Statistics for Particle Physics

Theory, methods, and examples

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What’s the big deal about Probability and Statistics?

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  - Topological Hausdorff Spaces
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  - Elementary Calculus
- Can be hard ...
  - Semicompact Lie Groups
  - Topological Hausdorff Spaces
- but it is essentially “done”:
  XIX century, early XX century at the latest...
Same thing when I studied Probability in school:

- To a large extent “closed”
- Fun
- Basically applicable to gaming theory
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Statistics was somewhat different (and murkier..)
- Basically simple sampling examples.
- The $\chi^2$ recipe.
- Not at all like the clean Mathematics I was used to.
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And then I became an experimental high energy physicists....
Lots of interesting recipes that help solve all kind of useful stuff.

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Lots of activity of people trying to understand:

▷ why we do what we do
▷ how to do it better
▷ what to do next
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In fact most of what I am going to tell in these three lectures comes from papers published by physicists in the last 10 years.
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**Unified approach to the classical statistical analysis of small signals**

Gary J. Feldman

Department of Physics, Harvard University, Cambridge, Massachusetts 02138

Robert D. Cousins

Department of Physics and Astronomy, University of California, Los Angeles, California 90095
The statistical analysis of Gaussian and Poisson signals near physical boundaries

Mark Mandelkern and Jonas Schultz

Department of Physics and Astronomy, University of California, Irvine, California 92697
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Including systematic uncertainties in confidence interval construction for Poisson statistics

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Division of High Energy Physics, Uppsala University, S-75121 Uppsala, Sweden
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Limits and confidence intervals in the presence of nuisance parameters

Wolfgang A. Rolke\textsuperscript{a,*}, Angel M. López\textsuperscript{b}, Jan Conrad\textsuperscript{c}
Statistical errors in Monte Carlo estimates of systematic errors

Byron P. Roe*
Statistical errors in Monte Carlo estimates of systematic errors

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Evaluation of three methods for calculating statistical significance when incorporating a systematic uncertainty into a test of the background-only hypothesis for a Poisson process

Robert D. Cousins, James T. Linnemann, and Jordan Tucker

Department of Physics and Astronomy, University of California, Los Angeles, CA 90095, USA
Department of Physics and Astronomy, Michigan State University, East Lansing, MI 48840, USA
Probability: Relation to Statistics

Statistics is to a large extent the inverse problem of Probability

Probability:
Know parameters that describe theory \(\Rightarrow\) predict probability of result

Statistics:
Know result \(\Rightarrow\) extract information on the parameters and/or the theory
Probability:

\( b \)-tagging efficiency is 97\% \Rightarrow \)

\[ P(\text{tag } 65 \leq n \leq 72 \text{ out of } N = 75 \text{ } b\text{-jets}) = 39.165\% \]
Probability:

$b$-tagging efficiency is 97%  \Rightarrow
P (\text{tag } 65 \leq n \leq 72 \text{ out of } N = 75 \text{ } b\text{-jets}) = 39.165\%$

Statistics:

$b$-tagging algorithm selects 73 out of 75 $b$-jets.
What can we say about the algorithm efficiency?
**Probability:**

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Well, we can say it’s in \([91.8, 99.5]\) with 90\% CL
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Well, we can say it’s in \([91.8,99.5]\) with 90% CL
or in \([93.9,99.1]\) with 68% CL, that is \(\varepsilon = 97.3^{+1.8}_{-3.4}\)
Something very common in HEP:
An experiment of probability $p$ is repeated $N$ times.
Binomial

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Examples:
- Coin tossing!
- Efficiencies (detector, method, selection)
- Branching Ratios
- Asymmetries
Poisson

Limit of binomial when \( N \to \infty \) and \( p \to 0 \) with \( N \cdot p = \mu \) finite

\[
\text{Poiss} (k \mid \mu) = \frac{e^{-\mu} \mu^k}{k!} \quad \sigma(k) = \sqrt{\mu}
\]

LOTS of examples.

Any counting observable in colliders.
Poisson

Limit of binomial when $N \to \infty$ and $p \to 0$ with $N \cdot p = \mu$ finite

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Any counting observable in colliders.

For instance, in LHC:

$$N = 1.30 \times 10^{+22}$$  \hspace{1cm} (p-p crossings per bunch)

$$p = 1.93 \times 10^{-21}$$  \hspace{1cm} (production of a minbias event)

$$\mu = N \cdot p = 25$$  \hspace{1cm} (av. minbias per bunch crossing)
Actually the number of $p$ per bunch is Poissonian itself because there is a tiny probability that a proton ends up in a bunch out of a huge number of starting protons.
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But at least somewhere we start with a true binomial experiment with (large) fixed $N$:

The bottle where it all starts ...
But don’t need to go up to $N = 10^{24}$!
At $N = 30$ Poisson and Binomial already equivalent.
Binomial → Poisson, in addition to “large” N, requires

\[ \frac{10}{N} \lesssim p \lesssim 1 - \frac{10}{N} \]

And we basically always forget about binomial errors, unless \( p \) gets very close to 0 or 1:
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**Example**

75 events out of 75 pass a given cut \( \Rightarrow \varepsilon = 100\% \)
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With what error?

\[ \varepsilon = 1 \quad \text{in} \quad \sigma = \sqrt{N \varepsilon (1 - \varepsilon)} \quad \text{yields} \quad \sigma = 0 \]
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In this case the result is $[0.976, 1.0] \@ 68\% \text{ CL}$
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✧ Need Confidence Intervals,
✧ A recipe for taking them into account in fits,
✧ No $\chi^2$ fit, but maximum likelihood...
Multinomial

Generalization of the Binomial distribution.

\(N_T\) repetitions of an experiment with \(n\) possible outcomes.

Most important example: Histogram with \(n\) bins and \(N_T\) total entries

\[
\text{Mult}(\mathbf{k} \mid N_T, \mathbf{p}) = \frac{N_T!}{k_1!k_2! \cdots k_n!} p_1^{k_1} p_2^{k_2} \cdots p_n^{k_n}, \quad \sigma(k_i) = \sqrt{N_T p_i (1 - p_i)}
\]

\(k_i\) is the number of events on the \(i\)-th bin, \(\sum_{i=1}^{n} k_i = N_T\).

\(p_i\) is the probability for an event to fall on the \(i\)-th bin, \(\sum_{i=1}^{n} p_i = 1\).
Composition of Binomial and Poisson

A Binomial experiment: $\text{Binom} (k \mid N, p)$
but $N$ itself a Poisson variable: $\text{Pois} (N \mid \mu)$

$$\implies k \text{ is } \text{Pois} (k \mid \mu p)$$

Example:
The number $k$ of $t\bar{t}$ triggered on a sample $N$ is $\text{Binom} (n \mid N, \varepsilon)$
The number $N$ of $t\bar{t}$ pairs during Run2a is $\text{Pois} (N \mid \sigma \mathcal{L})$

$$\implies k \text{ is } \text{Pois} (n \mid \varepsilon \sigma \mathcal{L})$$
Composition of Multinomial and Poisson

A multinomial experiment, $\text{Mult}(k_i \mid N, p_i)$, where $N$ itself is a Poisson variable $\text{Poiss}(N \mid \mu)$.

$\Rightarrow$ $k_i$ are $n$ independent Poisson variables

\[ k_i \text{ are } \text{Poiss}(k_i \mid \mu p_i) \Rightarrow \sigma(k_i) = \sqrt{\text{E}(k_i)} \]

$\Rightarrow$ The number of entries in each bin of an histogram is Poisson.
Joint Distribution of Poisson variables

Joint probability of two Poisson \( \{x, y\} \), is the product of single Poisson \( z = x + y \) times a Binomial for observing \( x \) events in \( z \) trials.

\[
\text{Poiss} (x \mid \mu) \times \text{Poiss} (y \mid \nu) =
\]

\[
= \frac{e^{-\mu} \mu^x}{x!} \times \frac{e^{-\nu} \nu^y}{y!}
\]

\[
= \frac{e^{-\mu} \mu^x}{x!} \times \frac{e^{-\nu} \nu^{z-x}}{(z-x)!}
\]

\[
= \frac{e^{-(\mu+\nu)} (\mu + \nu)^z}{z!} \times \frac{z!}{x!(z-x)!} \left( \frac{\mu}{\mu + \nu} \right)^x \left( 1 - \frac{\mu}{\mu + \nu} \right)^{z-x}
\]

\[
= \text{Poiss} (z \mid \mu + \nu) \times \text{Binom} (x \mid z, \frac{\mu}{\mu + \nu})
\]
Application to test of Poisson ratios

Measure \[ \begin{align*}
    n_P & \text{ in the peak region} \\
    n_C & \text{ in control region ("sidebands")}
\end{align*} \]

with \( \tau \) the ratio of expected backgrounds in control and peak region

\[ \begin{align*}
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Suppose we want to test \( H_0 : s = 0 \) via \( n_C/n_P \approx \tau. \)
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But if \( s = 0 \), \( n_P \sim \text{Poiss} (b) \) and \( n_C \sim \text{Poiss} (\tau b) \),
or \( n_P + n_C \sim \text{Poiss} (b + \tau b) \) and \( n_p \sim \text{Binom} (n_P + n_C, \frac{1}{1+\tau}) \)
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The fraction of measured events that are in the “peak” region, \( n_P/(n_P + n_C) \), is a Binomial variable that measures \( \frac{1}{1+\tau} \)
Application to test of Poisson ratios

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\( \Rightarrow \) Test on ratio of Poisson variables is test on a Binomial.
Story of a rediscovery ...

This standard method was elucidated for Botanics (testing clover seed for dodder) by
Przyborowski and Wilenski, Biometrika 31 (1940) 313

and generalized for Zoology (studying salmon fry migration)

The same result was obtained in the HEP community by
“Errors on Ratios of Small Numbers of Events”

and in the GRA community
“Confidence limits for small numbers of events in astrophysical data”
Chi-square

\[ y \equiv x^2: \]

If \( x \in (-\infty, \infty) \) is \( x \sim N(0, 1) \) then \( y \in [0, \infty) \) is \( y \sim \chi^2(1) \).

For \( n \) independent \( x_i \sim N(0, 1) \):

\[ y \equiv \sum_{i}^{n} x_i^2 \Rightarrow y \sim \chi^2(n). \]

The exponent in the \( n \)-dim multinormal

\[
f(x) = \frac{1}{\sqrt{(2\pi)^n|V|}} \exp \left[-\frac{1}{2} (x - \mu)^T V^{-1} (x - \mu) \right]
\]

is itself a \( \chi^2(n) \) random variable.
Central limit theorem

Given 2 random variables $x_1$ and $x_2$, its sum $y = x_1 + x_2$ will be a new random variable with a different distribution.

Example: the sum of two flat distributions is the triangular distribution.

Example 2:
Sum of $n$ independent random $x_i$, with $E(x_i) = \mu_i$ and $Var(x_i) = \sigma_i^2$. tends to a $N(\mu, \sigma)$, with $\mu = \sum_i^n \mu_i$ and $\sigma^2 = \sum_i^n \sigma_i^2$. 

![Histograms showing the distribution of the sum of independent random variables.](image)
Sum of $n$ independent random $x_i$, with $E(x_i) = \mu_i$ and $\text{Var}(x_i) = \sigma_i^2$. tends to a $N(\mu, \sigma)$, with $\mu = \sum_i^n \mu_i$ and $\sigma^2 = \sum_i^n \sigma_i^2$.
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Central limit theorem: Special cases

- Sum of Binomials with equal $p$ is Binomial:
  
  \[
  \text{Binom}(n_1, p) + \text{Binom}(n_2, p) = \text{Binom}(n_1 + n_2, p) \\
  \implies \text{Binom}(n, p) \to \mathcal{N}(np, \sqrt{np(1-p)}) \text{ for large } n
  \]

- Sum of Poissonians is Poisson:
  
  \[
  \text{Poiss}(\mu_1) + \text{Poiss}(\mu_2) = \text{Poiss}(\mu_1 + \mu_2) \\
  \implies \text{Poiss}(\mu) \to \mathcal{N}(\mu, \sqrt{\mu}) \text{ for large } \mu.
  \]

- Sum of Chi-squares is Chi-square:
  
  \[
  \chi^2(n_1) + \chi^2(n_2) = \chi^2(n_1 + n_2) \\
  \implies \chi^2(n) \to \mathcal{N}(n, \sqrt{2n}) \text{ for large } n.
  \]
The typical analysis we face is composed of roughly four steps

*Physics language*  
“Best fit” of parameters  
Errors on the parameters  
Judging quality of the fit  
Compare to theory

*Statisticians terminology*  
Point estimation  
Confidence region (at given C.L.)  
Goodness-of-fit testing  
Hypothesis testing (at significance level)
Point Estimation

A random variable depends on a parameter $\theta$: $f(x \mid \theta)$

By measuring a sample $x = \{x_1, x_2, \ldots, x_n\}$ we want to infer the value of $\theta$.

An estimator $\hat{\theta}$ of the parameter $\theta$

- is a random variable,
- function of the sample $x$: $\hat{\theta} = \hat{\theta}(x_1, \ldots, x_n)$
- that can have the following properties: Consistency, Bias, Efficiency, Sufficiency, Robustness

Consistency (for an infinite sample):

$$\lim_{n \to \infty} \hat{\theta} = \theta$$
Bias

Bias is defined for a finite sample: $b \equiv \mathbb{E}(\hat{\theta}) - \theta$

An estimator is unbiased if $\mathbb{E}(\hat{\theta}) = \theta$

Classical example: Two consistent estimators for $\sigma^2$

$$S^2 = \frac{1}{n} \sum_{i} (x_i - \bar{x})^2 \quad \text{biased estimator with} \quad b = -\frac{\sigma^2}{n}$$

$$s^2 = \frac{1}{n-1} \sum_{i} (x_i - \bar{x})^2 \quad \text{unbiased}$$
Efficiency

There can be numerous consistent unbiased estimators of $\theta$ in $f(x \mid \theta)$: $\hat{\theta}_1$, $\hat{\theta}_2$, $\hat{\theta}_3$, with different variances.

There is a minimum attainable variance given by Cramer-Rao bound:

$$\forall \hat{\theta}(x) \text{ with } E(\hat{\theta}) = \theta :$$

$$\text{Var}(\hat{\theta}) \geq \sigma_{\text{min}}^2 = \frac{1}{E \left[ (\frac{\partial}{\partial \theta} \sum_i \log f(x_i \mid \theta))^2 \right]}$$

Efficiency $\hat{\theta} \equiv \frac{\sigma_{\text{min}}^2}{\text{Var}(\hat{\theta})}$
Example: \( x_i \sim N(\mu, \sigma_i) \)

\( n \) measurements of same physical quantity, different errors.

Three unbiased estimators of \( \mu \):

\[
\hat{\mu}_2(x) = \frac{\sum (x_i / \sigma^2)}{\sum (1 / \sigma^2)}
\]
\[
\hat{\mu}_1(x) = \frac{\sum (x_i / \sigma)}{\sum (1 / \sigma)}
\]
\[
\hat{\mu}_0(x) = \frac{\sum x_i}{n}
\]

\( \sigma(\hat{\mu}_2) < \sigma(\hat{\mu}_1) < \sigma(\hat{\mu}_0) \)

\( \hat{\mu}_2 \) is 100\% Efficient only for \( x_i \) gaussian,

Sufficiency: we don’t lose information when replacing the \( n \) measurements \( x \), by the sole number \( \hat{\theta}(x) \).

Robustness: not unduly affected by small departures from model assumptions (e.g., insensitivity to what goes on at the tails of the distribution)
The likelihood function

Random variable that depends on $\theta$: $f(x \mid \theta)$

The probability to obtain the $n$ independent measurements $\{x_i\}$ is

$$f(x \mid \theta) = \prod_{i=1}^{n} f(x_i \mid \theta)$$

The likelihood function is exactly this same expression, but thought as a function of $\theta$, given the measurements $\{x_i\}$

$$L(\theta \mid x) \text{ or } L(x \mid \theta) \equiv \prod_{i=1}^{n} f(x_i \mid \theta)$$

The notation $L$ stresses that we mean fixed data $\{x_i\}$.

$L(\theta \mid x)$ in not a probability density for $\theta$: $\int L(\theta \mid x)\,d\theta \neq 1$
Maximum likelihood estimator

Obtain the estimator $\hat{\theta}$ by maximizing $\mathcal{L}$:

$$\frac{\partial \mathcal{L}(\theta \mid x_i)}{\partial \theta} \bigg|_{\theta = \hat{\theta}} = 0$$

Solution of this equation (analytical or numerical) yields $\hat{\theta} = \hat{\theta}(x)$.

Properties:

- ML estimators are consistent.
- ML will produce a sufficient, 100% efficient estimator, if it exists.
- ML estimators are asymptotically 100% efficient, sufficient and unbiased.
Method of least squares

When the probability $f(x \mid \theta)$ is gaussian, the maximum likelihood principle yields the method of least squares, also known as “minimizing” the $\chi^2$ (square of a gaussian)

$$\mathcal{L}(x \mid \theta) = C \prod_{i=1}^{n} e^{-\frac{1}{2} \left( \frac{x_i - \mu}{\sigma} \right)^2} \implies \log \mathcal{L} = -\frac{1}{2} \sum_{i=1}^{n} \left( \frac{x_i - \mu}{\sigma} \right)^2 + C'$$

Maximizing $\mathcal{L}$ equals minimizing the sum of gaussians squared.

If $f(x \mid \theta)$ is not gaussian, one can still apply least squares.

Gauss-Markov Theorem: Among all unbiased estimators that are linear in the data (gaussian or not gaussian), the Least Squares method produces the estimator with smallest variance.
The second step in you job, is to find the error on the parameter you have estimated
Confidence Interval: Simple gaussian case

Random variable $x$ with gaussian distribution $\mathcal{N}(x \mid \mu, \sigma)$

Assume that the precision of the instrument, $\sigma$ is known.

Perform a measurement and obtain $x$. Probability then states

$$P \left( \mu - \sigma \leq x \leq \mu + \sigma \right) = 0.6827 \approx 0.68$$

But

$$\mu - \sigma \leq x \implies \mu \leq x + \sigma \quad \text{and} \quad x \leq \mu + \sigma \implies x - \sigma \leq \mu$$

Then

$$P \left( x - \sigma \leq \mu \leq x + \sigma \right) = 0.68$$
Last equation again:

\[ P( x - \sigma \leq \mu \leq x + \sigma ) = 0.68 \]

This doesn’t mean that \( \mu \) has a 68% probability of being in \( x \pm \sigma \).

\( \mu \) is NO random variable, it is a FIXED parameter.

Here \([x - \sigma, x + \sigma]\) is a random interval, that will contain the fixed parameter \( \mu \), 68% of the time .

This is the frequentist interpretation of “error”

We write \( x \pm \sigma \) and \( x \pm 2\sigma \) meaning 68% and 95% CL intervals.
Neyman’s construction

It is not always possible to isolate analytically the parameter of interest. For instance, we have a $n$ measurements $x_i \sim N(\mu, \sigma)$. Want to estimate $\sigma^2$ with its error (confidence region at 68% CL). Use the well known unbiased estimator

$$s^2 = \frac{1}{n-1} \sum_{i}^{n} \left( x_i - \frac{\sum x_i}{n} \right)^2$$

To get the error need the distribution of the random variable $s^2$. $x_i \sim N(\mu, \sigma) \implies \frac{(n-1)s^2}{\sigma^2} = \frac{1}{\sigma^2} \sum_{i}^{n} (x_i - \bar{x})^2 \sim \chi^2_{n-1}$

Note that the distribution of $s^2$ depends on the unknown parameter $\sigma^2$.
For each $\sigma^2$, get $s_d^2$ and $s_u^2$: \[ \int_0^{s_d^2} \chi^2_{n-1} \, du = 0.16 \quad \int_{s_u^2}^\infty \chi^2_{n-1} \, du = 0.16 \]
For each $\sigma^2$, get $s_d^2$ and $s_u^2$: $\int_0^{s_d^2} \chi_{n-1}^2 \, du = 0.16$ $\int_{s_u^2}^{\infty} \chi_{n-1}^2 \, du = 0.16$
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Coverage

By construction, for all values of the unknown $\sigma^2$:

$$P(\sigma^2 \in [\sigma_d^2, \sigma_u^2]) = 0.68 \quad \forall \sigma^2$$

This expresses that the “confidence belt” we built has coverage:

A method is said to yield a $100 \alpha \%$ Confidence Interval if, were the experiment to be repeated many times, the resulting intervals would include (or cover) the true parameter at least $100 \alpha \%$ of the time, no matter what the value of the true parameter is.

Coverage is, in the frequentist approach, the main property which confidence intervals have to fulfill.
The construction of the confidence belt is far from unique.

In the example we have built the “central” C.I.

one could choose the “shortest”, or upper, or lower, limits.

The confidence belt depends also on which estimator you choose for your measurement.

Some choices for classical confidence intervals

| Central interval | $P(x \leq x_d \mid \theta) = P(x \geq x_u \mid \theta) = (1 - \alpha)/2$ |
| Equal probability densities | $f(x_d \mid \theta) = f(x_u \mid \theta)$ |
| Minimum size | $\theta_{\text{high}} - \theta_{\text{low}}$ is minimum |
| Symmetric | $\theta_{\text{high}} - \hat{\theta} = \hat{\theta} - \theta_{\text{low}}$ |
| Upper limit | $\theta_{\text{low}} = -\infty$ |
| Lower limit | $\theta_{\text{high}} = +\infty$ |
| Likelihood ratio ordering | $f(x_d \mid \theta)/f(x_d \mid \theta_{\text{best}}) = f(x_u \mid \theta)/f(x_u \mid \theta_{\text{best}})$ |
A few more confidence belts for free ...
A few more confidence belts for free ...
A few more confidence belts for free ...
A few more confidence belts for free ...
A few more confidence belts for free ...
A few more confidence belts for free ...
A few more confidence belts for free ...
Confidence Interval: Two-dimensional case
Central 68% confidence belt for a gaussian $N(\mu, 1)$ when for physics reasons we know $\mu \geq 0$ (like a mass or a production ratio) 

$\forall \mu \geq 0$, obtain $[x_1(\mu), x_2(\mu)]$ as $P(x < x_1 \mid \mu) = P(x > x_2 \mid \mu) = 0.16$. 

Confidence Interval near a bound
If measure: $x = +3.0 \implies 2 < \mu < 4$ at 68% CL
If measure: $x = +0.8 \implies 0 < \mu < 1.8$ at 68% CL
If measure: $x = -0.8 \implies 0 < \mu < 0.2$ at 68% CL
If measure: $x = -1.5 \implies$ Empty C.I at 68% CL
If measure: $x = +3.0$ $\implies$ $2 < \mu < 4$ at 68% CL

If measure: $x = +0.8$ $\implies$ $0 < \mu < 1.8$ at 68% CL

If measure: $x = -0.8$ $\implies$ $0 < \mu < 0.2$ at 68% CL

If measure: $x = -1.5$ $\implies$ Empty C.I at 68% CL

If you don’t like this, means you’re a potential Bayesian!
IS THIS WRONG?
IS THIS WRONG?  Nope.
IS THIS WRONG?  

Nope.

Frequentists say that in 68% of the cases your interval contains the true value of $\mu$ (remember *coverage*?)

This means 32% of the cases IT WILL NOT.

If you got an empty interval: TOO BAD, you fell in the unlucky 32%!

Trouble is you KNOW you were unlucky and you don’t like it
And what about $0 < \mu < 0.2$ with 68% C.L.?

How come we got so precise in an experiment when $\sigma = 1$?

Answer: It’s not supposed to mean that you have 68% belief that the true $\mu$ is in your interval.

It doesn’t say anything about your particular interval.

It says something about the set of CI of experiments you didn’t do.

In fact, in cases where $\mu$ is physically within a bounded domain, you could get a 68% CI that covers the whole domain!

Imagine publishing:

The branching ratio is between 0 and 1 with 68% CL!
The Bayesian way

Bayesians on the contrary do MEAN that
if you say $0 < \mu < 0.2$ (68% C.L.)
then it’s because you are ready to bet
with odds 68/32 ($\sim 2/1$) that $\mu$ IS in the interval.

And if your CI covers the whole domain,
for bayesians that is a 100% CL.

Of course in Bayesian statistics you can never get an empty interval.
Then ...
Then ...

Why isn’t every physicist a Bayesian?

Robert D. Cousins

Department of Physics, University of California, Los Angeles, California 90024-1547

(Received 1 June 1994; accepted 3 November 1994)
Then ...

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The price to pay is that you have to think of the charge of the electron as a random variable. But that’s not the only price.
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“Frequentists use impeccable logic to deal with an issue of no interest to anyone”

“Bayesians address the question everyone is interested in, by using assumptions no-one believes”
Discrete case: Poisson process with background

Observe $n$ events, from unknown signal $\mu$ and background $b = 3$

$$P(n \mid \mu) = \text{Poiss}(n \mid \mu + b) = \frac{e^{-(\mu+b)}(\mu + b)^n}{n!}$$

Confidence belt at 100 $\alpha$ % CL:
for each $\mu$ find $[n_1, n_2]$ such that $P(n \in [n_1, n_2] \mid \mu) = \alpha$

Central 90%: $P(n < n_1 \mid \mu) = 0.05$ and $P(n > n_2 \mid \mu) = 0.05$

Upper 90%: $P(n < n_1 \mid \mu) = 0.10$

Let’s look at $n_1$ for the upper limit

$$0.10 = P(n < n_1 \mid \mu) = \sum_{n=0}^{n_1-1} \frac{e^{-(\mu+3)}(\mu + 3)^n}{n!}$$
Since \( n_1 \) is discrete, only have exact solutions for certain \( \mu \).

\[
0.10 = P(n < n_1 | \mu)
\]

\( n_1 = 1 \):
\[
0.10 = e^{-(\mu+3)} \times 1 \quad \implies \text{no solution}
\]

\( n_1 = 2 \):
\[
0.10 = e^{-(\mu+3)} \times \left[ 1 + (\mu + 3) \right] \quad \implies \mu = 0.88972
\]

\( n_1 = 3 \):
\[
0.10 = e^{-(\mu+3)} \times \left[ 1 + (\mu + 3) + \frac{1}{2}(\mu + 3)^2 \right] \quad \implies \mu = 2.32232
\]

Exact coverage is not possible: either “overcover” or “undercover”.

Avoid undercoverage by replacing

\[
P(n \in [n_1, \infty) | \mu) = 0.90 \quad \implies \quad P(n \in [n_1, \infty) | \mu) \geq 0.90
\]

Thus the choice is

\[
0.0 \leq \mu < 0.88972 \quad \implies \quad n_1 = 2
\]
\[
0.88972 \leq \mu < 2.32232 \quad \implies \quad n_1 = 3
\]
Minimum overcoverage 90% C.L. confidence belts for central confidence intervals and upper limit, for unknown Poisson signal mean and Poisson background $b = 3$. 
With the choice \( P \left( n \in [n_1, n_2] \mid \mu \right) \geq \alpha \)

The intervals overcover and are conservative.

This is unavoidable for discrete distributions, but NO good.

A 90% C.I.interval *should* fail 10% of the time.

If want intervals that cover more than 90%, don’t add conservatism, but rather go to higher confidence levels.
Flip-Flopping

**Ideal Physicist**
- Choose Strategy
- Examine data
- Quote result

**Real Physicist**
- Examine data
- Choose Strategy
- Quote Result

Example:

You have a background of 3.2

Observe 5 events? No discovery: Quote one-sided upper limit

Observe 25 events? Discovery: Quote two-sided confidence interval.
An experiment designed to measure a positive quantity;

Which one to use?
One may choose the following strategy:

If the result $x$ is less than $3 \sigma$ above zero, state an upper limit.

If greater than $3 \sigma$, state a central confidence interval.

If measured value is negative, be conservative and pretend measured zero when calculating interval.
One may choose the following strategy:

If the result $x$ is less than $3 \sigma$ above zero, state an upper limit.

If greater than $3 \sigma$, state a central confidence interval.

If measured value is negative, be conservative and pretend measured zero when calculating interval.
For $\mu = 2.0$, acceptance interval is $x_1 = 2 - 1.28$ and $x_2 = 2 + 1.64$,

$$P(x_1 \leq x \leq x_2 \mid \mu = 2.0) = 85\% < 90\% \Rightarrow \text{intervals undercover}$$

They are not confidence intervals and certainly not “conservative” CI.
Problems:

- If you use the data to decide which plot to use, the hybrid method can undercover.
- Your CI can be the empty set, or unreasonably “precise”.
- “Worse” experiment with larger expected background can get “better” CI.

Let’s discuss briefly this 3\textsuperscript{rd} point.
CASE I: Experiment expects no background, and observes no signal. Frequentist 90% upper limit? Reject all values of $\mu$ for which

$$P(0 \mid \mu) = \text{Poiss}(0 \mid \mu) = \exp(-\mu) \text{ is less than 10\%}$$

$$P(0 \mid \mu_{\text{reject}}) < 0.10$$

$$\exp(-\mu_{\text{reject}}) < 0.10$$

$$-\mu_{\text{reject}} < \log 0.10 = -\log 10$$

$$\mu_{\text{reject}} > 2.30$$

CASE II: Experiment expects mean background $b$, observes no signal.

$$P(0 \mid \mu) = \text{Poiss}(0 \mid \mu + b) = \exp[-(\mu + b)]$$

$$P(0 \mid \mu_{\text{reject}}) < 0.10$$

$$\exp[-(\mu_{\text{reject}} + b)] < 0.10$$

$$-(\mu_{\text{reject}} + b) < \log 0.10$$

$$\mu_{\text{reject}} > 2.30 - b$$
90% CL frequentist and Bayesian upper limits for $n = 0$ observed events and background expectation $b$

<table>
<thead>
<tr>
<th></th>
<th>$b = 0$</th>
<th>$b = 1$</th>
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<th>$b = 4$</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Standard Classical</strong></td>
<td>2.30</td>
<td>1.30</td>
<td>0.30</td>
<td>$\emptyset$</td>
<td>$\emptyset$</td>
</tr>
<tr>
<td><strong>Unified Classical</strong></td>
<td>2.44</td>
<td>1.61</td>
<td>1.26</td>
<td>1.08</td>
<td>1.01</td>
</tr>
<tr>
<td><strong>Uniform Bayesian</strong></td>
<td>2.30</td>
<td>2.30</td>
<td>2.30</td>
<td>2.30</td>
<td>2.30</td>
</tr>
</tbody>
</table>

The same problem that in the gaussian case.

If the experiment measures $n = 0$ it yields an empty set.

Should the experiment report “No result at 90% CL”?
The “unified” approach: Feldman-Cousins

Back to the confidence belt for a Poisson experiment with $b = 3$

Consider the horizontal acceptance interval at signal mean $\mu = 0.5$

The probability of obtaining $n = 0$ events is $\exp[-(0.5 + 3)] = 0.03$

Pretty low. But, compared to what?

If we got $n = 0$, our best bet for $\mu$ is $\mu_{\text{best}} = 0$

And for our best bet, the probability is $P(0 \mid \mu_{\text{best}}) = 0.05$

Now, 0.03 is not much smaller than 0.05, so $\mu = 0$ is not that bad.

Take the ratio $0.03/0.05 = 0.607$ as figure of merit for $\mu = 0$ hypothesis.
For each $n$ let $\mu_{\text{best}}$ be that value of $\mu$ which maximizes $P(n \mid \mu)$ within the physically allowed region (non-negative $\mu$).

Thus, $\mu_{\text{best}} = \max(0, n - b)$.

Choose what values of $n$ to include in the confidence belt following a merit ordering based on the ratio of likelihoods

$$R = \frac{L(n \mid \mu)}{L(n \mid \mu_{\text{best}})}$$
Confidence Interval

The “unified” approach: Feldman-Cousins

R.Piegaia  HCPSS08/Statistics

Construction of confidence belt for signal mean $\mu = 0.5$
in the presence of known mean background $b = 3.0$.

<table>
<thead>
<tr>
<th>$n$</th>
<th>$P(n \mid \mu)$</th>
<th>$\mu_{\text{best}}$</th>
<th>$P(n \mid \mu_{\text{best}})$</th>
<th>$R$</th>
<th>rank</th>
<th>U.L.</th>
<th>central</th>
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</thead>
<tbody>
<tr>
<td>0</td>
<td>0.030</td>
<td>0.0</td>
<td>0.050</td>
<td>0.607</td>
<td>6</td>
<td></td>
<td></td>
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<tr>
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<td>0.0</td>
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<tr>
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<tr>
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</tr>
<tr>
<td>5</td>
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<tr>
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<tr>
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</tr>
<tr>
<td>9</td>
<td>0.007</td>
<td>6.0</td>
<td>0.132</td>
<td>0.050</td>
<td></td>
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<td></td>
</tr>
<tr>
<td>10</td>
<td>0.002</td>
<td>7.0</td>
<td>0.125</td>
<td>0.018</td>
<td></td>
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<td></td>
</tr>
<tr>
<td>11</td>
<td>0.001</td>
<td>8.0</td>
<td>0.119</td>
<td>0.006</td>
<td></td>
<td>✓</td>
<td></td>
</tr>
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</table>
This process is repeated for each $\mu$ and yields

Because of the discreteness of $n$, the acceptance region contains a summed probability greater than 90%.
Comparison of standard and unified confidence confidence belts

\[ \text{Signal Mean } \mu \]

\begin{align*}
\text{Measured } n & \quad 15 & 14 & 13 & 12 & 11 & 10 & 9 & 8 & 7 & 6 & 5 & 4 & 3 & 2 & 1 & 0 \\
0 & 1 & 2 & 3 & 4 & 5 & 6 & 7 & 8 & 9 & 10 & 11 & 12 & 13 & 14 & 15
\end{align*}
**FC: Gaussian case near physical boundary**

For a particular \( x \), \( \mu_{\text{best}} \) is the physically allowed value of \( \mu \) for which \( P(x \mid \mu) \) is maximum. This is \( \mu_{\text{best}} = \max(0, x) \)

\[
P(x \mid \mu_{\text{best}}) = \begin{cases} 
1/\sqrt{2\pi}, & x \geq 0 \\
\exp\left(-x^2/2\right)/\sqrt{2\pi}, & x < 0.
\end{cases}
\]

And the likelihood ratio \( R \) :

\[
R(x) = \frac{P(x \mid \mu)}{P(x \mid \mu_{\text{best}})} = \begin{cases} 
\exp\left(-(x - \mu)^2/2\right), & x \geq 0 \\
\exp(x\mu - \mu^2/2), & x < 0.
\end{cases}
\]

For a given \( \mu \), the acceptance interval \([x_1, x_2]\) satisfies

\[
R(x_1) = R(x_2) \quad \text{and} \quad \int_{x_1}^{x_2} P(x \mid \mu) \, dx = \alpha
\]

Here the coverage is exactly 90% by construction.
Comparison of standard and unified confidence confidence belts
FC does not solve the problem of shrinking CI for increasing background

90% CL frequentist and Bayesian upper limits for $n = 0$ observed events and background expectation $b$

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FC advocate to inform also the sensitivity of the experiment:
the average upper limit one would get from an ensemble of
experiments with your expected background and no true signal.
Preliminary result from CDF on the top quark charge

$f^+$ is fraction of pairs with top charge assigned to $+\frac{2}{3}$ via a jet charge algorithm using the charge of the tracks associated to the jet weighted by their momentum projection on the jet axis.

The measured value 0.87 yields a lower bound 0.6 @68% CL

Notice that a measurement above 1.2 would give extremely narrow confidence intervals.
Feldman and Cousins Summary

- Avoids forbidden regions and empty results in a Frequentist way
- Solves flip-flopping, it “unifies” central and upper limit belts
- Makes us more honest (a bit)
- Can lead to 2-tailed limits where you don’t want claim discovery
- Not easy to calculate and extend to systematic errors
- Unphysically small Confidence intervals still present
- Shrinking CI for increasing background
- Upper limits may tighten when including systematic errors
| Bayes’ theorem | R.Piegaia | HCPSS08/Statistics | 68 |
Bayes’ theorem

Conditional probability: given two events $x$ and $y$

$$P(x \mid y) = \frac{P(x \cap y)}{P(x)}$$

Example, rolling dice:

$$P(n < 3 \mid n \text{ even}) = \frac{P(n < 3 \cap n \text{ even})}{P(n \text{ even})} = \frac{1/6}{3/6} = \frac{1}{3}$$

Let $S$ be a sample (set) that can be divided in exclusive events $Y_i$:

$$Y_i \cap Y_j = \varnothing, \ i \neq j \quad \text{and} \quad \sum_i P(Y_i) = 1$$

For any event $X$, Bayes theorem states:

$$P(Y_k \mid X) = \frac{P(X \mid Y_k) P(Y_k)}{\sum_i (X \mid Y_i) P(Y_i)}$$
Example:
Particles entering a threshold Cerenkov detector can be $e$, $\pi$ or $K$, with $P(e) = 1\%$, $P(\pi) = 70\%$ and $P(K) = 29\%$.
The probabilities that the detector fires (efficiencies) are $P(C \mid e) = 99\%$, $P(C \mid \pi) = 2\%$, $P(C \mid K) = 1\%$.
A particle fired the detector, what is the probability that it’s an $e$?

$$P(e \mid C) = \frac{P(C \mid e)P(e)}{P(C \mid e)P(e) + P(C \mid \pi)P(\pi) + P(C \mid K)P(K)}$$

$$= \frac{0.99 \times 0.01}{0.99 \times 0.01 + 0.02 \times 0.70 + 0.01 \times 0.29} = 0.37$$

A rather selective detector, but 63\% of signals will be background.
Notice that $P(C \mid e, \pi, K)$ is what we know about our detector),
$C$ or $\bar{C}$ is the result of the experiment, and
$P(e, \pi, K \mid C$ or $\bar{C}$) is what we want to learn from our experiment.
With the Bayesian extension of the interpretation of probability, if we have several competing hypothesis $H_i$ and the respective theoretical expectations $P(E \mid H_i)$, we can calculate the probability of hypothesis $H_k$, given that the result of the experiment was $E$

$$P(H_k \mid E) = \frac{P(E \mid H_k) P(H_k)}{\sum_i P(E \mid H_i) P(H_i)}$$

$P(E \mid H_i) \rightarrow$

Theoretical prediction: Probability of result $E$ assuming hypothesis $H_i$

$P(H_i \mid E) \rightarrow$

Experimental inference: Degree of belief on $H_i$ given we obtained $E$. 
Bayes’ theorem

- \( P(\text{Data} \mid \text{Theory}) \neq P(\text{Theory} \mid \text{Data}) \)
  - Theory = female or male
  - Data = pregnant or non-pregnant
  - \( P(\text{pregnant} \mid \text{female}) = 1\% \)
  - \( P(\text{female} \mid \text{pregnant}) \gg 1\% \)
- To invert probabilities \( P(E \mid H_k) \rightarrow P(H_k \mid E) \), need \( P(H_i) \)
Instead of discrete probabilities $P(Y)$, we have density functions $f(y)$.

Conditional probability:

$$P(X \mid Y) \equiv \frac{P(X \cap Y)}{P(X)} \quad \text{Continuous case} \quad f(x \mid y) \equiv \frac{f(x, y)}{f(x)}$$

Bayes Theorem:

$$P(Y_k \mid X) = \frac{P(X \mid Y_k) P(Y_k)}{\sum_i P(X \mid Y_i) P(Y_i)} \quad \text{Continuous case} \quad f(y \mid x) = \frac{f(x \mid y) f(y)}{\int f(x \mid y) f(y) \, dy} \propto$$
Example: The 200 GeV CERN muon beam had an approximately gaussian energy distribution

\[ f(E_b) = \frac{1}{\sqrt{2\pi}\sigma_b} \exp\left[-\frac{1}{2} \left( \frac{E_b - \mu_b}{\sigma_b} \right)^2 \right] \]

with \( \mu_b = 200 \text{ GeV} \) and \( \sigma_b = 5 \text{ GeV} \).

The EMC spectrometer measured the energy of *each* incoming muon with a gaussian uncertainty of 0.5\% (\( \sigma_b = 1 \text{ GeV} \)), basically due to the spatial resolution of the chambers and the magnetic field calibration.

\[ f(E_m \mid E_b) = \frac{1}{\sqrt{2\pi}} \exp\left[-\frac{(E_m - E_b)^2}{2} \right] \]

Question: For a certain event the measured energy is \( E_m = 208 \text{ GeV} \). What’s the probability distribution of the true energy \( E_b \) *after* the measurement?

Plug \( f(E_b) \) and \( f(E_m \mid E_b) \) into

\[ f(E_b \mid E_m) = \frac{f(E_m \mid E_b) f(E_b)}{\int f(E_m \mid E_b) f(E_b) \, dE_b} \]

to find it’s a Gaussian \( N(207.5, 0.9) \).

An undisputed *frequentist* use of Bayes’ theorem.