  - Data X with model M and statistic $T(X)$ with model M' provide the same inference
- Rao-Blackwell theorem: if $g(X)$ is an estimator for θ and T is sufficient, then $E[g(X)|T(X)]$ is never a worse estimator of θ
  - Build a ballpark estimator $g(X)$, then condition on some $T(X)$ to obtain a better estimator
- Sufficiency Principle: if $T(X) = T(Y)$, then X and Y provide same inference about θ
  - Implications for data storage, computation requirements, etc.



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Images from AmStat magazine and illinois.edu

The Maximum Likelihood Method

- $x = (x_1, ..., x_N)$ of N statistically independent observations $x_i \sim f(x)$

$$L(x;\theta) = \prod_{i=1}^{N} f(x_i, \theta)$$

- Maximum-likelihood estimator is θ_{ML} such that

$$\theta_{ML} := argmax\theta\Big(L(x,\theta)\Big)$$

- Numerically, best to minimize: $-lnL(x;\theta) = -\sum_{i=1}^{N} lnf(xi, \theta)$
  - Fred James' Minuit's MINOS routine powers e.g. RooFit
- The MLE is:
  - Consistent: $\lim_{N\to\infty} \theta_{ML} = \theta_{true}$;
  - Unbiased: only asymptotically. $\vec{b} \propto \frac{1}{N}$, so $\vec{b} = 0$ only for $N \to \infty$;
  - Efficient: $V[\theta_{ML}] = \frac{1}{I(\theta)}$
  - Invariant under $\psi = g(\theta)$: $\hat{\psi}_{ML} = g(\theta_{ML})$

MLE for Nuclear Decay

- Nuclear decay with half-life τ
  $f(t;\tau) = \frac{1}{\tau}e^{-\frac{t}{\tau}}$
  $E[f] = \tau$
  $V[f] = \tau^2$
- Sample $t_i \sim f(t;\tau)$, obtaining $f(t_1, ...t_N; \tau) = \prod_i f(t_i;\tau) = L(\tau)$

$$\frac{\partial lnL(\tau)}{\partial\tau} = \sum_i \left(-\frac{1}{\tau} + \frac{t_i}{\tau^2} \right) \equiv 0 \qquad \Longrightarrow \qquad \hat{\tau}(t_1, ..., t_N) = \frac{1}{N}\sum_i t_i$$

- Unbiased: $b = E[\hat{\tau}] - E[f] = \tau - \tau = 0$
- Variance depends on samples: $V[\hat{\tau}] = V\left[\frac{1}{N}\sum_i t_i\right] = \frac{1}{N^2}\sum_i V[t_i] = \frac{\tau^2}{N}$

Estimator	Consistent	Unbiased	Efficient
$\hat{\tau} = \hat{\tau}_{ML} = \frac{t_1+...+t_N}{N}$	Yes	Yes	Yes
$\hat{\tau} = \frac{t_1+...+t_N}{N-1}$	Yes	No	No
$\hat{\tau} = t_i$	No	Yes	No

Bias-variance tradeoff

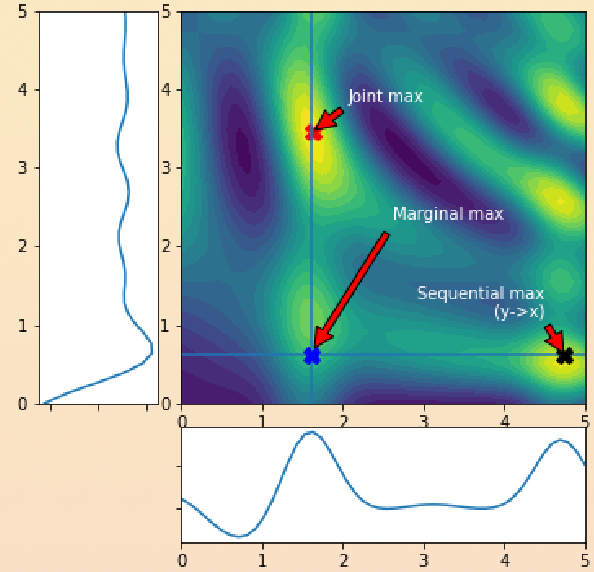
- Cannot have both zero bias and the smallest variance
- Information acts on the curvature of the likelihood, which represents the precision
  - Information is a limiting factor for the variance
- Rao-Cramer-Frechet (RCF) bound

$$V[\hat{\theta}] \geq \frac{(1+\partial b/\partial\theta)^2}{-E\left[\partial^2 lnL/\partial\theta^2\right]}$$

- Fisher Information Matrix

$$I_{ij} = E\left[\partial^2 lnL/\partial\theta_i\partial\theta_j\right]$$

$$argmin_{x,y}\Big(f(x,y)\Big)_y \neq argmin_y\Big(f(x,y)\Big)$$



Approximate variance

$$V[\hat{\theta}] \geq \frac{\left(1+\frac{\partial b}{\partial \theta}\right)^2}{-E\left[\frac{\partial^2 lnL}{\partial \theta^2}\right]}$$

- MLE is efficient and asymptotically unbiased

$$V[\theta_{ML}] \simeq \frac{1}{-E\left[\frac{\partial^2 lnL}{\partial \theta^2}\right]}\Bigg|\theta = \theta ML$$

- For a Gaussian pdf $f(x;\theta) = N(\mu, \sigma)$

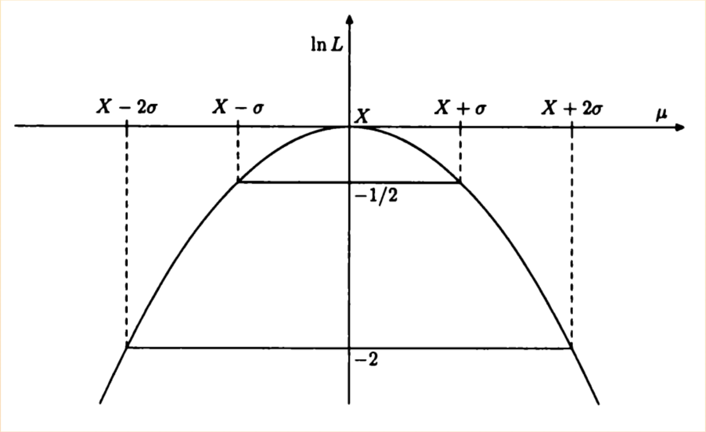
$$L(\theta) = ln\left[-\frac{(x-\theta)^2}{2\sigma^2}\right]$$

- $L(\theta_{1\sigma}) - \hat{\theta}_{ML} = 1/2$, and the area enclosed in $[\theta_{ML} - \sigma, \theta_{ML} + \sigma]$ will be 68.3%.

Confidence interval

- An interval with a fixed probability content
  $$P\Big((\theta_{ML}-\theta_{true})^2 \leq \sigma)\Big) = 68.3\%$$
  $$P(-\sigma \leq \theta_{ML}-\theta_{true} \leq \sigma) = 68.3\%$$
  $$P(\theta_{ML}-\sigma \leq \theta_{true} \leq \theta_{ML}+\sigma) = 68.3\%$$

- Practical prescription
  - Point estimate by computing the MLE
  - Confidence interval by taking the range delimited by the crossings of the likelihood function with $\frac{1}{2}$ (for 68.3% probability content, or 2 for 95% probability content), etc)



- MLE is invariant for monotonic transformations of θ
  - Likelihood crossings can be used also for asymmetric likelihood functions
  - Intervals exact only to $\mathcal{O}(\frac{1}{N})$

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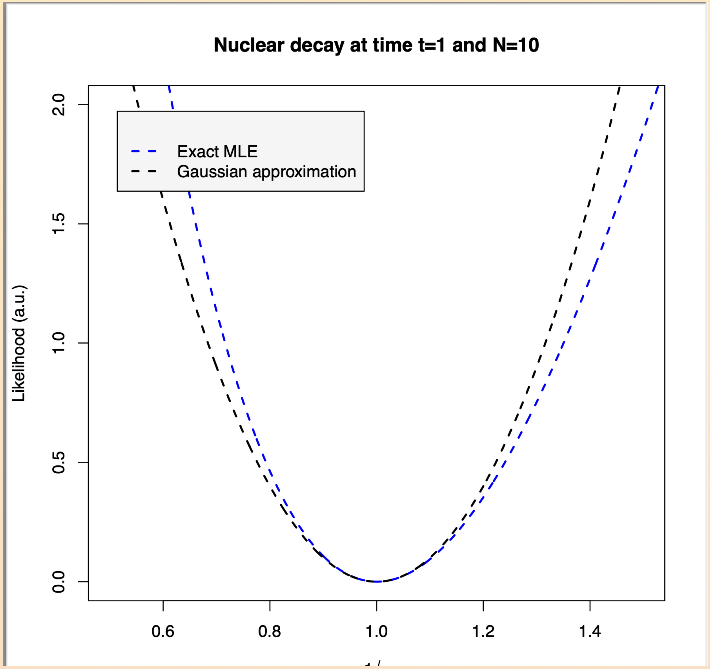
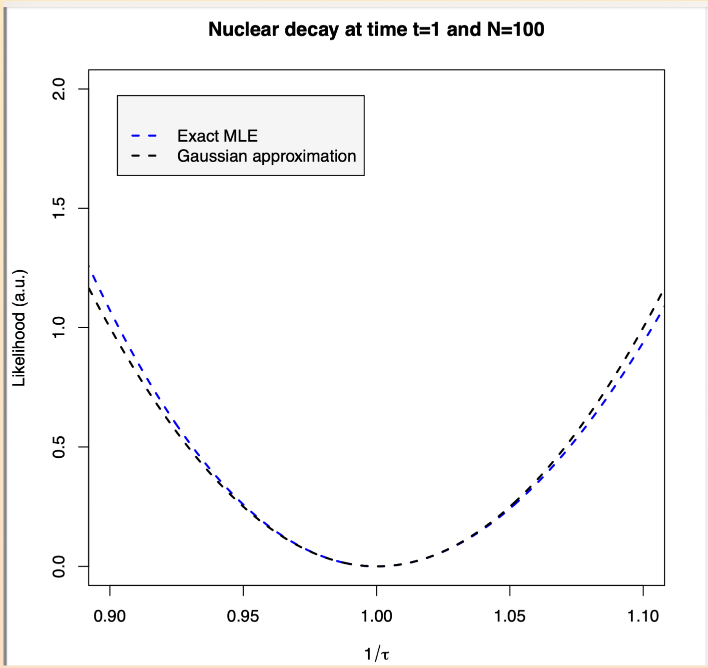
Image from James, 2nd ed.

Normal approximation

- Good only to $\mathcal{O}(\frac{1}{N})$:

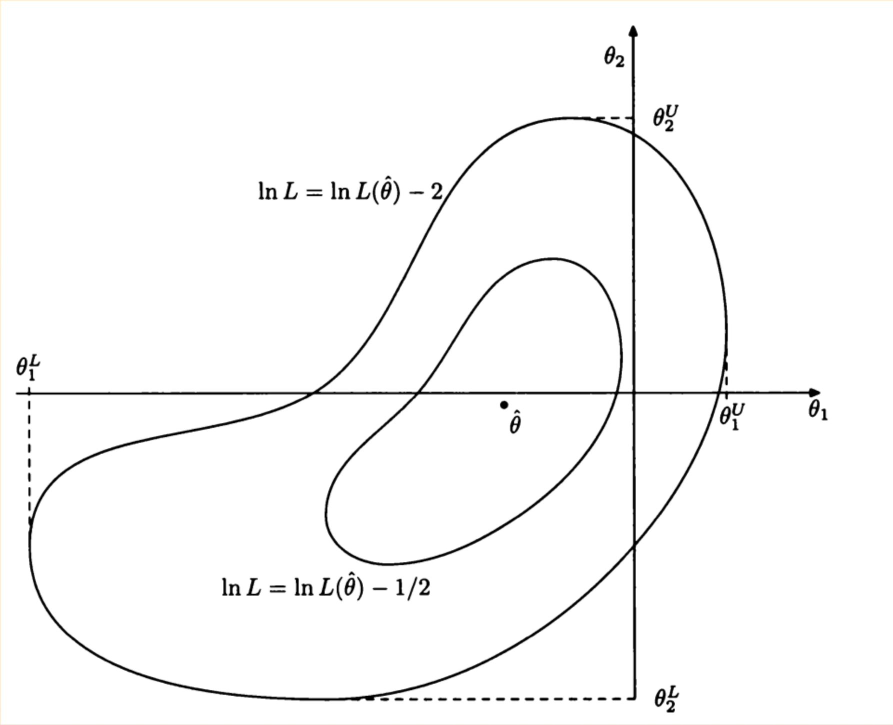
$$L(x;\theta) \propto exp\Big[-\frac{1}{2}(\theta-\theta_{ML})^T H(\theta-\theta_{ML})\Big]$$





Likelihood in many dimensions

- Elliptical contours correspond to gaussian Likelihoods
  - The closer to MLE, the more elliptical the contours, even in nonlinear problems
  - Minimizers just follow the contour regardless of nonlinearity
- Crossings (contours) adapted to areas under N-dimensional gaussians



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Plots from James, 2ed.

Profiling for systematic uncertainties

- Once upon a time, cross sections were: $\sigma = \frac{N_{data} - N_{bkg}}{\epsilon L}$
  - N_{sig} estimated from $N_{data} - N_{bkg}$ for the measured integrated luminosity L
  - Uncertainties in the acceptance ϵ propagated to the result for σ
- Nowadays, $p(x|\mu, \theta)$ pdf for the observable x to assume a certain value in a single event
  - $\mu := \frac{\sigma}{\sigma_{pred}}$ parameter of interest
  - θ nuisance parameters representing all the uncertainties affecting the measurement
  - Many events: $\prod_{e=1}^{n} p(x_e|\mu, \theta)$
- The number of events in the data set is however a Poisson random variable itself!
  - Marked Poisson Model $f(X|\nu(\mu, \theta), \mu, \theta) = Pois(n|\nu(\mu, \theta)) \prod_{e=1}^{n} p(x_e|\mu, \theta)$

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Pleasant read Vischia, 2019

Uncertainties as nuisance parameters

- Incorporate systematic uncertainties as nuisance parameter θ (Conway, 2011)
  - constraint interpreted as (typically Gaussian) prior coming from the auxiliary measurement
- MLE still depends on nuisance parameters: $\hat{\mu} := argmax_{\mu}\mathcal{L}(\mu, \theta; X)$

$$\mathcal{L}(\boldsymbol{n}, \boldsymbol{\alpha}^{\mathbf{0}} | \mu, \boldsymbol{\alpha}) = \prod_{i \in bins} \mathcal{P}(n_i | \mu S_i(\boldsymbol{\alpha}) + B_i(\boldsymbol{\alpha})) \times \prod_{j \in syst} \mathcal{G}(\alpha_j^0 | \alpha_j, \delta\alpha_j)$$

$$\downarrow$$

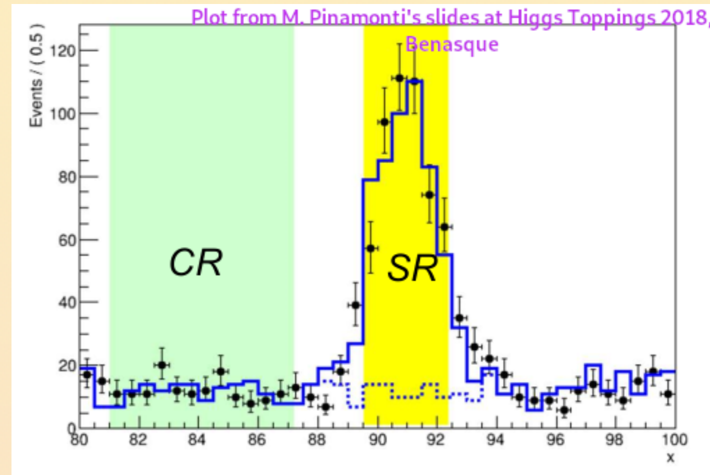
$$\mathcal{L}(\boldsymbol{n}, 0 | \mu, \boldsymbol{\alpha}) = \prod_{i \in bins} \mathcal{P}(n_i | \mu S_i(\boldsymbol{\alpha}) + B_i(\boldsymbol{\alpha})) \times \prod_{j \in syst} \mathcal{G}(0 | \alpha_j, 1)$$

Sidebands

- Sideband measurement

$$L_{SR}(s,b) = Poisson(N_{SR} \mid s+b)$$

$$L_{CR}(b) = Poisson(N_{CR} \mid \tilde{\tau} \cdot b)$$



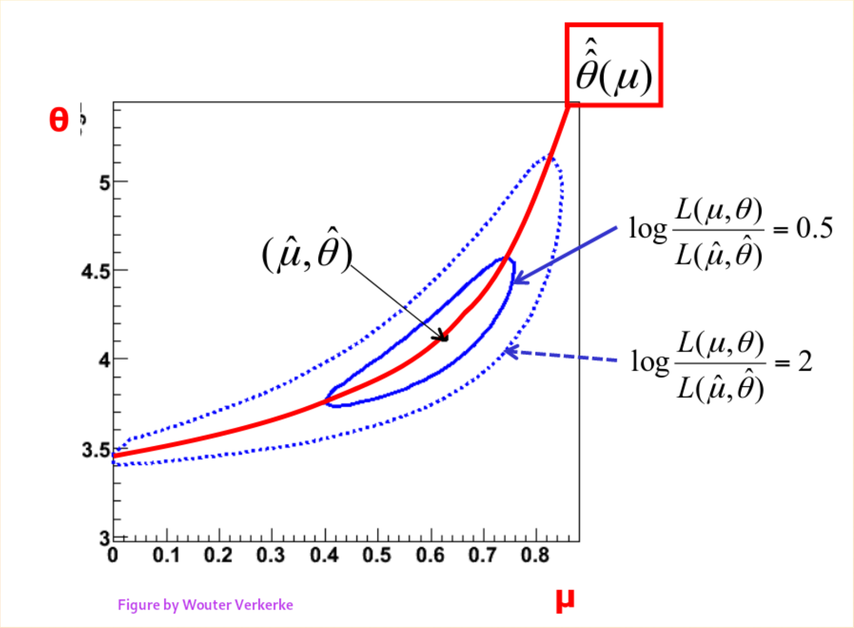
$$\mathcal{L}_{full}(s,b) = \mathcal{P}(N_{SR}|s+b) \times \mathcal{P}(N_{CR}|\tilde{\tau} \cdot b)$$

- Example subsidiary measurement of the background rate:
  - 8% systematic uncertainty in the MC rates
  - $\tilde{b}$: measured background rate
  - $\mathcal{G}(\tilde{b}|b, 0.08)\, \mathcal{L}_{full}(s,b) = \mathcal{P}(N_{SR}|s+b) \times \mathcal{G}(\tilde{b}|b, 0.08)$

The Likelihood Ratio:

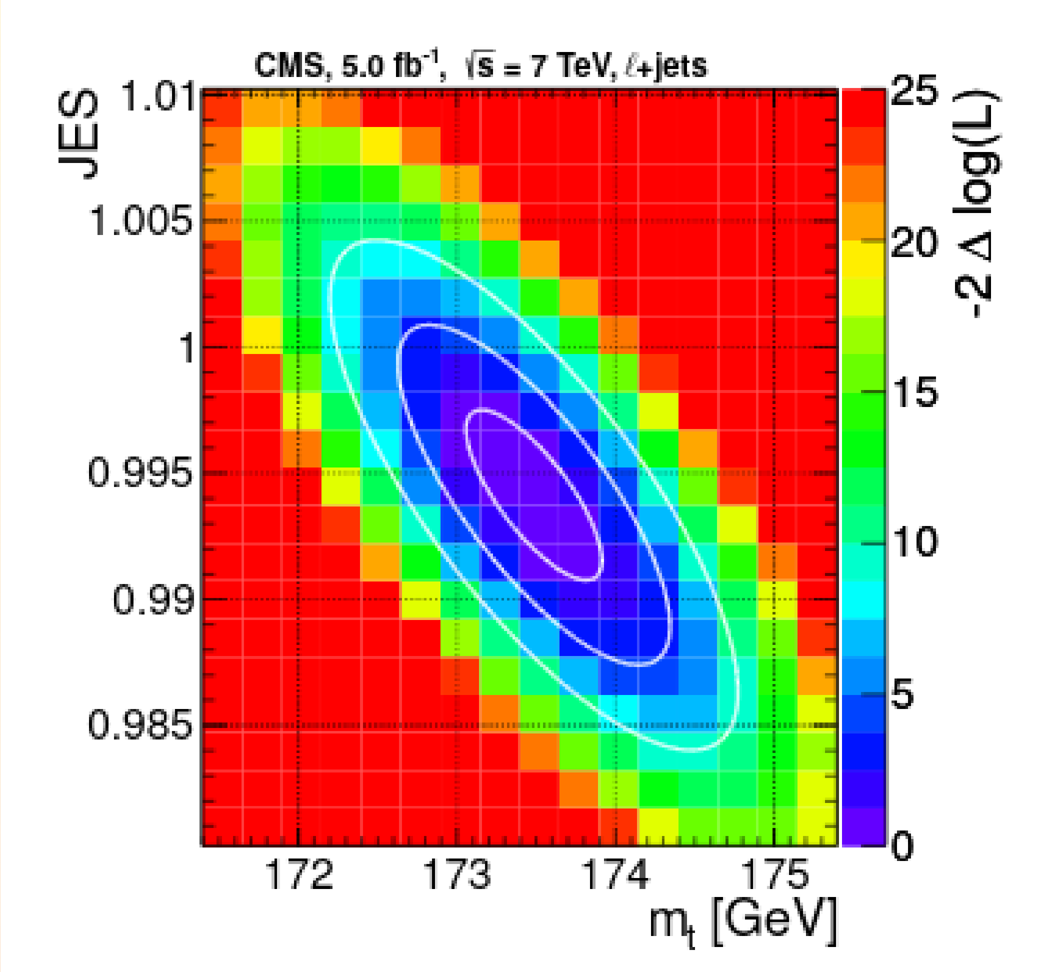
$$\lambda(\mu) := \frac{\mathcal{L}(\mu,\hat{\hat{\theta}})}{\mathcal{L}(\hat{\mu},\hat{\theta})}$$

- Profiling: eliminate dependence on θ by taking conditional MLEs
    - Bayesian marginalize Demortier, 2002



- $\lambda(\mu)$ distribution by toy data, or use Wilks theorem: $\lambda(\mu) \sim exp\Big[-\frac{1}{2}\chi^2\Big]\Big(1+\mathcal{O}(\frac{1}{\sqrt{N}})\Big)$ under some regularity conditions

What is a nuisance parameter?



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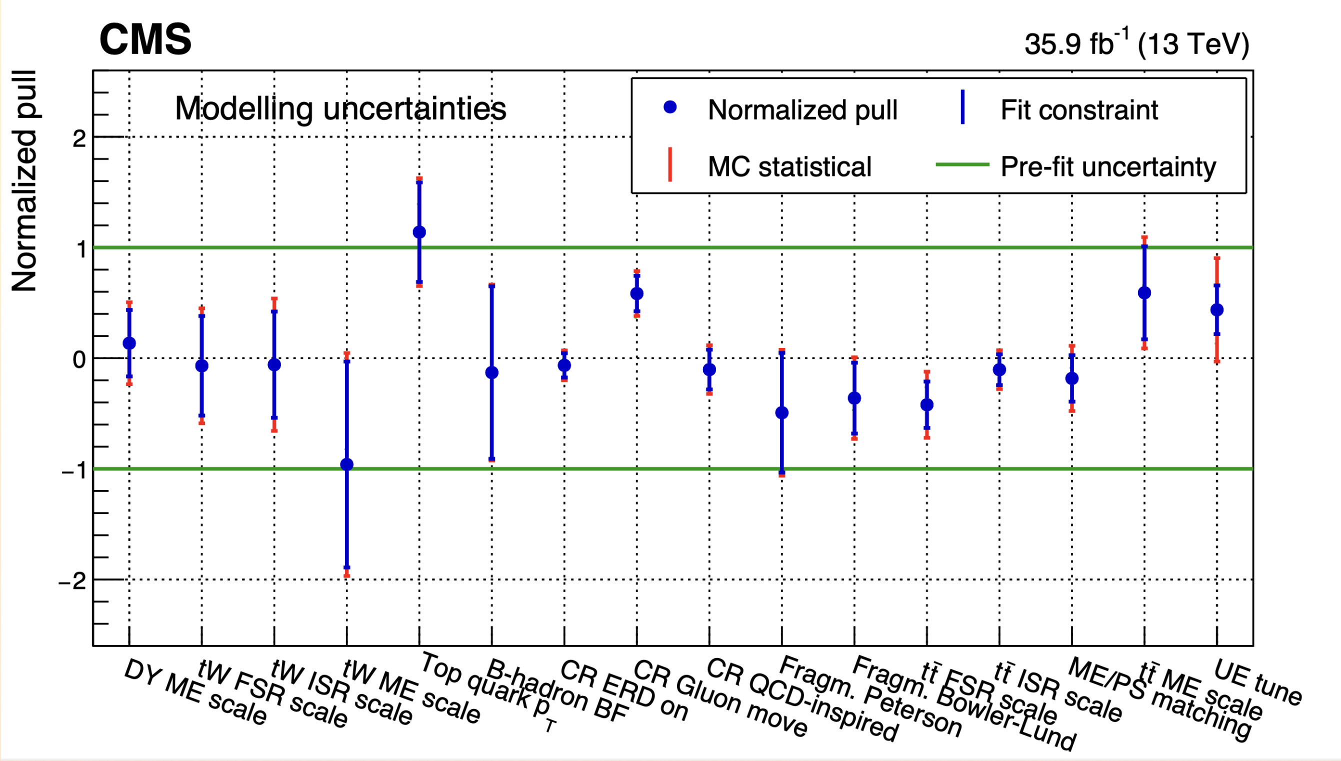
Plot from doi:10.1007/JHEP12(2012)105105)

Pulls and Constraints

- Pull: difference of the post-fit and pre-fit values of the parameter, normalized to the pre-fit uncertainty: $pull := \frac{\hat{\theta}-\theta}{\delta\theta}$
- Constraint: the ratio between the post-fit and the pre-fit uncertainty in the nuisance parameter.



Correlation and Significance

- What worries you the most?
  - A pull with very small constraint: $\theta_{prefit} = 0 \pm 1, \theta_{postfit} = 1 \pm 0.9$
  - The same pull with a strong constraint: $\theta_{prefit} = 0 \pm 1, \theta_{postfit} = 1 \pm 0.2$

Correlation and Significance

- What worries you the most?
  - A pull with very small constraint: $\theta_{prefit} = 0 \pm 1, \theta_{postfit} = 1 \pm 0.9$
  - The same pull with a strong constraint: $\theta_{prefit} = 0 \pm 1, \theta_{postfit} = 1 \pm 0.2$
- Compare the shift to its uncertainty
- Indipendent measurements: the compatibility C is

$$C = \Delta\theta / \sigma_{\Delta\theta} = \frac{\theta_2 - \theta_1}{\sqrt{\sigma_1^2 + \sigma_2^2}}$$

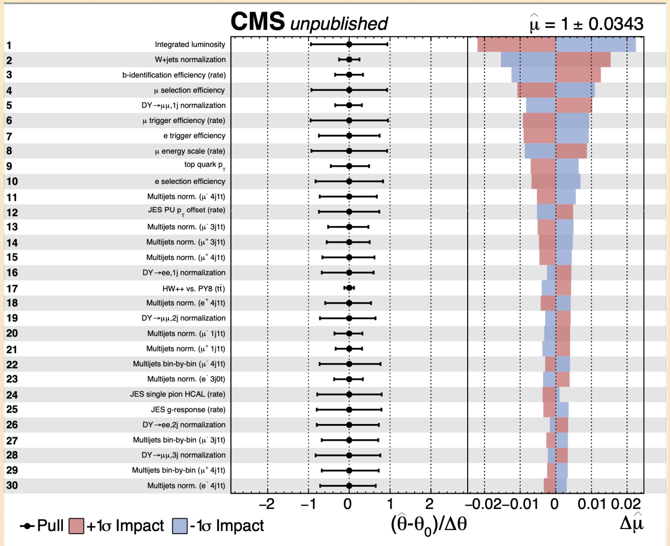
- First case $C = 0.74$, second case $C = 0.98$ (larger, still within uncertainty)
- These are not independent measurements! Worst-case scenario formula:

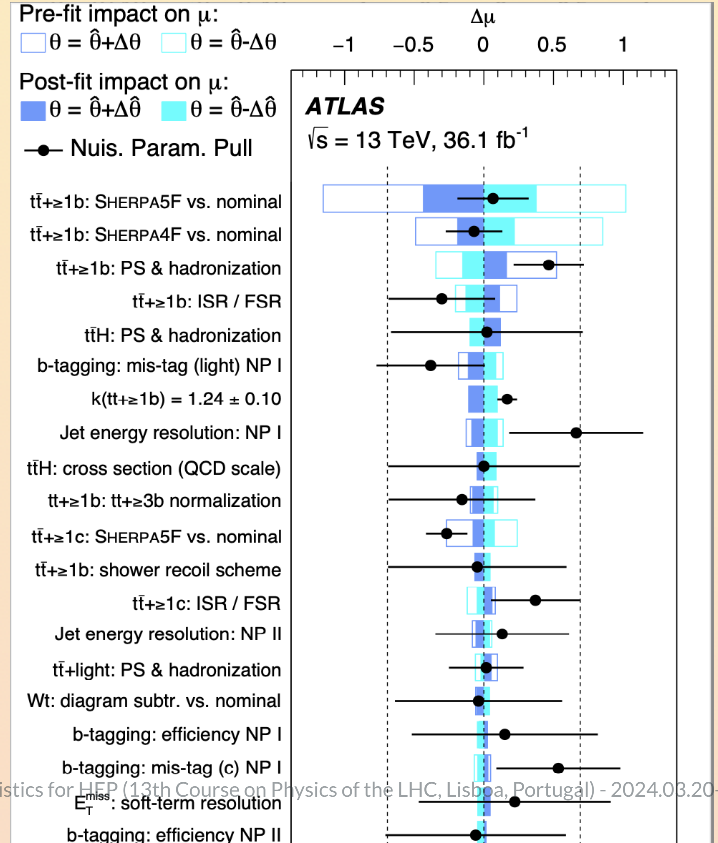
$$C = \Delta\theta / \sigma_{\Delta\theta} = \frac{\theta_2 - \theta_1}{\sqrt{\sigma_1^2 - \sigma_2^2}}$$

- First case, $C = 2.29$, second case $C = 1.02$
- The same pull is more significant if there is (almost no) constraint!!!

Impacts on the post-fit μ

- Fix each θ to its post-fit value $\hat{\theta}$ plus/minus its pre(post)fit uncertainty $\delta\theta$ ($\delta\hat{\theta}$)
- Reperform the fit for μ
- Impact is $\hat{\mu} - \hat{\mu}(\hat{\theta})$ (should give perfect result on Asimov dataset)

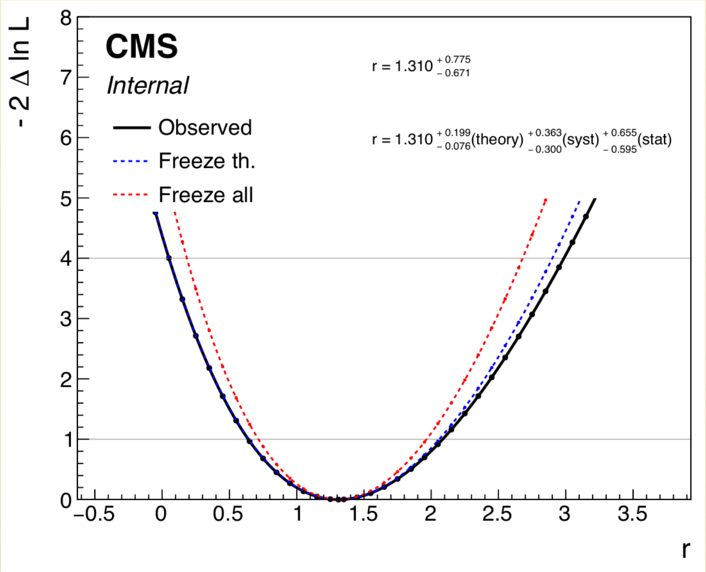




Breakdown of uncertainties

- Amount of uncertainty on μ imputable to a given source of uncertainty
  - Modern version of Fisher's formalization of the ANOVA concept
  - the constituent causes fractions or percentages of the total variance which they together produce (Fisher, 1919)
  - the variance contributed by each term, and by which the residual variance is reduced when that term is removed (Fisher, 1921)

- Freeze a set of θ_i to $\hat{\theta}_i$
- Repeat the fit, uncertainty on μ is smaller
- Contribution of θ_i to the overall uncertainty as squared difference
- Statistical uncertainty by freezing all nuisance parameters



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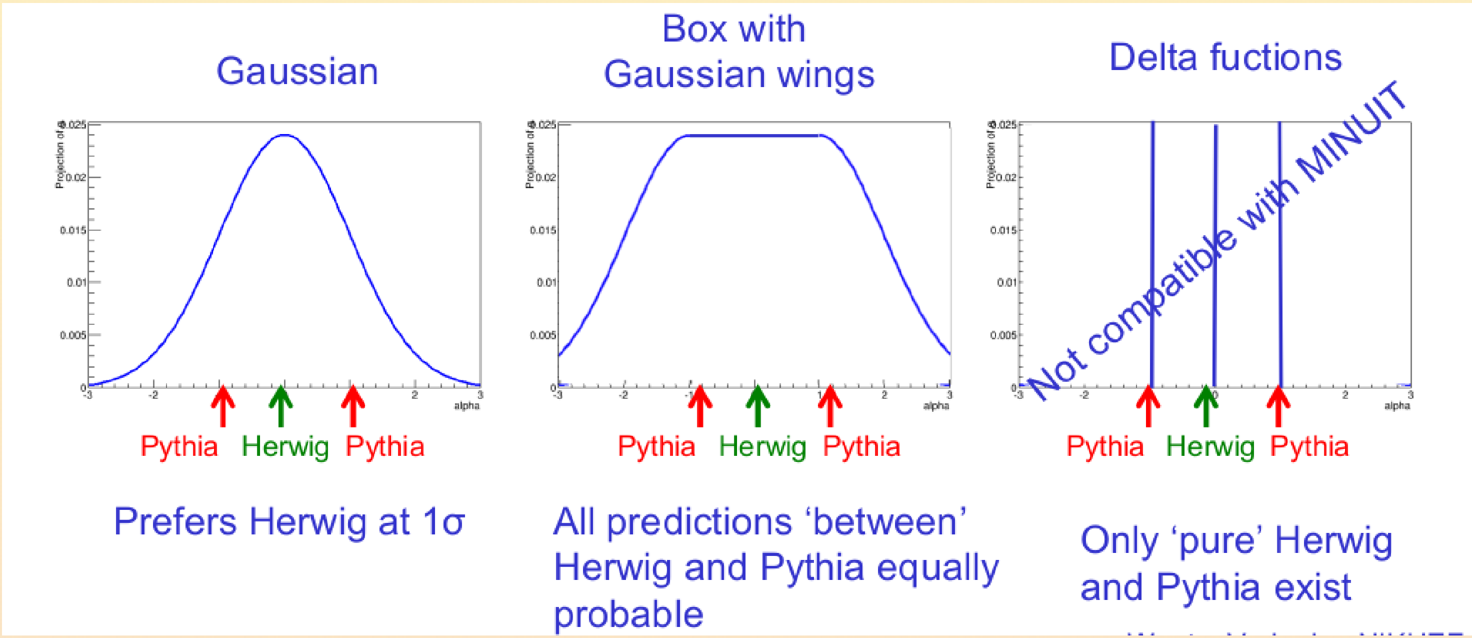
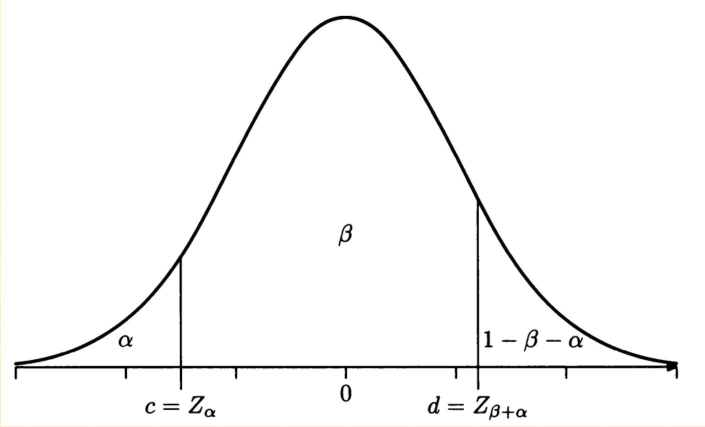
Toy data

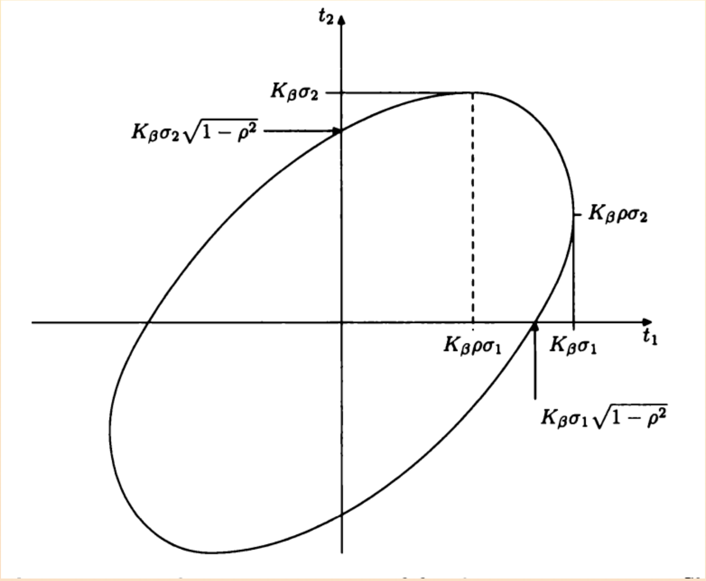
Which is the "correct" constraint?



Confidence intervals

- Probability content: solve $\beta = P(a \leq X \leq b) = \int_a^b f(X|\theta)dX$ for a and b
  - A method yielding interval with the desired β, has coverage





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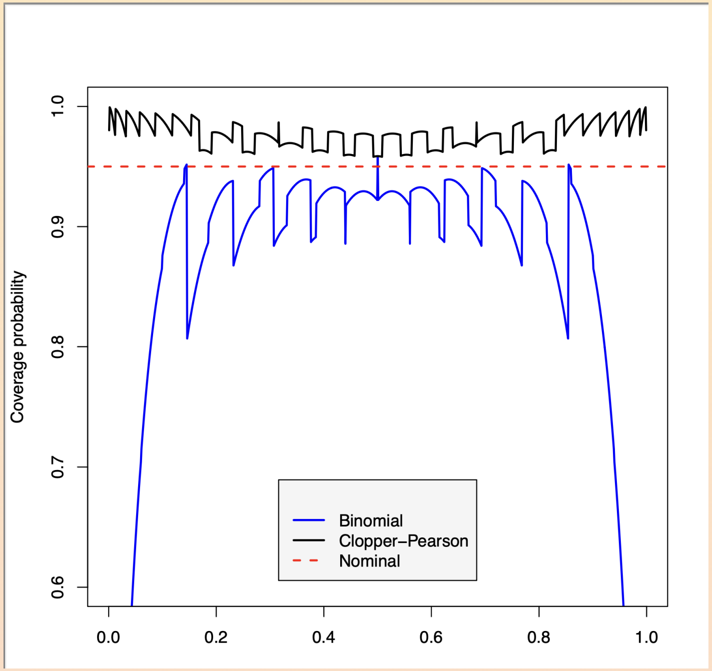
Plots from James, 2nd ed.

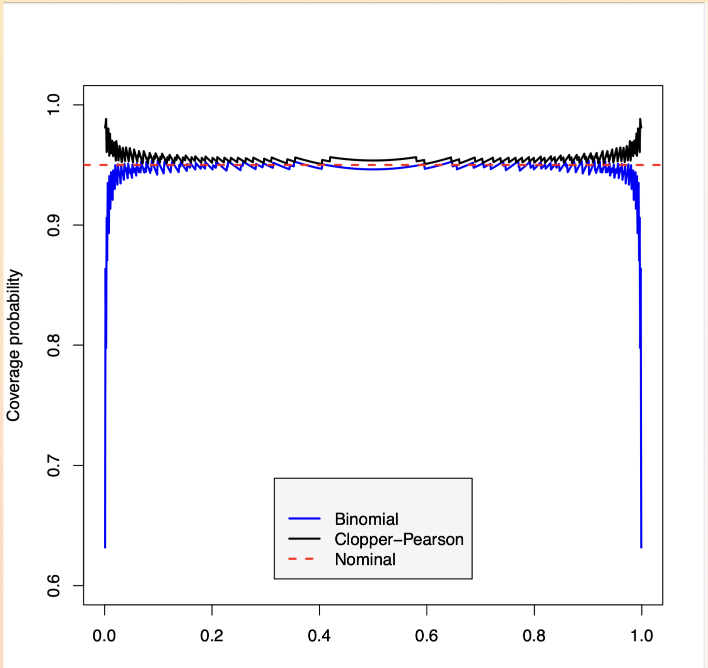
Checking for coverage

- Operative definition of coverage probability
  - Fraction of times, over a set of (usually hypothetical) measurements, that the resulting interval covers the true value of the parameter
  - Obtain the sampling distribution of the confidence intervals using toy data
- Nominal coverage: the one you have built your method around
- Actual coverage: the one you calculate from the sampling distribution
  - Toy experiment: sample N times for a known value of θ_{true}
  - Compute interval for each experiment
  - Count fractions of intervals containing θ_{true}
- Nominal and actual coverage should agre if all assumptions of method are valid
  - Undercoverage: intervals smaller than proper ones
  - Overcoverage: intervals larger than proper ones

Discrete Case

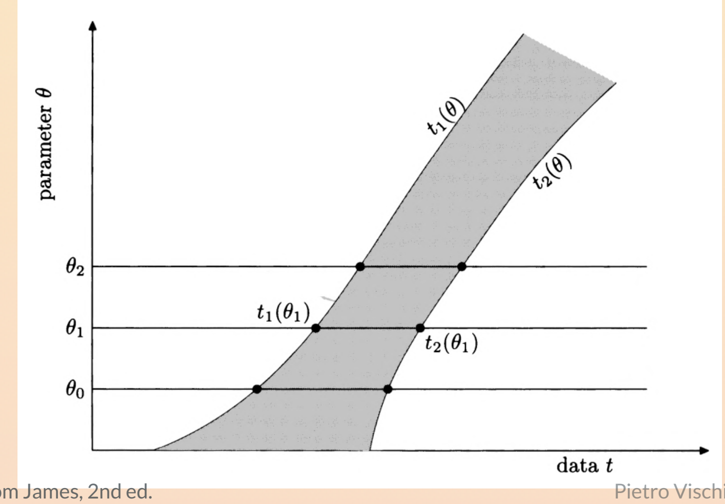
- Probability content $P(a \leq X \leq b) = \sum_a^b f(X|\theta)dX \leq \beta$
- Binomial: find (r_{low}, r_{high}) such that $\sum_{r=r_{low}}^{r=r_{high}} \binom{r}{N} p^r (1-p)^{N-r} \leq 1-\alpha$
  - Gaussian approximation: $p \pm Z_{1-\alpha/2}\sqrt{\frac{p(1-p)}{N}}$
  - Clopper Pearson: invert two single-tailed binomial tests

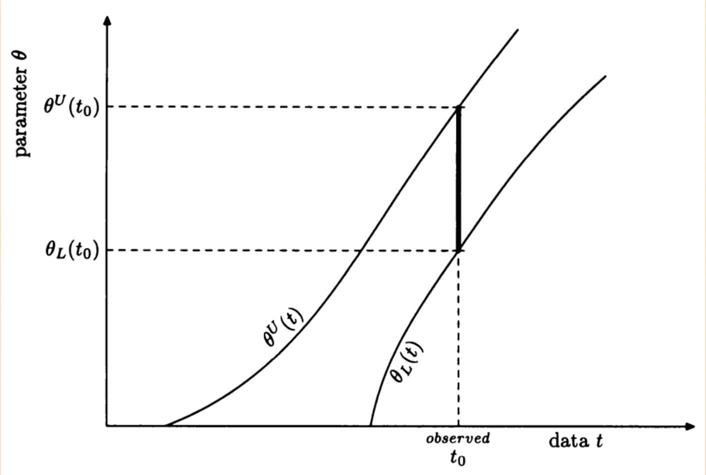




The Neyman construction

- Unique solutions to finding confidence intervals are infinite
  - Let's suppose we have chosen a way
- Build horizontally: for each (hypothetical) value of θ, determine $t_1(\theta), t_2(\theta)$ such that $\int_{t_1}^{t_2} P(t|\theta)dt = \beta$
- Read vertically: from the observed value t_0, determine $[\theta_L, \theta^U]$ by intersection
- Intrinsically frequentist procedure





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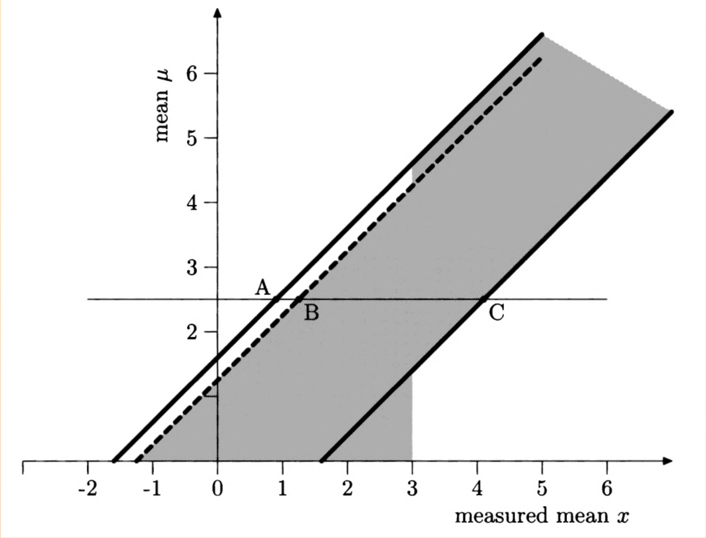
Figures from James, 2nd ed.

Flip-flopping

- Gaussian measurement (variance 1) of $\mu > 0$ (physical bound)
- Individual prescriptions are self-consistent
  - 90% central limit (solid lines)
  - 90% upper limit (single dashed line)

- Mixed choices (after looking at data) are problematic
- Unphysical values and empty intervals: choose 90% central interval, measure $x_{obs} = -2.0$
  - Interval empty, yet with the desired coverage



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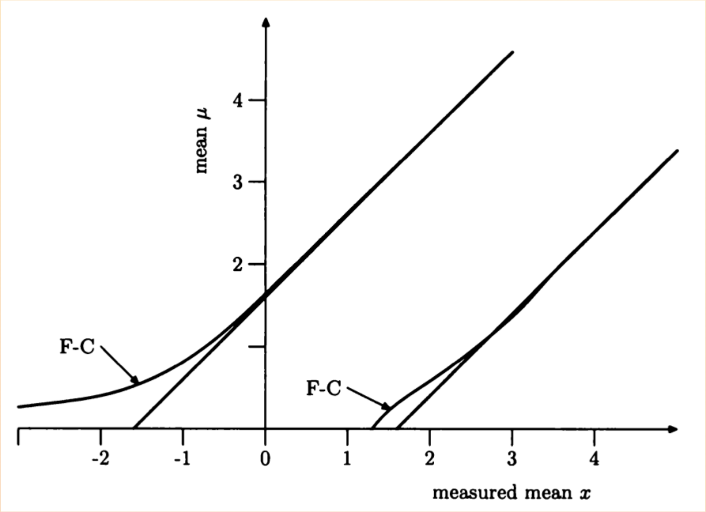
Figures from James, 2nd ed.

The Feldman-Cousins Ordering Principle

- Unified approach for determining interval for $\mu = \mu_0$
  - Include in order by largest $\ell(x) = \frac{P(x|\mu_0)}{P(x|\hat{\mu})}$
  - $\hat{\mu}$ value of μ which maximizes $P(x|\mu)$ within the physical region
  - $\hat{\mu}$ remains equal to zero for $\mu < 1.65$, yielding deviation w.r.t. central intervals

- Minimizes Type II error (likelihood ratio for simple test is the most powerful test)
- Solves the problem of empty intervals
- Avoids flip-flopping in choosing an ordering prescription



Bayesian intervals

- Often numerically identical to frequentist confidence intervals
    - Much simple derivation
    - Interpretation is different: {\em credible intervals}
    - Posterior density summarizes the complete knowledge about θ
- Highest Probability Density intervals
    - Work out of the box for multimodal distributions and for physical constraints

Fig. 1 Simple examples of central (*black*) and highest probability density (*red*) intervals. The intervals coincide for a symmetric distribution, otherwise the HPD interval is shorter. The three examples are a normal distribution, a gamma with shape parameter 3, and the marginal posterior density for a variance parameter in a hierarchical model. (Color figure online)

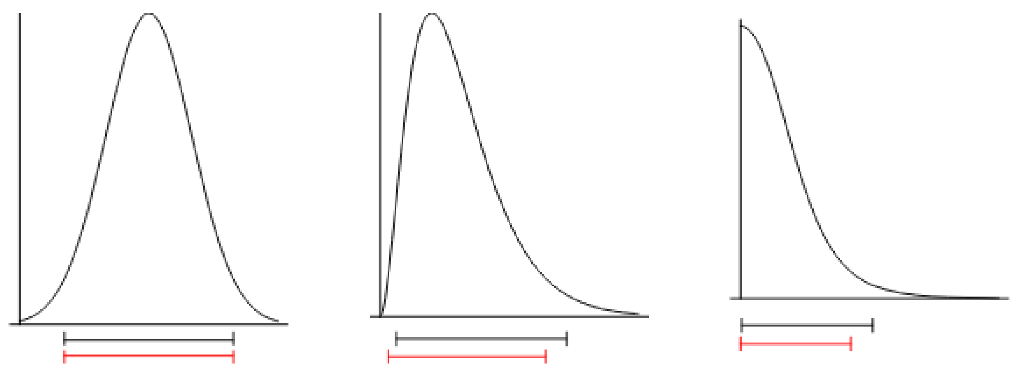


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Figure from Stat Comput (2015) 25:809--819

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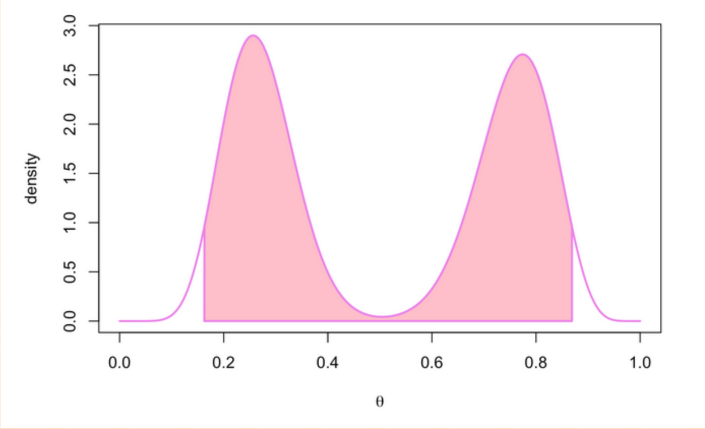

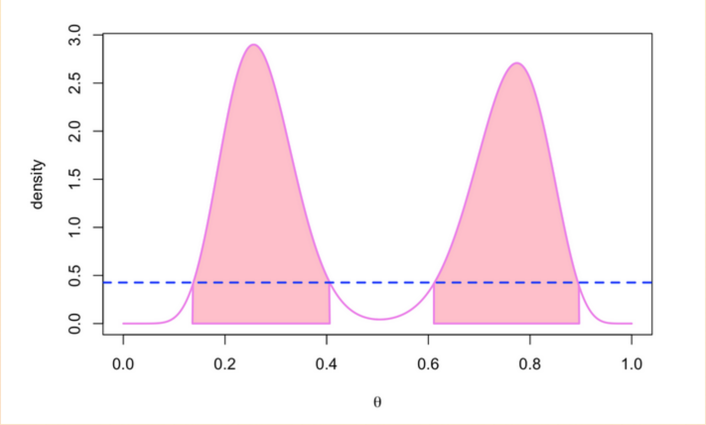

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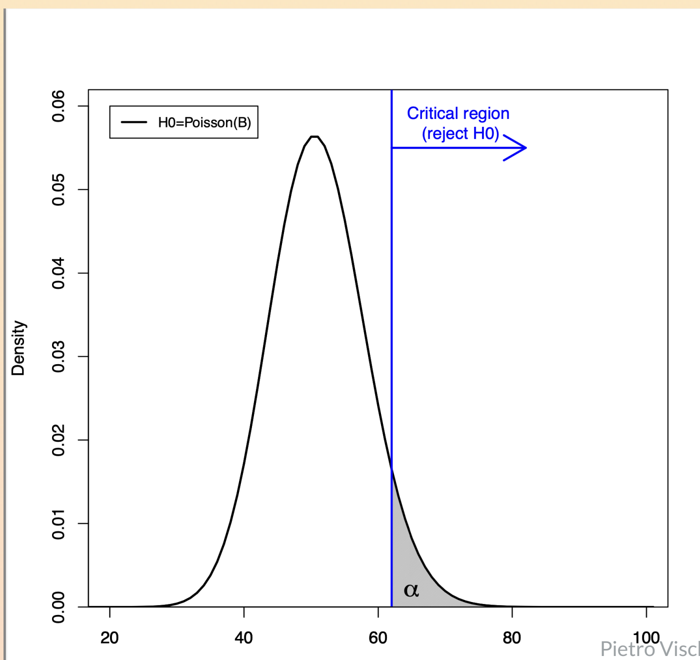
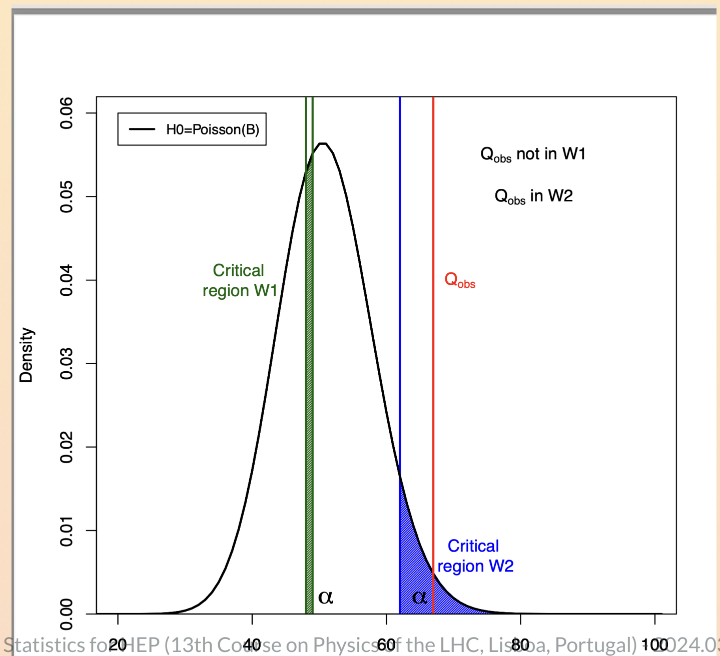
Figure from vioshyvo.github.io

Test of hypotheses

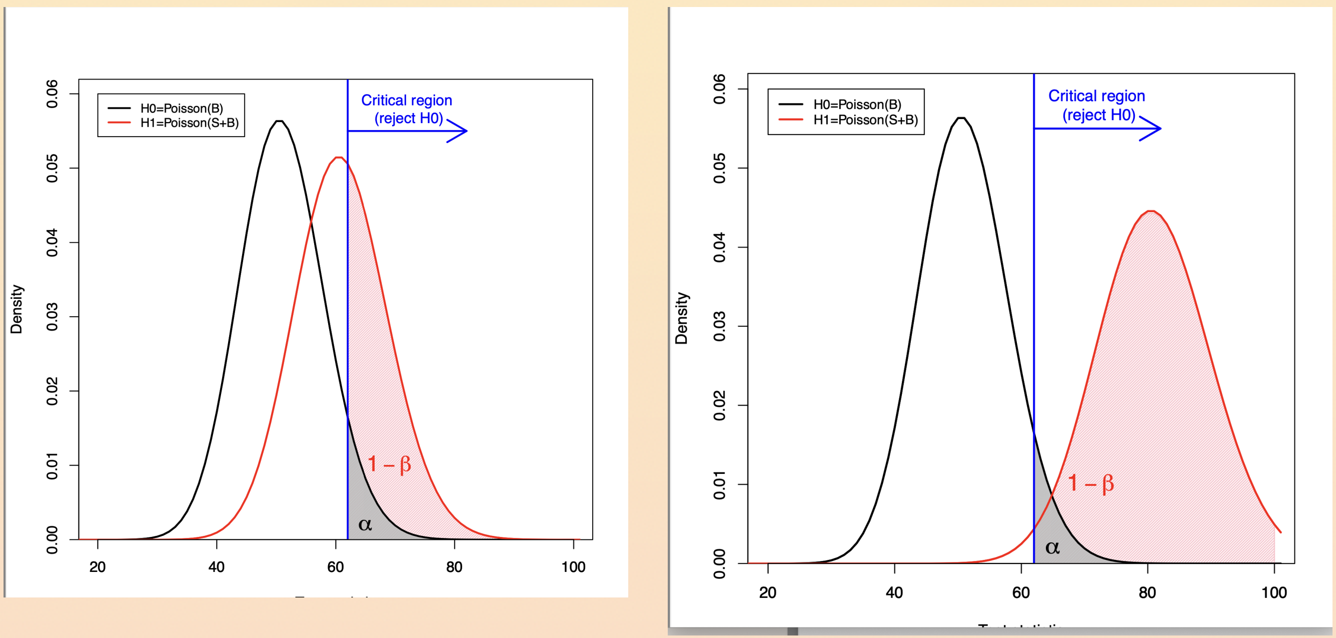
- Hypothesis: a complete rule that defines probabilities for data.
- Statistical test: a proposition on compatibility of H_0 with the available data.
  - $X \in \Omega$ a test statistic
  - Critical region W: if $X \in W$, reject H_0, Acceptance region>: if $X \in \Omega - W$, accept H_0
  - Level of significance (size of the test): $P(X \in W|H_0) = \alpha$





Alternative hypothesis and power

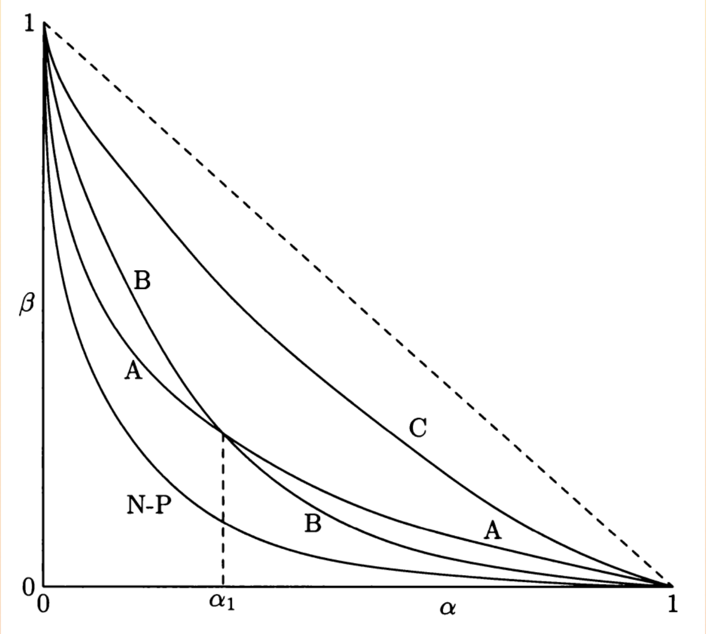
- Need an alternative to solve ambiguities
- Power of the test
  - $P(X \in W | H_1) = 1 - \beta$
  - Power β is such that $P(X \in \Omega - W | H_1) = \beta$



Families of Tests

- Varying α and β results in families of tests
- In one dimension, likelihood ratio (Neyman-Pearson) test is the most powerful test, given by

$$\ell(X,\theta_0,\theta_1) := \frac{f(X|\theta_1)}{f(X|\theta_0)} \geq c_\alpha$$



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Images from Statistical Statistics Memes and James, 2nd ed.

Bayesian Model Selection

- M_0 and M_1 predict θ> : $P(\theta|x,M) = \frac{P(x|\theta,M)P(\theta|M)}{P(x|M)}$
  - Bayesian evidence (Model likelihood) $P(x|M) = \int P(x|\theta,M)P(\theta|M)d\theta$
  - Posterior for M_0: $P(M_0|x) = \frac{P(x|M_0)\pi(M_0)}{P(x)}$, posterior for M_1: $P(M_1|x) = \frac{P(x|M_1)\pi(M_1)}{P(x)}$
  - Posterior odds: $\frac{P(M_0|x)}{P(M_1|x)} = \frac{P(x|M_0)\pi(M_0)}{P(x|M_1)\pi(M_1)}$
  - Bayes factor: $B_{01} := \frac{P(x|M_0)}{P(x|M_1)}$
  - Posterior odds = Bayes Factor $\times$ prior odds
- Turing (IJ Good, 1975): deciban as the smallest change of evidence human mind can discern

Jeffreys

K	dHart	bits	Strength of evidence
$< 10^0$	0	—	Negative (supports M_2)
10^0 to $10^{1/2}$	0 to 5	0 to 1.6	Barely worth mentioning
$10^{1/2}$ to 10^1	5 to 10	1.6 to 3.3	Substantial
10^1 to $10^{3/2}$	10 to 15	3.3 to 5.0	Strong
$10^{3/2}$ to 10^2	15 to 20	5.0 to 6.6	Very strong
$> 10^2$	> 20	> 6.6	Decisive

Kass and Raftery

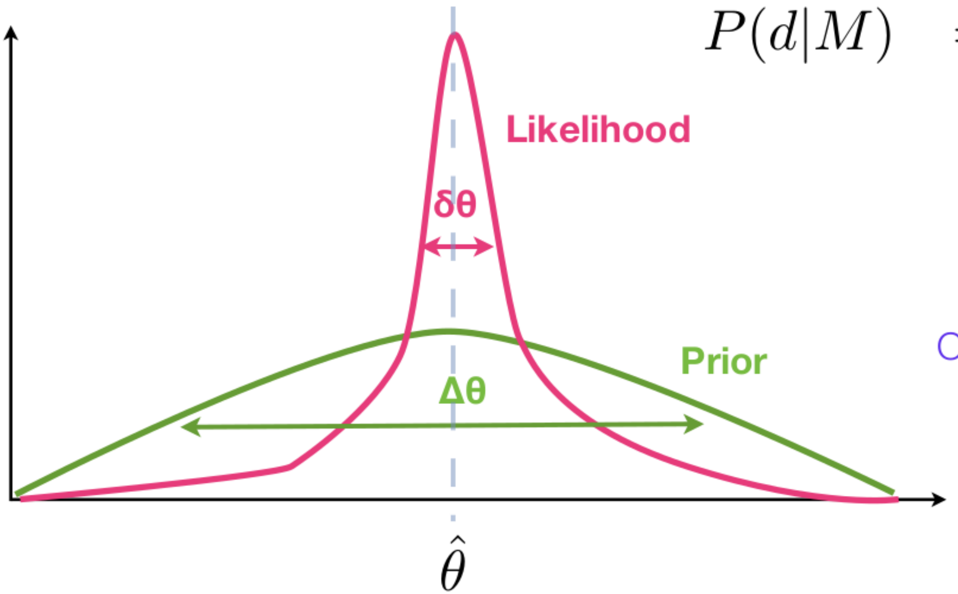
$\log_{10} K$	K	Strength of evidence
0 to 1/2	1 to 3.2	Not worth more than a bare mention
1/2 to 1	3.2 to 10	Substantial
1 to 2	10 to 100	Strong
> 2	> 100	Decisive

Trotta

|lnB|	relative odds	favoured model's probability	Interpretation
< 1.0	< 3:1	< 0.750	not worth mentioning
< 2.5	< 12:1	0.923	weak
< 5.0	< 150:1	0.993	moderate
> 5.0	> 150:1	> 0.993	strong

Discourage nonpredictive models

- The Bayes Factor penalizes excessive model complexity
- Highly predictive models are rewarded, broadly-non-null priors are penalized

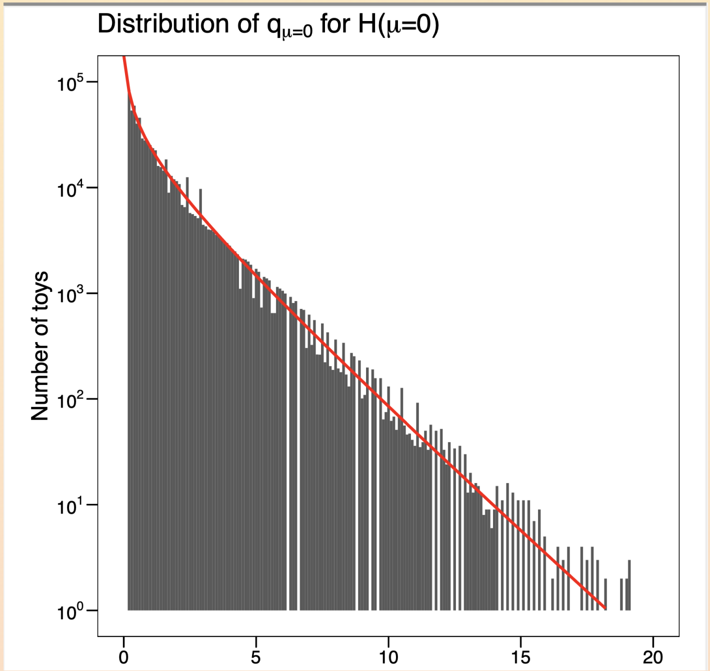


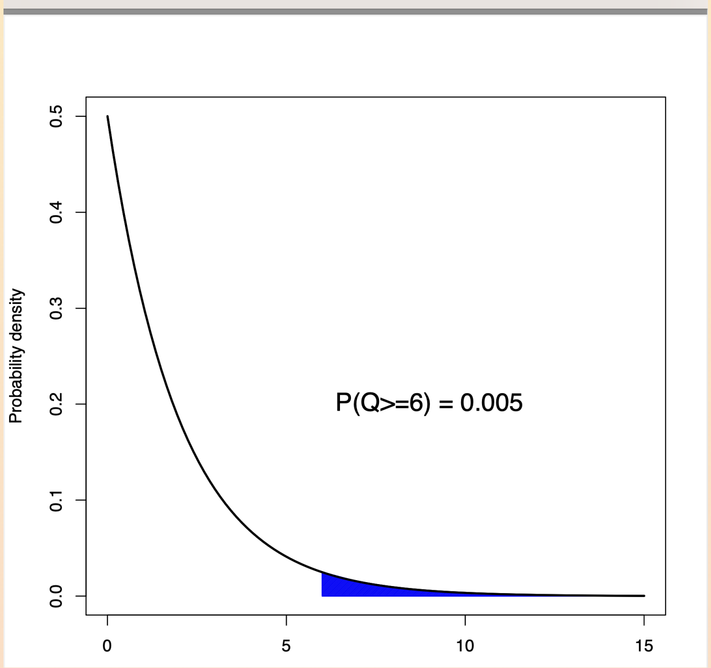
$$P(d|M) = \int d\theta L(\theta) P(\theta|M)$$
$$\approx P(\hat{\theta}) \delta\theta L(\hat{\theta})$$
$$\approx \frac{\delta\theta}{\Delta\theta} L(\hat{\theta})$$

Image from Trotta, Chair Lemaitre 2018

P-values

- Probability of obtaining a fluctuation with test statistic q_{obs} or larger, under the null hypothesis H_0
  - Need the distribution of test statistic under \hzero either with toys or asymptotic approximation (if N_{obs} is large, then $q \sim \chi^2(1)$)





Beyond frequentism: CLs

- $CL_s := \frac{CL_{s+b}}{CL_b}$
- Exclude the signal hypothesis at confidence level CL if $1 - CL_s \leq CL$

- Ratio of p-values is not a p-value
- Denominator prevents excluding signals for which there is no sensitivity
- Formally corresponds to have $H_0 = H(\theta! = 0)$ and test it against $H_1 = H(\theta = 0)$

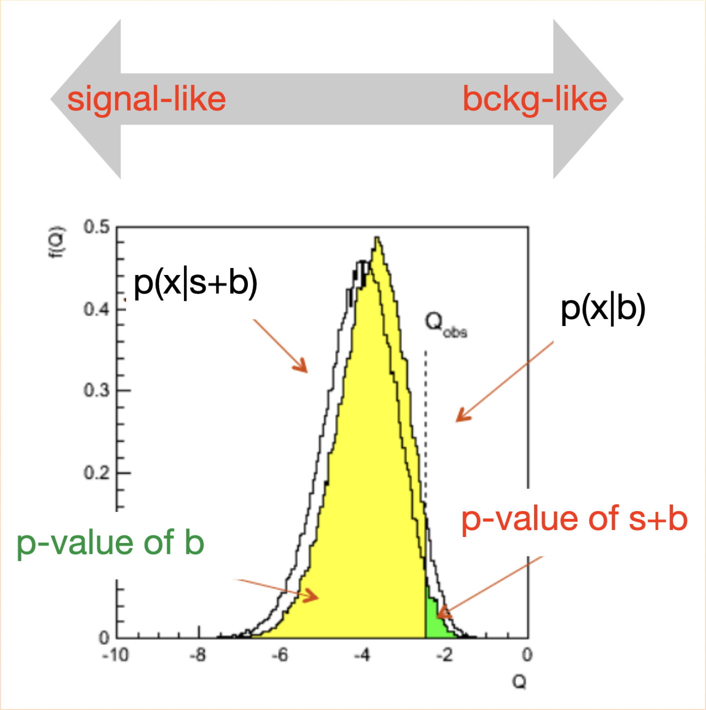


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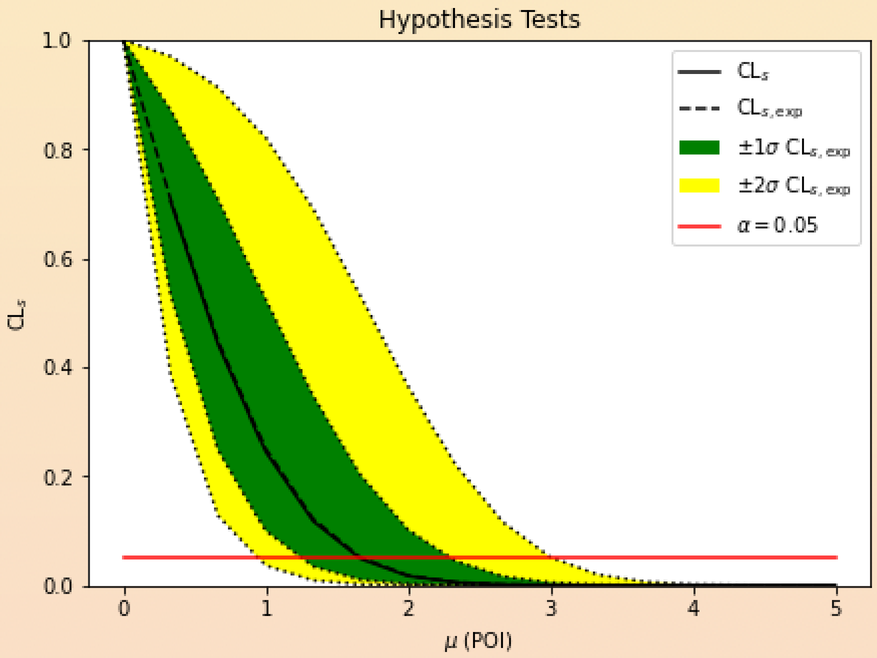
Image by Diego Tonelli

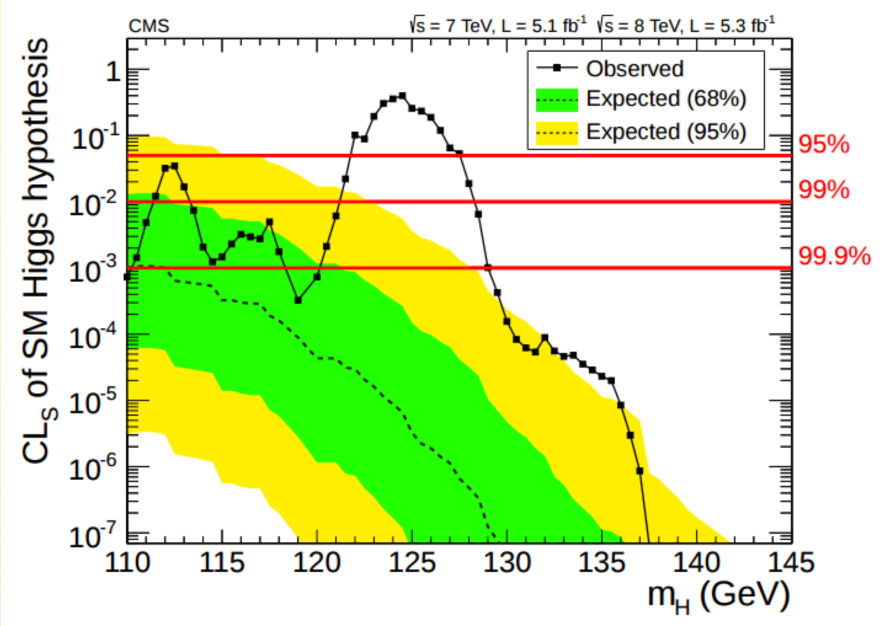
From a scans to limits

- Scan the $CLs test statistic as a function of the POI (typically \mu = \sigma{obs}/\sigma{pred}$)
- Find intersection with the desired confidence level
- (eventually) convert the limit on μ back to a cross section



From a limit to hypothesis testing

- Apply the CL_s method to each Higgs mass hypothesis
- Show the CL_s test statistic for each value of the fixed hypothesis
- Green/yellow bands indicate the $\pm1\sigma$ and $\pm2\sigma$ intervals for the expected values under B-only hypothesis
  - Obtained by taking the quantiles of the B-only hypothesis



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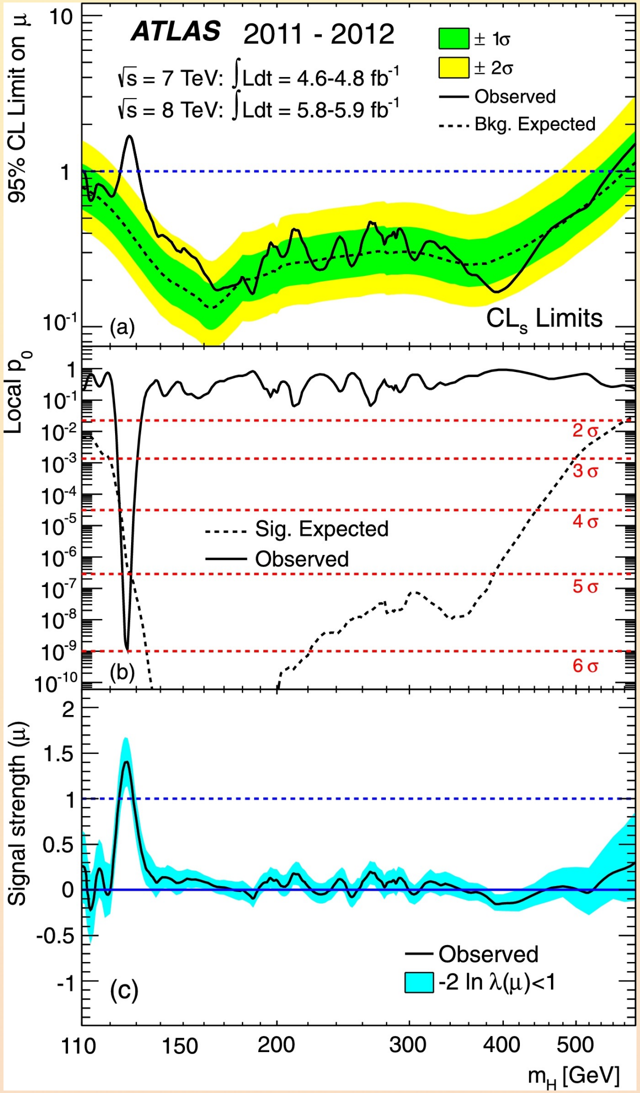
Plot from the CMS Higgs discovery paper

From a limit to hypothesis testing

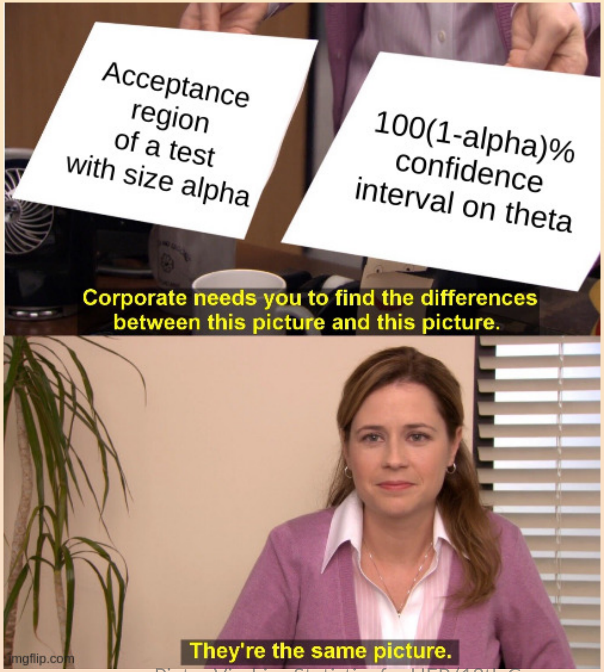
- CLs limit on μ as a function of mass hypothesis
- p-value of excess
- Fitted signal strength peaks at excess



Duality

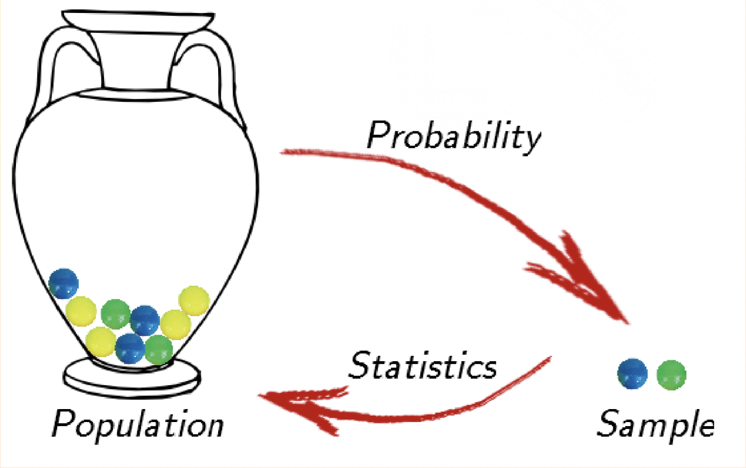
Meme generated with memegenerator

- Acceptance region set of values of the test statistic for which we don't reject H_0 at significance level α
- $100(1-\alpha)\%$ confidence interval: set of *values of the parameter θ for which we don't reject H_0 (if H_0 is assumed true)



Summary

- Statistics is the way we connect experiment and models
  - Estimate parameters
  - Quantify uncertainties
  - Test theories



- All models are wrong, some models are useful
  (George E. P. Box, Science and Statistics)

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Picture by Rob Hall