Lectures on Statistics in Theory: Prelude to Statistics in Practice

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August 29, 2023

Abstract

This is a writeup of lectures on “statistics” that have evolved from the 2009 Hadron Collider Physics Summer School at CERN to the forthcoming 2018 school at Fermilab. The emphasis is on foundations, using simple examples to illustrate the points that are still debated in the professional statistics literature. The three main approaches to interval estimation (Neyman confidence, Bayesian, likelihood ratio) are discussed and compared in detail, with and without nuisance parameters. Hypothesis testing is discussed mainly from the frequentist point of view, with pointers to the Bayesian literature. Various foundational issues are emphasized, including the conditionality principle and the likelihood principle.
Contents

1 Introduction 6

2 Preliminaries 7
  2.1 Why foundations matter 7
  2.2 Definitions are important 7
  2.3 Key tasks: Important to distinguish 8

3 Probability 9
  3.1 Definitions, Bayes’s theorem 9
  3.2 Example of Bayes’s theorem using frequentist $P$ 11
  3.3 Example of Bayes’s theorem using Bayesian $P$ 11
  3.4 A note re Decisions 13
  3.5 Aside: What is the “whole space”? 13

4 Probability, probability density, likelihood 13
  4.1 Change of observable variable (“metric”) $x$ in pdf $p(x|\mu)$ 14
  4.2 Change of parameter $\mu$ in pdf $p(x|\mu)$ 15
  4.3 Probability integral transform 16
  4.4 Bayes’s theorem generalized to probability densities 16

5 Bayesian analysis 17
  5.1 Can “subjective” be taken out of “degree of belief”? 18
  5.2 “Uniform prior” requires a choice of metric 18
  5.3 Jeffreys’s choice of metric in which prior is uniform 18
    5.3.1 Reference priors of Bernardo and Berger 19
  5.4 What to call such non-subjective priors? 19
  5.5 Whatever you call them, non-subjective priors cannot represent ignorance! 20
  5.6 Priors in high dimensions 20
  5.7 Types of Bayesians 21
  5.8 Do “Bayesians” care about frequentist properties of their results? 22
  5.9 Analysis of sensitivity to the prior 22
  5.10 Bayesian must-read list for HEP/Astro/Cosmo (including discussion!) 22
  5.11 Pseudo-Bayesian analyses 23

6 Frequentist estimation: confidence intervals 24
  6.1 Notation 25
  6.2 The basic idea of confidence intervals in two sentences 25
    6.2.1 Ordering principle is required for possible values of $x$ 25
    6.2.2 A “confidence level” must be specified 26
    6.2.3 One-sentence summary 26
  6.3 Correspondence between upper/lower limits and central confidence intervals 26
  6.4 Gaussian pdf $p(x|\mu, \sigma)$ with $\sigma$ a function of $\mu$: $\sigma = 0.2\mu$ 26
    6.4.1 What is the central confidence interval for $\mu$? 28
    6.4.2 Contrast Wilson reasoning with “Wald interval” reasoning 30
6.5 Confidence intervals for binomial parameter $\rho$ ........................................... 30
6.5.1 What central confidence interval should we report for $\rho$? ...................... 31
6.5.2 Gaussian approximation for binomial confidence intervals: Wilson score
interval of 1927 ........................................................... 32
6.5.3 Gaussian approximation for binomial confidence intervals: potentially
disastrous Wald interval to avoid ............................................. 33
6.5.4 HEP applications of confidence intervals for binomial parameter ........ 33
6.6 Perceived problems with upper/lower limits and hence for central confidence
intervals ........................................................................ 33
6.7 Beyond upper/lower limits and central confidence intervals .................. 34
6.8 Neyman’s Construction of Confidence Intervals ........................................ 34
6.9 Famous confusion re Gaussian $p(x|\mu)$ where $\mu$ is mass $\geq 0$ ............ 35
6.10 Confidence belts .............................................................. 37
6.11 Confidence intervals and coverage ......................................................... 38
6.11.1 Over-coverage when observable $x$ is discrete ........................................ 38

7 Frequentist (classical) hypothesis testing ..................................................... 39
7.1 The choice of Type I error probability $\alpha$ ............................................... 39
7.2 Frequentist hypothesis testing: Simple hypotheses .................................. 40
7.2.1 Testing Simple hypotheses: Neyman–Pearson lemma .......................... 40
7.3 Nested hypothesis testing ........................................................................ 41
7.4 Nested hypothesis testing: Duality with intervals .................................... 41
7.5 Feldman-Cousins ...................................................................................... 42
7.6 Post-data $p$-values and $Z$-values ............................................................. 42
7.6.1 Interpreting $p$-values and $Z$-values ................................................... 42
7.6.2 Early CMS Higgs boson spin-parity test of $0^+ \text{ vs. } 0^-$ ...................... 43
7.6.3 Post-data choice of the C.L. ................................................................. 45
7.7 Classical frequentist goodness of fit (g.o.f.) .............................................. 45

8 Likelihood (ratio) intervals for 1 parameter ............................................... 46
8.1 LR interval example: Gaussian pdf $p(x|\mu, \sigma)$ with $\sigma = 0.2\mu$ ............ 46
8.2 Binomial likelihood-ratio interval example .............................................. 46
8.3 Poisson likelihood-ratio interval example ................................................. 46

9 Likelihood principle ...................................................................................... 47
9.1 Likelihood principle example #1: the “Karmen problem” ......................... 48
9.2 Likelihood principle example #2: binomial stopping rule ......................... 49
9.3 Stopping rule principle ............................................................................. 50
9.4 Likelihood principle discussion ................................................................. 50

10 Summary of three ways to make intervals ............................................... 50

11 1D parameter space, 2D observation space ............................................. 52
11.1 Conditioning: Restricting the sample space used
by frequentists ............................................................................ 52
C Look-elsewhere effect 81

D Bayesian hypothesis testing (model selection) 81

E Point estimation 82
   E.0.1 Point estimation: Traditional desiderata . . . . . . . . . . . . . . . . . . . . . . . 82
   E.0.2 Alternatives to the arithmetic mean when model is non-Gaussian . . 83
1 Introduction

This is a writeup of slides that I first prepared for two hours of lectures at the Hadron Collider Physics Summer School (HCPSS) at CERN in 2009, and which eventually grew to about four hours of lectures within the CMS collaboration in summer of 2017. I will prepare a shortened version of the slides for lectures at the 2018 HCPSS at Fermilab. Unlike commonly available lectures by many of my colleagues on practical statistics for data analysis, my lectures focus on discussion of the foundational aspects, for which there is much less secondary literature written by physicists. [Note added August 29, 2023: I added some references and Appendix B with further discussion on goodness of fit.]

I first got interested in the foundations of statistics in the late 1980’s, when I learned that deep issues of great importance to science, such as “Is there a statistically significant departure from expectations in my data?” were not at all settled. The issue is not merely, “How many sigma is a discovery?”, but rather, “Is the (equivalent) number of sigma even the right figure of merit for inferring the presence of a discovery?” The more I read about the Bayesian–frequentist debates in the primary statistics literature (which has the wonderful practice of including commentary and a rejoinder in many major papers), the more it became a “hobby” to browse this literature and (thanks to the PhyStat series organized by Louis Lyons and colleagues) to discuss these issues with preeminent statisticians and other interested physicists.

The style here is rather terse, reflecting the origin in the slides [1], with each subsection drawing attention to a point of interest or controversy, including pointers to more literature. I do not assume much advanced statistics knowledge, but the reader will may well find the subject to be surprisingly difficult. That is correct (!), and in fact is one of the main points of my lectures. Of course, a familiarity with examples of plots from various HEP analyses will be helpful.

By concentrating on the “theoretical” underpinnings, I hope to provide the reader with what one must know in order to choose appropriate methods from the many possibilities. This includes the hope that by studying these topics, one will learn to avoid common pitfalls (and even silly statements) that can trip up professionals in the field.

This is a dense writeup, and I do not expect one to pick it all up in a quick read-through. It should however be extremely useful to study the topics, referring to the references. I have also tried to put in enough sub-headings so that one can use it as a reference on specific topics. After some preliminaries, I begin with definitions and the Bayesian approach. That should help to understand what the frequentist approach (described next) is not! The frequentist discussion includes interval estimation, hypothesis testing, conditional frequentist estimation, and the much-debated issue of downward fluctuations in a search for an excess. After discussing likelihood-ratio intervals, I compare the three approaches, including major foundational issues such as the likelihood principle (Sections 9, 10). Finally I add nuisance parameters in the context of each of the approaches. I conclude with a word about current practice at the LHC.

The appendices have a detailed worked example of a hypothesis test for two simple hypotheses; a brief discussion of the look-elsewhere effect; some further notes on Bayesian model selection; and some remarks on point estimation. All of these are are important topics that did not make it into my lectures.
2 Preliminaries

2.1 Why foundations matter

In the “final analysis”, we often make approximations, take a pragmatic approach, or follow a convention. To inform such actions, it is important to understand some foundational aspects of statistical inference. In Quantum Mechanics, we are used to the fact that for all of our practical work, one’s philosophical interpretation (e.g., of collapse of the wave function) does not matter. In statistical inference, however, *foundational differences result in different answers*: one cannot ignore them!

The professional statistics community went through the topics of many of our discussions starting in the 1920’s, and revisited them in the resurgence of Bayesian methods in recent decades. I attempt to summarize some of the things that we should understand from that debate. *Most importantly*: One needs to understand both frequentist and Bayesian methods!

2.2 Definitions are important

As in physics, much confusion can be avoided by being precise about definitions, and much confusion can be generated by being imprecise, or (especially) by assuming every-day definitions in a technical context. By the end of these notes, you should see just as much confusion in these statements:

1. “The confidence level tells you how much confidence one has that the true value is in the confidence interval,”

2. “A noninformative prior probability density contains no information.”

...As you have learned to see in the statement, “I did a lot of work today by carrying this big stone around the building and then putting it back in its original place.”

Confusion is also possible because the statistics literature uses some words differently than does the HEP literature. A few examples are in Table 1, adapted from James [2]. Here I tend to use words from both columns, with nearly exclusive use of the statisticians’ definition of “estimation”, as discussed below.

| Physicists say... | Statisticians say... |
|------------------|---------------------|
| Determine, Measure | Estimate           |
| Estimate         | (Informed) Guess   |
| Gaussian         | Normal              |
| Breit-Wigner, Lorentzian | Cauchy |
2.3 Key tasks: Important to distinguish

The most common tasks to be performed in statistical inference are typically classified as follows.

- **Point estimation**: What single “measured” value of a parameter do you report? While much is written about point estimation, in the end it is not clear what the criteria are for a “best” estimator. Decision Theory can be used to specify criteria and choose among point estimators. However, in HEP this is only implicitly done, and point estimation is usually not a contentious issue: typically the maximum-likelihood (point) estimator (MLE) serves our needs rather well, sometimes with a small correction for bias if desired. (See Appendix E.) We generally put a “hat” (accent circumflex) over a variable to denote a point estimate, e.g., $\hat{\mu}$.

- **Interval estimation**: What interval (giving a measure of uncertainty of the parameter inference) do you report? This is crucial in HEP (and in introductory physics laboratory courses), and as discussed below, is deeply connected to frequentist hypothesis testing. In HEP it is fairly mandatory that there is a confidence level that gives the frequentist coverage probability (Section 6.11) of a method, even if it is a Bayesian-inspired recipe.

  Point estimation and interval estimation can be approached consistently by insisting that the interval estimate contain the point estimate; in that case one can construct the point estimate by taking the limit of interval estimates as intervals get smaller (limit of confidence level going to zero).

  For many problems in HEP, there is reasonable hope of approximate reconciliation between Bayesian and frequentist methods for point and interval estimation, especially with large sample sizes.

- **Hypothesis testing**: There are many special cases, including a test of:

  (a) A given functional form (“model”) vs another functional form. Also known as “model selection”;  

  (b) A single value of a parameter (say 0 or 1) vs all other values;  

  (c) Goodness of Fit: A given functional form against all other (unspecified) functional forms (also known as “model checking”)

  Bayesian methods for hypothesis testing generally attempt to calculate the probability that a hypothesis is true. Frequentist methods cannot do this, and often lead to results expressed as $p$-values (Section 7.6). There is a large literature bashing $p$-values, but they are still deemed essential in HEP.

- **Decision making**: What action should I take (tell no one, issue press release, propose new experiment, . . . ) based on the observed data? Decision making is rarely performed formally in HEP, but it is important to understand the outline of the formal theory, in order to avoid confusion with statistical inference that stops short of a decision, and to inform informal application.
In frequentist statistics, the above hypothesis testing case (b) maps identically onto interval estimation. This is called the duality of “inversion of a hypothesis test to get confidence intervals”, and vice versa. I discuss this in more detail in Section 7.4.

In contrast, in Bayesian statistics, hypothesis testing case (b) is an especially controversial form of case (a), model selection. The model with fixed value of the parameter is considered to be a lower-dimensional model in parameter space (one fewer parameter) than the model with parameter not fixed. I just mention this here to foreshadow a very deep issue. Because of the completely different structure of the approaches to testing, there be dramatic differences between frequentist and Bayesian hypothesis testing methods, with conclusions that apparently disagree, even in the limit of large data sets. Beware! See Appendix D and my paper on the Jeffreys-Lindley paradox [3].

3 Probability

3.1 Definitions, Bayes’s theorem

Abstract mathematical probability $P$ can be defined in terms of sets and axioms that $P$ obeys, as outlined in Ref. [4] (Chapter 1) and discussed in much more detail in Ref. [5] (Chapter 5). Conditional probabilities $P(B|A)$ (read “$P$ of $B$ given $A$”) and $P(A|B)$ are related by Bayes’s Theorem (or “Bayes’s Rule”):

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

(1)

A cartoon illustration of conditional probabilities and a “derivation” of Bayes’s theorem is in Fig. 1.

Two established incarnations of $P$ (still argued about, but to less practical effect) are:

- **Frequentist $P$**: the limiting frequency in an ensemble of imagined repeated samples (as usually taught in Q.M.). $P$(constant of nature) and $P$(SUSY is true) do not exist (in a useful way) for this definition of $P$ (at least in one universe).

- **(Subjective) Bayesian $P$**: subjective (personalistic) degree of belief (as advocated by de Finetti [6], Savage [7], and others). $P$(constant of nature) and $P$(SUSY is true) exist for You. (In the literature, “You” is often capitalized to emphasize the personalistic aspect.) This has been argued to be a basis for coherent personal decision-making (where “coherent” has a technical meaning).

It is important to be able to work with either definition of $P$, and to know which one you are using!

The descriptive word “Bayesian” applies to use of the above definition of probability as degree of belief! The adjective “Bayesian” thus also normally applies to the use of a probability density for any parameter (such as a constant of nature) whose true value is **fixed but unknown**, even in a context where the practitioner is not really aware of the degree-of-belief definition.

In contrast, Bayes’s theorem applies to any definition of probability that obeys the axioms and for which the probabilities are defined in the relevant context! The distinction
Figure 1: A cartoon explanation of probability, conditional probability, and Bayes’s Theorem, using picture arithmetic.
was noted by statistician Bradley Efron in his keynote talk at the 2003 PhyStat meeting at SLAC [8]:

“Bayes’ rule is satisfying, convincing, and fun to use. But using Bayes’ rule does not make one a Bayesian; always using it does, and that’s where difficulties begin.” (Emphasis in original.)

Clearly Bayes’s theorem has more applications for Bayesian $P$ than for frequentist $P$, since Bayesian $P$ can be used in more contexts. But one of the sillier things one sometimes sees in HEP is the use of a frequentist example of Bayes’s Theorem as a foundational argument for “Bayesian” statistics! Below I give a simple example for each definition of $P$.

### 3.2 Example of Bayes’s theorem using frequentist $P$

A b-tagging method is developed, and one measures:

- $P(b\text{-}tag|b\text{-}jet)$, i.e., efficiency for tagging b-jets
- $P(b\text{-}tag|\text{not a b-jet})$, i.e., efficiency for background
- $P(\text{no b-tag}|b\text{-}jet) = 1 - P(b\text{-}tag|b\text{-}jet)$
- $P(\text{no b-tag}|\text{not a b-jet}) = 1 - P(b\text{-}tag|\text{not a b-jet})$.

**Question:** Given a selection of jets tagged as b-jets, what fraction of them is b-jets? I.e., what is $P(\text{b-jet}|b\text{-}tag)$?

**Answer:** Cannot be determined from the given information!

One needs in addition: $P(\text{b-jet})$, the true fraction of all jets that are b-jets. Then Bayes’s Theorem inverts the conditionality:

$$P(\text{b-jet}|b\text{-}tag) \propto P(b\text{-}tag|b\text{-}jet)P(\text{b-jet}),$$

(2)

(where I suppress the normalization denominator).

As noted, in HEP $P(b\text{-}tag|b\text{-}jet)$ is called the efficiency for tagging b-jets. Meanwhile $P(b\text{-}jet|b\text{-}tag)$ is often called the purity of a sample of b-tagged jets. As this should be a conceptually easy distinction for experienced data analysts in HEP, it is helpful to keep it in mind when one encounters cases where it is perhaps tempting to make the logical error of equating $P(A|B)$ and $P(B|A)$.

### 3.3 Example of Bayes’s theorem using Bayesian $P$

In a background-free experiment, a theorist uses a “model” to predict a signal with Poisson mean of 3.0 events. From the Poisson formula (Eqn. 9) we know:

$$P(0 \text{ events}|\text{model true}) = 3.0^0 e^{-3.0}/0! = 0.05$$

$$P(0 \text{ events}|\text{model false}) = 1.0$$
The experiment is performed, and zero events are observed.

**Question:** Given the result of the experiment, what is the probability that the model is true? I.e., What is \( P(\text{model true} | 0 \text{ events}) \)?

**Answer:** Cannot be determined from the given information!

One needs in addition: \( P(\text{model true}) \), the degree of belief in the model prior to the experiment. Then Bayes’s Theorem inverts the conditionality:

\[
P(\text{model true} | 0 \text{ events}) \propto P(0 \text{ events} | \text{model true})P(\text{model true})
\]  
(again suppressing the normalization). It is instructive to apply Bayes’s Theorem in a little more detail, with the normalization. In Eqn. 1, let “\( A \)” correspond to “0 events” and “\( B \)” correspond to “model true”. Similarly, with \( P(\text{not } B) = 1 - P(B) \), we can write a version of Bayes’s Theorem (replacing \( B \) with “not \( B \)”)

\[
P(\text{not } B | A) = P(A | \text{not } B) \times P(\text{not } B) / P(A).
\]  
(As a check, we can add Eqns. 1 and 4 and get unity, confirming that \( P(A) \) is the correct normalization.) Solving Eqn. 4 for \( P(A) \) and substituting into Eqn. 1, and inserting numerical values from above, yields \( P(B | A) = 0.05P(B)/(1 - 0.95P(B)) \), i.e.,

\[
P(\text{model true} | 0 \text{ events}) = \frac{0.05 \times P(\text{model true})}{(1 - 0.95P(\text{model true}))}.
\]  

We can examine the limiting cases of strong prior belief in the model and very low prior belief. If we let the “model” be the Standard Model, then we could express our high prior belief as \( P(\text{model true}) = 1 - \epsilon \), where \( \epsilon \ll 1 \). Plugging in gives, to lowest order,

\[
P(\text{model true} | 0 \text{ events}) \approx 1 - 20\epsilon.
\]  
This is still very high degree of belief in the SM. Unfortunately, one still finds (in the press and even among scientists) the fallacy that is analogous to people saying, “\( P(0 \text{ events} | \text{model true}) = 5\% \), with 0 events observed, means there is 5\% chance the SM is true.” (UGH!)

In contrast, let the “model” be large extra dimensions, so that for a skeptic, the prior belief can be expressed as \( P(\text{model true}) = \epsilon \), for some other small \( \epsilon \). Then to lowest order we have,

\[
P(\text{model true} | 0 \text{ events}) \approx 0.05\epsilon.
\]  
Low prior belief becomes even lower.

More realistic examples are of course more complex. But this example is good preparation for avoiding misinterpretation of \( p \)-values in Section 7.6.
3.4 A note re Decisions

Suppose that as a result of the previous experiment, your degree of belief in the model is \( P(\text{model true} | 0 \text{ events}) = 99\% \), and you need to decide on an action (making a press release, or planning next experiment), based on the model being true.

**Question:** What should you decide?

**Answer:** Cannot be determined from the given information!

One needs in addition: The utility function (or its negative, the loss function), which quantifies the relative costs (to You) of

- **Type I error:** declaring model false when it is true; and of
- **Type II error:** not declaring model false when it is false.

Thus, Your decision requires two subjective inputs: Your prior probabilities, and the relative costs (or benefits) to You of outcomes.

Statisticians often focus on decision-making. In HEP, the tradition thus far is to communicate experimental results (well) short of formal decision calculations. It is important to realize that frequentist (classical) “hypothesis testing” as discussed in Section 7 below (especially with conventions like 95% C.L. or 5\( \sigma \)) is not a complete theory of decision-making! One must always keep this in mind, since the traditional “accept/reject” language of frequentist hypothesis testing is too simplistic for “deciding”.

3.5 Aside: What is the “whole space”? 

For probabilities to be well-defined, the “whole space” needs to be defined. This can be difficult or impossible for both frequentists and Bayesians. For frequentists, specification of the whole space may require listing the experimental protocol in detail, including the experimenters’ reaction to potentially unexpected results that did not occur! For Bayesians, normalization of probabilities of hypotheses requires enumerating all possible hypotheses and assigning degree of belief to them, including hypotheses not yet formulated!

Thus, the “whole space” itself is more properly thought of as a conditional space, conditional on the assumptions going into the model (Poisson process, whether or not total number of events was fixed, etc.), and simplifying assumptions or approximations.

Furthermore, it is widely accepted that restricting the “whole space” to a relevant (“conditional”) subspace can sometimes improve the quality of statistical inference. The important topic of such “conditioning” in frequentist inference is discussed in detail in Section 11.1.

In general I do not clutter the notation with explicit mention of the assumptions defining the “whole space”, but some prefer to do so. In any case, it is important to keep them in mind, and to be aware of their effect on the results obtained.

4 Probability, probability density, likelihood

These are key building blocks in both frequentist and Bayesian statistics, and it is crucial distinguish among them. In the following we let \( x \) be an observed quantity; sometimes we
use \( n \) if the observation is integer-valued and we want to emphasize that (to aging Fortran programmers). A \"(statistical) model\" is an equation specifying probabilities or probability densities for observing \( x \). We use \( \mu \) for parameters (sometimes vector-valued) in the model.

In Bayesian statistics, the parameters themselves are considered to be \"random variables\". The notation for such a general model is \( p(x|\mu) \), where the vertical line (read \"given\") means conditional probability, conditional on a particular value of \( \mu \). (In the statistical literature, \( \theta \) is more common.) In frequentist statistics, typically the dependence on \( \mu \) is not a proper conditional probability, and thus many experts advocate using notation with a semicolon: \( p(x; \mu) \). The modern text by George Casella and Roger Berger \[9\] (p. 86) however uses the vertical line for \"given\" in the context where the parameter is not a random variable being conditioned on. I do not know of any examples where this causes trouble, so at the risk of offending some, I use a vertical line throughout for both Bayesian and frequentist models. Then the most common examples in HEP are:

- Binomial probability for \( n_{\text{on}} \) successes out of \( n_{\text{tot}} \) trials (Section 6.5):
  \[
  \text{Bi}(n_{\text{on}}|n_{\text{tot}}, \rho) = \frac{n_{\text{tot}}!}{n_{\text{on}}!(n_{\text{tot}} - n_{\text{on}})!} \rho^{n_{\text{on}}} (1 - \rho)^{(n_{\text{tot}} - n_{\text{on}})}
  \]  
  (8)

- Poisson probability for \( n \) events to be observed:
  \[P(n|\mu) = \frac{\mu^n e^{-\mu}}{n!}\]  
  (9)

- Gaussian probability \textit{density} function (pdf):
  \[
p(x|\mu, \sigma) = \frac{1}{\sqrt{2\pi\sigma^2}} e^{-(x-\mu)^2/2\sigma^2},
  \]  
  so that \( p(x|\mu, \sigma)dx \) is a differential of probability \( dP \).

(A typical course in statistical physics shows how the latter two can be viewed as limiting cases of the first.) The binomial and Poisson formulas are sometimes called probability \textit{mass} functions in the statistics literature.

In the Poisson case, suppose that \( n = 3 \) is observed. Substituting this \textit{observed value} \( n = 3 \) into \( P(n|\mu) \) yields the \textit{likelihood function}, \( \mathcal{L}(\mu) = \mu^3 \exp(-\mu)/3! \), plotted in Fig. 2.

It is tempting to consider the area under \( \mathcal{L} \) as meaningful, but \( \mathcal{L}(\mu) \) is \textit{not} a probability density in \( \mu \). The area under \( \mathcal{L} \) (or parts of it) is meaningless! The Poisson example makes this particularly clear, since the definition of \( \mathcal{L}(\mu) \) starts with a probability (not a probability density); it makes no sense to multiply \( \mathcal{L}(\mu) \) by \( d\mu \) and integrate.

As we shall see, likelihood \textit{ratios} \( \mathcal{L}(\mu_1)/\mathcal{L}(\mu_2) \) are useful and frequently used.

### 4.1 Change of observable variable (\textit{\"metric\"}) \( x \) in pdf \( p(x|\mu) \)

For pdf \( p(x|\mu) \) and a 1-to-1 change of variable (metric) from (vector) \( x \) to (vector) \( y(x) \), the volume element is modified by the Jacobian. For a 1D function \( y(x) \), we have \( p(y)dy = p(x)dx \), so that

\[
p(y(x)|\mu) = p(x|\mu) / |dy/dx|.
\]  
(11)
The likelihood obtains its maximum (ML) at $\mu = 3$.

The Jacobian modifies the probability density in such a way to guarantee that

$$P(y(x_1) < y < y(x_2)) = P(x_1 < x < x_2),$$

(12)

(or equivalent with decreasing $y(x)$). That is, the Jacobian guarantees that probabilities are invariant under change of variable $x$.

Because of the Jacobian in Eqn. 11, the mode of probability density is in general not invariant under change of metric. That is, the value of $y$ for which $p(y(x))$ is a maximum is not trivially related to the value of $x$ for which $p(x)$ is a maximum.

Another consequence of the Jacobian in Eqn. 11 is that the likelihood function $\mathcal{L}(\mu)$ differs for different choices of the data variable. However, likelihood ratios such as $\mathcal{L}(\mu_1)/\mathcal{L}(\mu_2)$ are invariant under change of variable $x$ to $y(x)$. The Jacobian in the denominator cancels that in the numerator. Thus, for example, the value of $\mu$ that maximizes $\mathcal{L}(\mu)$ will be independent of the choice of data variable, but the value of $\mathcal{L}(\mu)$ at that maximum is different. The latter point also explains why the value of $\mathcal{L}(\mu)$ at its maximum is not an appropriate test statistic for goodness of fit; useful tests based on the likelihood function use likelihood ratios, as discussed in Appendix B.

### 4.2 Change of parameter $\mu$ in pdf $p(x|\mu)$

The pdf for $x$ given parameter $\mu = 3$ is the same as the pdf for $x$ given $1/\mu = 1/3$, or given $\mu^2 = 9$, or given any specified function of $\mu$. They all imply the same $\mu$, and hence the same pdf for $x$.

In slightly confusing notation, that is what we mean by changing the parameter from $\mu$ to $f(\mu)$, and saying that

$$p(x|f(\mu)) = p(x|\mu).$$

(13)
Inserting an observed value of $x$, we see the important result that the likelihood $L(\mu)$ is invariant (!) under reparameterization from parameter $\mu$ to $f(\mu)$: $L(f(\mu)) = L(\mu)$. The absence of a Jacobian reinforces the fact that $L(\mu)$ is not a pdf in $\mu$. Furthermore, the mode of $L(\mu)$ is thus also invariant: if we let $\hat{\mu}$ be the value of $\mu$ for which $L(\mu)$ is a maximum, and if we let $\hat{f}$ be the value of $f(\mu)$ for which $L(f)$ is a maximum, then

$$\hat{f} = f(\hat{\mu}).$$

(14)

This is an important property of the popular ML technique of point estimation. (See discussion in Ref. [10], Section 5.3.1.)

4.3 Probability integral transform

In 1938 Egon Pearson commented on a paper of his father Karl (of $\chi^2$ fame), noting that the probability integral transform “...seems likely to be one of the most fruitful conceptions introduced into statistical theory in the last few years” [11]. Indeed this simple transform makes many issues more clear (or trivial). Given continuous $x \in (a, b)$, and its pdf $p(x)$, one transforms to $y$ given by

$$y(x) = \int_a^x p(x')dx'.$$

Then trivially $y \in (0, 1)$, and with the chain rule and the fundamental theorem of calculus, it follows that the pdf for $y$ is $p(y) = 1$ (uniform) for all $y$! (If $x$ is discrete, there are complications.)

So for continuous variables, there always exists a metric $y$ in which the pdf is uniform. (As an aside, the inverse transformation can provide for efficient Monte Carlo (MC) generation of $p(x)$ starting from a pseudo-random number generator uniform on (0,1). See Section 40.2 in Ref. [12] .)

Looking ahead to Section 5, I mention here that the specification of a Bayesian prior pdf $p(\mu)$ for parameter $\mu$ is thus equivalent to the choice of the metric $g(\mu)$ in which the pdf is uniform. This is a deep issue, not always recognized by users of uniform prior pdf’s in HEP!

4.4 Bayes’s theorem generalized to probability densities

Recall (Eqn. 1) that $P(B|A) \propto P(A|B)P(B)$. For Bayesian $P$, continuous parameters such as $\mu$ are random variables with pdf’s.

Let pdf $p(\mu|x)$ be the conditional pdf for parameter $\mu$, given data $x$. As usual $p(x|\mu)$ is the conditional pdf for data $x$, given parameter $\mu$. Then Bayes’s Theorem becomes $p(\mu|x) \propto p(x|\mu)p(\mu)$. Substituting in a particular set of observed data $x_0$, we have $p(\mu|x_0) \propto p(x_0|\mu)p(\mu)$.

Recognizing the likelihood (variously written as $\mathcal{L}(x_0|\mu)$, $\mathcal{L}(\mu)$, or unfortunately even $\mathcal{L}(\mu|x_0)$), then

$$p(\mu|x_0) \propto \mathcal{L}(x_0|\mu)p(\mu).$$

(16)

where:
\( p(\mu|x_0) \) = the *posterior pdf* for \( \mu \), given the results of this experiment,
\( \mathcal{L}(x_0|\mu) \) = the *likelihood function* of \( \mu \) from this experiment,
\( p(\mu) \) = the *prior pdf* for \( \mu \), before applying the results of this experiment.

Note that there is one (and only one) probability *density in \( \mu \) on each side of the equation, consistent with \( \mathcal{L}(x_0|\mu) \) *not* being a density in \( \mu \)!

(Aside: occasionally someone in HEP refers to the prior pdf as “*a priori*”. This is incorrect, as is obvious when one considers that the posterior pdf from one experiment can serve as the prior pdf for the next experiment.)

5 Bayesian analysis

All equations up until now are true for *any* definition of probability \( P \) that obeys the axioms, including frequentist \( P \), as long as the probabilities exist. For example, if \( \mu \) is sampled from an ensemble with known “prior” pdf, then it has a frequentist interpretation. (This is however unusual.) The word “Bayesian” refers *not* to these equations, but to the choice of definition of \( P \) as personal subjective degree of belief. For example, if \( \mu \) is a constant of nature, its Bayesian pdf expresses one’s relative belief in different values.

Bayesian \( P \) applies to hypotheses and constants of nature (while frequentist \( P \) does not), so there are many Bayesian-only applications of Bayes’s Theorem. Bayesian analysis is based on the Bayesian posterior pdf \( p(\mu|x_0) \), as sketched here.

- **Point estimation**: Some Bayesians use the posterior mode (maximum posterior density) as the point estimate of \( \mu \). This has the problem that it is metric dependent: the point estimate of the mean lifetime \( \tau \) will not be the inverse of the point estimate of the decay rate \( \Gamma \). This is because the Jacobian moves the mode around under change of parameter from lifetime \( \tau \) to decay rate \( \Gamma = 1/\tau \). (Recall Section 4.1.) The posterior median can be used in 1D, and is metric-independent. There are also Bayesians (as well as frequentists) who think that emphasis on point estimation is misguided.

- **Interval estimation**: The *credibility* of \( \mu \) being in any interval \([\mu_1, \mu_2]\) can be calculated by integrating \( p(\mu|x_0) \) over the interval. For reporting a default interval with, say, 68% credibility, one needs in addition a convention for which 68% to use (lower, upper, or central quantiles are common choices). It is preferable to refer to such intervals as “credible intervals”, as opposed to “confidence intervals”, unless the Bayesian machinery is used just as a technical device to obtain valid (at least approximate) frequentist confidence intervals (as is often the case in HEP).

- **Hypothesis testing**: Unlike frequentist statistics, testing credibility of whether or not \( \mu \) equals a particular value \( \mu_0 \) is *not* performed by examining interval estimates (at least assuming a regular posterior pdf). One starts over with Bayesian model selection, as discussed in Appendix D. (Dirac \( \delta \)-functions in the prior and posterior pdfs can however connect interval estimation to model selection, with its issues.)

- **Decision making**: All decisions about \( \mu \) require not only \( p(\mu|x_0) \) but also further input: the utility function (or its negative, the loss function). See, e.g., Ref. [2] (Chapter 6) and Ref. [13] (Chapter 2).
Since Bayesian analysis requires a prior pdf, big issues in Bayesian estimation include:

- What prior pdf to use, and how sensitive is the result to the prior?
- How to interpret posterior probability if the prior pdf is not Your personal subjective belief?

*Frequentist tools can be highly relevant to both questions!*

### 5.1 Can “subjective” be taken out of “degree of belief”?

There are compelling arguments (Savage [7], De Finetti [6] and others) that Bayesian reasoning with personal subjective $P$ is the uniquely “coherent” way (with technical definition of coherent) of updating personal beliefs upon obtaining new data and making decisions based on them. (These foundational works are very heavy going. For a more accessible review by an outspoken subjectivist, with more complete references, see Lindley’s 2000 review [14]. A 2018 book by Diaconis and Skyrms [5] is also very detailed and at a deep level that seems mostly comprehensible to physicists.)

A huge question is: *Can the Bayesian formalism be used by scientists to report the results of their experiments in an “objective” way (however one defines “objective”), and does any of the glow of coherence remain when subjective $P$ is replaced by something else?*

An idea vigorously pursued by physicist Harold Jeffreys [15] in the mid-20th century is: *Can one define a prior $p(\mu)$ that contains as little information as possible?*

The really really thoughtless idea (despite having a fancy name, “Laplace’s Principle of Insufficient Reason”), recognized by Jeffreys as such, but dismayingly common in HEP is: just choose prior $p(\mu)$ uniform in whatever metric you happen to be using!

### 5.2 “Uniform prior” requires a choice of metric

Recall that the probability integral transform *always* allows one to find a metric in which $p$ is uniform (for continuous $\mu$). Thus the question, “What is the prior pdf $p(\mu)$?” is equivalent to the question, “For what function $g(\mu)$ is $p(g)$ uniform?” There is usually no reason to choose $g$ arbitrarily as $g(\mu) = \mu$ (!).

### 5.3 Jeffreys’s choice of metric in which prior is uniform

The modern foundation of the vast literature on prior pdfs that one may hope (in vain) to be uninformative is the monograph by Harold Jeffreys [15]. He proposes more than one approach, but the one that is commonly referred to as “Jeffreys Prior” (and considered the default “noninformative” prior by statisticians for estimation in 1-parameter problems) is derived from the statistical model $p(x|\mu)$.

*This means that the prior pdf depends on the measurement apparatus!* For example, if the measurement apparatus has a resolution function that is Gaussian for mass $m$ (with $\sigma$ independent of $m$), then the Jeffreys prior pdf $p(m)$ for the mass is uniform in $m$. If a different measurement apparatus has a resolution function that is Gaussian for $m^2$, then the
Jeffreys prior pdf $p(m^2)$ is uniform in $m^2$. In the latter case, by the rules of probability (Eqn. 11), the prior pdf $p(m)$ is not uniform, but rather proportional to $m$ (!).

Jeffreys’s derivation of his eponymous prior is based on the idea that the prior should be uniform in a metric related to the Fisher information, calculated from curvature of the log-likelihood function averaged over sample space. Some examples are:

Poisson signal mean $\mu$, no background: $p(\mu) = 1/\sqrt{\mu}$

Poisson signal mean $\mu$, mean background $b$: $p(\mu) = 1/\sqrt{\mu + b}$

Mean $\mu$ of Gaussian with fixed $\sigma$ (unbounded or bounded $\mu$): $p(\mu) = 1$

rms deviation $\sigma$ of a Gaussian when mean fixed: $p(\sigma) = 1/\sigma$

Binomial parameter $\rho$, $0 \leq \rho \leq 1$: $p(\rho) = \rho^{-1/2}(1 - \rho)^{-1/2} = \text{Beta}(1/2, 1/2)$

If parameter $\mu$ is changed to $f(\mu)$, the recipe for obtaining the Jeffreys prior for $f(\mu)$ yields a different-looking prior that corresponds to the same choice of uniform metric. So if you use Jeffreys’s recipe to obtain a prior pdf for $\mu$, and your friend uses Jeffreys’s recipe to obtain a prior pdf for $f(\mu)$, then those pdfs will be correctly related by the appropriate Jacobian. (This is not true for some other rules, in particular if each of you takes a uniform prior in the metric you are using.) Thus probabilities (integrals of pdfs over equivalent endpoints) using Jeffreys prior are invariant under choices of different parameterizations.

For a detailed modern review of Jeffreys’s entire book, including his prior, with discussion by six prominent statisticians (including outspoken subjectivist Lindley), and rejoinder, see Ref. [16].

5.3.1 Reference priors of Bernardo and Berger

As Jeffreys noted, his recipe encounters difficulties with models having more than one parameter. José Bernardo [17] and J.O. Berger [18, 19] advocate an approach that they argue works well in higher dimensions, with the crucial observation one must choose an ordering of the parameters in order to well-define the multi-dimensional prior pdf. Their so-called “Reference prior” reduces to the Jeffreys prior in 1D, with a different rationale, namely the prior that leads to a posterior pdf that is most dominated by the likelihood.

There are many subtleties. Beware! See also Bernardo’s talk at PhyStat-2011, which includes hypothesis testing, and discussion following [20]. Demortier, Jain, and Prosper pioneered the use of Bernardo/Berger reference priors in a case of interest in HEP [21], with about 30 citations thus far at inspirehep.net.

5.4 What to call such non-subjective priors?

- “Noninformative priors”? Traditional among statisticians, even though they know it is a misnomer. (You should too!)
- “Vague priors”?
- “Ignorance priors”?
• “Default priors”? 

• “Reference priors”? (Unfortunately also refers to the specific recipe of Bernardo and Berger) 

• “Objective priors”? Despite the highly questionable use of the word, Jeffreys prior and its generalization by Bernardo and Berger are now widely referred to as “objective priors”.

Kass and Wasserman [22] give the best (neutral) name in my opinion: Priors selected by “formal rules”. Their article is required reading for anyone using Bayesian methods! Whatever the name, the prior pdf in one metric determines it in all other metrics: be careful in the choice of metric in which it is uniform!

For one-parameter models, the “Jeffreys Prior” is the most common choice among statisticians for a non-subjective “default” prior—so common that statisticians can be referring to the Jeffreys prior when they say “flat prior” (e.g., D.R. Cox in discussion at PhyStat 2005 [23], p. 297).

A key point: priors such as the Jeffreys Prior are based on the likelihood function and thus inherently derived from the measurement apparatus and procedure, not from thinking about the parameter! This may seem strange, but does give advantages, particularly for frequentist (!) coverage (Section 6.11), as mentioned in Section 12.7 and emphasized to us by Jim Berger at the Confidence Limits Workshop at Fermilab in 2000 [24].

5.5 Whatever you call them, non-subjective priors cannot represent ignorance!

Although some authors have claimed that various invariance principles can be invoked to yield priors that represent complete “ignorance”, I do not know of any modern statistician who thinks that this is possible. On the contrary, (subjectivist) Dennis Lindley wrote, [25], “the mistake is to think of them [Jeffreys priors or Bernardo/Berger’s reference priors] as representing ignorance.” This Lindley quote is emphasized in the monograph by prominent Bayesian Christian Robert [26] (p. 29).

Objectivist Jose Bernardo says, regarding his reference priors, “[With non-subjective priors.] The contribution of the data in constructing the posterior of interest should be ‘dominant’. Note that this does not mean that a non-subjective prior is a mathematical description of ‘ignorance’. Any prior reflects some form of knowledge.”

Nonetheless, Berger [13] (p. 90) argues that Bayesian analysis with noninformative priors (older name for objective priors), such as those of Jeffreys and Bernardo/Berger, “is the single most powerful method of statistical analysis, in the sense of being the ad hoc method most likely to yield a sensible answer for a given investment of effort.” [emphasis in original].

5.6 Priors in high dimensions

Is there a sort of informational “phase space” that can lead us to a sort of probability Dalitz plot? I.e., the desire is that structure in the posterior pdf represents information in the data, not the effect of Jacobians in the priors. This is a notoriously hard problem!
Be careful: Uniform priors push the probability away from the origin to the boundary! (The volume element goes as \( r^2 \mathrm{dr} \).) The state of the art for “objective” priors may be the “reference priors” of Bernardo and Berger, but multi-D tools have been lacking. Subjective priors are also very difficult to construct in high dimensions: human intuition is poor.

Subjective Bayesian Michael Goldstein [27] told us in 2002 at Durham, “…meaningful prior specification of beliefs in probabilistic form over very large possibility spaces is very difficult and may lead to a lot of arbitrariness in the specification…”.

Bradley Efron at PhyStat-2003 [8] concluded: “Perhaps the most important general lesson is that the facile use of what appear to be uninformative priors is a dangerous practice in high dimensions.”

Sir David Cox [28], p. 46: “With multi-dimensional parameters…naive use of flat priors can lead to procedures that are very poor from all perspectives…” Also p. 83: “…the notion of a flat or indifferent prior in a many-dimensional problem is untenable.”

5.7 Types of Bayesians

The broad distinction between the subjective and objective Bayesians is far from the complete story. At PhyStat-LHC in 2007, Sir David Cox described “Five faces of Bayesian statistics” [29]:

- empirical Bayes: number of similar parameters with a frequency distribution
- neutral (reference) priors: Laplace, Jeffreys, Jaynes, Berger and Bernardo
- information-inserting priors (evidence-based)
- personalistic priors
- technical device for generating frequentist inference

Currently in HEP, the main application is the last “face” on his list: we typically desire good frequentist properties for point or interval estimation when using a nominally “Bayesian” recipe. In particular, for upper limits on a Poisson mean, we use a uniform prior (i.e., not what objective statisticians recommend), for frequentist reasons. (See Section 10 and Ref. [30].) Cox’s third “face” also arises in HEP when likelihoods are incorporated from subsidiary measurements, and are used to provide evidence-based priors. Unfortunately, some people in HEP have in effect also added to Cox’s list a 6th “face”:

- Priors uniform in arbitrary variables, or in “the parameter of interest”.

I know of no justification for this in modern subjective or objective Bayesian theory. It is an “ignorance” prior only in the sense that it betrays ignorance of the modern Bayesian literature!
5.8 Do “Bayesians” care about frequentist properties of their results?

Another claim that is dismaying to see among some physicists is the blanket statement that “Bayesians do not care about frequentist properties”. While that may be true for pure subjective Bayesians, most of the pragmatic Bayesians that we have met at PhyStat meetings do use frequentist methods to help calibrate Bayesians statements. That seems to be essential when using “objective” priors to obtain results that are used to communicate inferences from experiments.

A variety of opinions on this topic are in the published comments in the inaugural issue of the journal *Bayesian Analysis*, following the papers by Jim Berger [31] and Michael Goldstein [32] that advocate the objective and subjective points of view, respectively. In particular, Robert Kass [33] provided a list of nine questions for which answers “may be used to classify various kinds of Bayesians”.

The first question is, “Is it important for Bayesian inferences to have good frequentist operating characteristics?” The questions, the explicit answers from Kass, Berger, and Goldstein, and other commentary (from which answers can be gleaned) from other prominent statisticians, are part of my list of “required reading” for physicists. They should go a long way toward broadening the view of any physicists who have swallowed some of the extreme polemics about Bayesian analysis (as found for example in Jaynes [34], which unfortunately seems to have been read uncritically by too many scientists).

5.9 Analysis of sensitivity to the prior

Since a Bayesian result depends on the prior probabilities, which are either personalistic or with elements of arbitrariness, it is widely recommended by Bayesian statisticians to study the *sensitivity* of the result to varying the prior.

- “Objective” Bayesian José Bernardo, quoted in Ref. [35]: “Non-subjective Bayesian analysis is just a part—an important part, I believe —of a healthy sensitivity analysis to the prior choice. . .”.

- “Subjective” Bayesian Michael Goldstein, from the Proceedings [27]: “. . . Again, different individuals may react differently, and the sensitivity analysis for the effect of the prior on the posterior is the analysis of the scientific community. . .” In his transparencies at the conference, he put it simply: “Sensitivity Analysis is at the heart of scientific Bayesianism.”

I think that too little emphasis to this important point is given by Bayesian advocates in HEP.

5.10 Bayesian must-read list for HEP/Astro/Cosmo (including discussion!)

In my experience, some high energy physicists and astrophysicists appear to be overly influenced by the polemical book by E.T. Jaynes [34], (which, for example, argues for the existence
priors representing ignorance). I strongly urge anyone diving into Bayesian statistics to read as well the following minimal set of papers by Bayesian subjectivists and objectivists, and the associated discussion, and rejoinders. (If there is one thing that HEP journals could learn from statisticians, it is to publish such discussion and rejoinder accompanying major papers and reviews!) As I made this list over ten years ago, I would welcome suggestions for more recent additions.

Robert E. Kass and Larry Wasserman, “The Selection of Prior Distributions by Formal Rules,” [22]

Telba Z. Irony and Nozer D. Singpurwalla, “Non-informative priors do not exist: A dialogue with Jose M. Bernardo,” [35]

James Berger, “The Case for Objective Bayesian Analysis,” [31]

Michael Goldstein, “Subjective Bayesian Analysis: Principles and Practice,” [32]

J.O. Berger and L.R. Pericchi, “Objective Bayesian Methods for Model Selection: Introduction and Comparison,” [36]

5.11 Pseudo-Bayesian analyses

Jim Berger in 2006 [31]:

“One of the mysteries of modern Bayesianism is the lip service that is often paid to subjective Bayesian analysis as opposed to objective Bayesian analysis, but then the practical analysis actually uses a very adhoc version of objective Bayes, including use of constant priors, vague proper priors, choosing priors to ‘span’ the range of the likelihood, and choosing priors with tuning parameters that are adjusted until the answer ‘looks nice.’ I call such analyses pseudo-Bayes because, while they utilize Bayesian machinery, they do not carry with them any of the guarantees of good performance that come with either true subjective analysis (with a very extensive elicitation effort) or (well-studied) objective Bayesian analysis... I do not mean to discourage this approach. It simply must be realized that pseudo-Bayes techniques do not carry the guarantees of proper subjective or objective Bayesian analysis, and hence must be validated by some other route.”

Berger goes on to give examples of pseudo-Bayes analyses, with the first being (what else?), “Use of the constant prior density”.

Pseudo-Bayes analyses pop up from time to time in HEP, for example by those using priors “uniform in the parameter of interest”. Here I mention three examples of “pseudo-Bayes” in HEP that have been criticized by me and others. I previously discussed them at the PhyStat-nu workshop in Tokyo in 2016 [37] (slides 62–68).

The first example was exposed in Luc Demortier’s talk in 2002 at Durham [38]. In a method of Bayesian upper limit calculation that was common at the Tevatron at the time, the use of a uniform prior for a Poisson mean, along with a Gaussian truncated at the origin for a systematic uncertainty in efficiency, led to an integral that Luc showed “by hand” to diverge! The integral was typically evaluated numerically, without first checking that it exists. The answer thus depended on the choice of cutoff that was used in the numerical evaluation. Alternatives to the truncated Gaussian prior are mentioned in Section 12.3.1.
The second example comes from Joel Heinrich at the Oxford PhyStat in 2005 [39]. It had been known a long time that a uniform prior for a Poisson mean of a signal yields good frequentist properties for upper limits (but not lower limits). (See Section 10.) Joel showed the dangers of naively using uniform prior for the means of several background processes.

The third example is in the category that I find has some of the worst pseudo-Bayes examples, namely Bayesian model selection (Appendix D), which is however not attempted as often as Bayesian estimation in HEP. Practitioners are sometimes unaware that:

1. In model selection, unlike estimation, the dependence on some prior pdfs for parameters does not become negligible as the amount of data increases without bound (even for so-called Bayes factors that attempt to separate out the prior probabilities of the hypotheses).

2. Improper priors (such as uniform over a line or half-line) are a disaster, and if they are made proper by adding a cutoff, then the model selection answer is directly proportional to the (often arbitrary) cutoff. Using “1” for the prior just hides the problem.

3. In fact, Jeffreys and followers use priors for model selection that are different from those used for estimation (!).

Thus, Bayesian model selection should not be approached naively. For an example in PRL that I criticized, see my Comment in Ref. [40].

Harrison Prosper (an early and sustained advocate of Bayesian methods in HEP) has provided an excellent discussion of the care needed in Bayesian analyses in Chapter 12 of *Data Analysis in High Energy Physics*, edited by O. Behnke et al. [41].

### 6 Frequentist estimation: confidence intervals

What can be computed without using a prior, with only the frequentist definition of $P$?

- Not $P$ (constant of nature is in some specific interval $|$ data)
- Not $P$ (SUSY is true $|$ data)
- Not $P$ (SM is false $|$ data)

Rather:

1. **Confidence Intervals** for constants of nature or other parameter values, as defined in the 1930’s by Jerzy Neyman. Statements are made about probabilities in *ensembles* of intervals (fraction containing unknown true value). Confidence intervals have further applications in frequentist hypothesis testing.

2. Likelihoods and thus *likelihood ratios*, the basis for a large set of techniques for point estimation, interval estimation, and hypothesis testing.
Both can be constructed using the frequentist definition of $P$. In this section, we introduce confidence intervals, and in Section 8, introduce likelihood ratios for interval estimation.

“Confidence intervals”, and this phrase to describe them, were invented by Jerzy Neyman in 1934-37 [42]. Statisticians typically mean Neyman’s intervals (or an approximation thereof) when they say “confidence interval”. In HEP the language is a little loose. I highly recommend using “confidence interval” (and “confidence regions” when multi-D) only to describe intervals and regions corresponding to Neyman’s construction, described below, or by recipes of other origin (including Bayesian recipes) only if they yield good approximations thereof.

The following subsections use upper/lower limits and closely related central confidence intervals to introduce and illustrate the basic notions, and then discuss Neyman’s more general construction (used e.g. by Feldman and Cousins). Then, after introducing frequentist hypothesis testing (Section 7), we return to make the connection between confidence intervals and hypothesis testing of a particular value of parameter vs other values (Section 7.4).

6.1 Notation

$x$ denotes observable(s). More generally, $x$ is any convenient or useful function of the observable(s), and is called a “statistic” or “test statistic”.

$\mu$ denotes parameter(s). (Statisticians often use $\theta$.)

$p(x|\mu)$ is the probability or pdf (from context) characterizing everything that determines the probabilities/densities of the observations, from laws of physics to experimental setup and protocol. The function $p(x|\mu)$ is called “the statistical model”, or simply “the model”, by statisticians.

6.2 The basic idea of confidence intervals in two sentences

Given the model $p(x|\mu)$ and the observed value $x_0$, we ask: For what values of $\mu$ is $x_0$ an “extreme” value of $x$? Then we include in the confidence interval $[\mu_1, \mu_2]$ those values of $\mu$ for which $x_0$ is not “extreme”.

(Note that this basic idea sticks strictly to the frequentist probability of obtaining $x$, and makes no mention of probability (or density) for $\mu$.)

6.2.1 Ordering principle is required for possible values of $x$

In order to define “extreme”, one needs to choose an ordering principle that ranks the possible values of $x$ applicable to each $\mu$. By convention high rank means not extreme.

Some common ordering choices in 1D (when $p(x|\mu)$ is such that higher $\mu$ implies higher average $x$) are:

- Order $x$ from largest to smallest: the smallest values of $x$ are the most extreme. Given $x_0$, the confidence interval that contains $\mu$ for which $x_0$ is not extreme will typically not contain the largest values of $\mu$. This leads to confidence intervals known as upper limits on $\mu$. 

• Order $x$ from smallest to largest. This leads to lower limits on $\mu$.

• Order $x$ using central quantiles of $p(x|\mu)$, with the quantiles shorter in $x$ (least integrated probability of $x$) containing higher-ranked $x$, with lower-ranked $x$ added as the central quantile gets longer (contains more integrated probability of $x$). This leads to central confidence intervals for $\mu$.

These three orderings apply only when $x$ is 1D. A fourth ordering, using a particular likelihood ratio advocated by Feldman and Cousins, is still to come (Section 6.7); it is applicable in both 1D and multi-D.

6.2.2 A “confidence level” must be specified

Given model $p(x|\mu)$ and an ordering of $x$, one chooses a particular fraction of highest-ranked values of $x$ that are not considered as “extreme”. This fraction is called the confidence level (C.L.), say 68% or 95%.

(In this discussion, 68% is more precisely 68.27%; 84% is 84.13%; etc. Also, in the statistics literature there is a fine distinction between confidence level and confidence coefficient, which we ignore here.)

We also define $\alpha = 1 - $C.L., i.e., the fraction that is the lower-ranked, “extreme” set of values.

6.2.3 One-sentence summary

Then the confidence interval $[\mu_1, \mu_2]$ contains those values of $\mu$ for which $x_0$ is not “extreme” at the chosen C.L., given the chosen ordering of $x$. E.g., at 68% C.L., $[\mu_1, \mu_2]$ contains those $\mu$ for which $x_0$ is in the highest-ranked (least extreme) 68% values of $x$ for each respective $\mu$, according probabilities obtained from the model $p(x|\mu)$.

6.3 Correspondence between upper/lower limits and central confidence intervals

As illustrated in Fig. 3, the 84% C.L. upper limit $\mu_2$ excludes $\mu$ for which $x_0$ is in the lowest 16% values of $x$. The 84% C.L. lower limit $\mu_1$ excludes $\mu$ for which $x_0$ is in the highest 16% values of $x$. Then, the interval $[\mu_1, \mu_2]$ includes $\mu$ for which $x_0$ is in the central 68% quantile of $x$ values. It is a 68% C.L. central confidence interval (!).

For general C.L., the endpoints of central confidence intervals are, by the same reasoning, the same as upper/lower limits with confidence level given by $1 - (1 - $C.L.$)/2 = (1 + $C.L.$)/2$.

Examples follow for a couple illustrative models, first with continuous $x$, then with discrete $x$.

6.4 Gaussian pdf $p(x|\mu, \sigma)$ with $\sigma$ a function of $\mu$: $\sigma = 0.2\mu$

It is common in HEP to express uncertainties as a percentage of a mean $\mu$ (even though situations in which this is rigorously motivated are rare). Thus, instead of the most trivial
Figure 3: Sketch to illustrate the relationship among 84% C.L. upper limits, 84% C.L. lower limits, and 68% C.L. central confidence interval. The two one-sided tails of 16% compose the two-sided tails totaling 32%. 
example of Gaussian with unknown mean $\mu$ and known rms $\sigma$, let’s assume that $\sigma$ is 20% of the unknown true value $\mu$:

$$p(x|\mu, \sigma) = \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{(x-\mu)^2}{2\sigma^2}} = \frac{1}{\sqrt{2\pi(0.2\mu)^2}} e^{-\frac{(x-\mu)^2}{2(0.2\mu)^2}},$$  \hspace{1cm} (17)

as illustrated in Fig. 4.

With $\mu$ (and hence $\sigma$) unknown, suppose $x_0 = 10.0$ is observed. What can one say about $\mu$? Regardless of what else is done, it is always useful to plot the likelihood function, in this case obtained by plugging $x_0$ into Eqn. 17:

$$\mathcal{L}(\mu) = \frac{1}{\sqrt{2\pi(0.2\mu)^2}} e^{-\frac{(10.0-\mu)^2}{2(0.2\mu)^2}},$$  \hspace{1cm} (18)

as illustrated in Fig. 5. The first thing one notices is that the likelihood is asymmetric and obtains it maximum at $\mu$ less than the $x_0$. (There is food for thought here, but we move on.)

### 6.4.1 What is the central confidence interval for $\mu$?

First we find $\mu_1$ such that 84% of $p(x|\mu_1, \sigma = 0.2\mu_1)$ is below $x_0 = 10.0$; 16% of the probability is above. Solve: $\mu_1 = 8.33$, as in Fig. 6(left). So $[\mu_1, \infty]$ is an 84% C.L. confidence interval, and $\mu_1$ is 84% C.L. lower limit for $\mu$.

Then we find $\mu_2$ such that 84% of $p(x|\mu_2, \sigma = 0.2\mu_2)$ is above $x_0 = 10.0$; 16% of the probability is below. Solve: $\mu_2 = 12.52$, as in Fig. 6(right). So $[-\infty, \mu_2]$ is an 84% C.L. confidence interval, and $\mu_2$ is 84% C.L. upper limit for $\mu$.

Then the 68% C.L. central confidence interval is $[\mu_1, \mu_2] = [8.33, 12.52]$. This is “exact”. In fact, the reasoning used here was already laid out by E.B. Wilson in 1927 [43] in his discussion of intervals in the Gaussian approximation of the binomial model (Section 6.5.2).
Figure 5: Plot of $\mathcal{L}(\mu)$ for observed $x_0 = 10$, for the model in Eqn. 17. The maximum is at $\mu_{ML} = 9.63$.

Figure 6: (left) The model in Eqn. 17, with $\mu$ chosen such that 84% of the probability is below $x_0 = 10$. (right) The model in Eqn. 17, with $\mu$ chosen such that 84% of the probability is above $x_0 = 10$. 
6.4.2 Contrast Wilson reasoning with “Wald interval” reasoning

The Wilson-inspired reasoning is crucial. Note the difference from the superficially attractive reasoning that proceeds as follows, leading to so-called Wald intervals:

1. For \( x_0 = 10.0 \), the “obvious” point estimate \( \hat{\mu} \) (perhaps thought to be justified by minimum-\( \chi^2 \)) is \( \hat{\mu} = 10.0 \). (This makes the mistake of interpreting the sampled value of \( x \) as being the “measured value of \( \mu \)”, and hence as the point estimate of \( \mu, \hat{\mu} \).)

2. Then one estimates \( \sigma \) by \( \hat{\sigma} = 0.2 \times \hat{\mu} = 2.0 \). (This is potentially dangerous, since it estimates one parameter by plugging the point estimate of another parameter into a relationship between true values of parameters.)

3. Then \( \hat{\mu} \pm \hat{\sigma} \) yields the interval \([8.0, 12.0]\). (Again this is potentially dangerous, as it evaluates tail probabilities of a model having true parameters via plugging in estimates of the parameters.)

Such “Wald intervals” are at best only approximations to exact intervals. For (“exact”) confidence intervals, the reasoning must always involve probabilities for \( x \) calculated considering particular possible true values of parameters, as in the Wilson reasoning! Clearly the validity of the approximate Wald-interval reasoning (i.e., how dangerous the “potentially dangerous” steps are) depends on how much \( \sigma(\mu) \) changes for \( \mu \) relevant to problem at hand. The important point is that the Wald reasoning is not the correct reasoning for confidence intervals. Beware!

6.5 Confidence intervals for binomial parameter \( \rho \)

The binomial model is directly relevant to efficiency calculations in HEP, as well as other contexts. Recall the binomial distribution \( \text{Bi}(n_{on}|n_{tot}, \rho) \) from Eqn. 8 for the probability of \( n_{on} \) successes in \( n_{tot} \) trials, each with binomial parameter \( \rho \). In repeated trials, \( n_{on} \) has mean

\[ n_{tot} \rho \tag{19} \]

and rms deviation

\[ n_{tot} \rho (1 - \rho). \tag{20} \]

For asymptotically large \( n_{tot} \), \( \text{Bi}(n_{on}|n_{tot}, \rho) \) can be approximated by a normal distribution with this mean and rms deviation.

With observed number of successes \( n_{on} \), the likelihood function \( L(\rho) \) follows from reading Eqn. 8 as a function of \( \rho \). The maximum is at

\[ \hat{\rho} = n_{on}/n_{tot}. \tag{21} \]

Suppose one observes \( n_{on} = 3 \) successes in \( n_{tot} = 10 \) trials. The likelihood function \( L(\rho) \) is plotted in Fig. 7.
Figure 7: (left) Likelihood function $\mathcal{L}(\rho)$ for $n_{\text{on}} = 3$ successes in $n_{\text{tot}} = 10$ trials in the binomial model of Eqn. 8. (right) Looking ahead to Section 8, the plot of $-2 \ln \mathcal{L}(\rho)$.

6.5.1 What central confidence interval should we report for $\rho$?

We have $n_{\text{on}} = 3$, $n_{\text{tot}} = 10$. Let us find the “exact” 68% C.L. central confidence interval $[\rho_1, \rho_2]$. Recall the shortcut in Section 6.4.1 for central intervals: Find the lower limit $\rho_1$ with C.L. = $(1 + 0.68)/2 = 84\%$; and find upper limit $\rho_2$ with C.L. = 84\%. Then $[\rho_1, \rho_2]$ is a 68\% C.L. central confidence interval.

1. For lower limit at 84\% C.L., find $\rho_1$ such that $\text{Bi}(n_{\text{on}} < 3 | \rho_1) = 84\%$, i.e., $\text{Bi}(n_{\text{on}} \geq 3 | \rho_1) = 16\%$. Solve: $\rho_1 = 0.142$ as in Fig. 8 (left).

2. For upper limit at 84\% C.L.), find $\rho_2$ such that $\text{Bi}(n_{\text{on}} > 3 | \rho_2) = 84\%$, i.e., $\text{Bi}(n_{\text{on}} \leq 3 | \rho_2) = 16\%$. Solve: $\rho_2 = 0.508$ as in Fig. 8 (right).

3. Then $[\rho_1, \rho_2] = [0.142, 0.508]$ is a central confidence interval with 68\% C.L.

This is the same result as obtained by Clopper and Pearson (C-P) in 1934 [44], citing Fisher, Neyman, and Neyman’s students. In HEP, such C-P intervals are the standard for a binomial parameter; they have been in PDG RPP since 2002 [12] (although the connection of the given formula with C-P is obscure).

The same method was applied to confidence intervals for a Poisson mean by Garwood in his 1934 thesis, and published in 1936. (See Ref. [30], and references therein.) They are also the standard in HEP when there is no background. There is controversy when there is background; see PDG RPP (Section 39.4.2.4).

Many tables and online calculators for C-P intervals and Garwood intervals exist; I usually use Ref [45].

The use of the word “exact” (dating to Fisher) for intervals such as C-P refers to the construction above. But the discreteness of observed $x$ ($n_{\text{on}}$ in this case) causes the frequentist coverage (defined and discussed Section 6.11 below) not to be exact, but rather generally greater than the chosen C.L. C-P intervals are thus criticized by some as “wastefully conservative”. For a comprehensive review of both central and non-central confidence
intervals for a binomial parameter and for the ratio of Poisson means, see Cousins, Hymes, and Tucker [46]. Many choices, including C-P, are implemented in ROOT [47].

For the closely related construction of upper/lower limits and central confidence intervals for a Poisson mean, see Ref. [30].

6.5.2 Gaussian approximation for binomial confidence intervals: Wilson score interval of 1927

As mentioned above, $n_{on}$ has mean and rms deviation given by Eqns. 19 and 20, and for asymptotically large $n_{tot}$, Bi($n_{on}$|$n_{tot}$, $\rho$) converges to a Gaussian with mean $\mu(\rho) = n_{tot}\rho$ and rms $\sigma(\rho) = \sqrt{n_{tot}\rho(1 - \rho)}$.

We can thus compute approximate confidence intervals for $\rho$ while invoking this Gaussian approximation to the binomial distribution.

The idea is not to substitute $\hat{\rho}$ for $\rho$ in Eqns. 19 and 20 (potentially big mistake!), but rather to follow the logic already used above from E.B. Wilson in 1927 [43]. (This is in fact the example that he was illustrating in that paper!) That is, we use the above recipe for upper and lower limits:

1. Find $\rho_1$ such that Gauss($x \geq 3$|mean $\rho_1$, $\sigma(\rho_1)$) = 0.16.

2. Find $\rho_2$ such that Gauss($x \leq 3$|mean $\rho_2$, $\sigma(\rho_2)$) = 0.16.

This consistently uses the (different) values of $\sigma$ associated with each $\rho$, not $\sigma(\hat{\rho})$. It leads to a quadratic equation that, for our example, has solution [$\rho_1, \rho_2$] = [0.18, 0.46]. This is the approximate 68% C.L. confidence interval known as the Wilson score interval. (See Ref. [46] and references therein.)
Although this Wilson score interval needs only the quadratic formula, it is for some reason relatively unknown, as students are taught the Wald interval (UGH) of the next subsection.

6.5.3 Gaussian approximation for binomial confidence intervals: potentially disastrous Wald interval to avoid

It is tempting instead to follow the so-called “Wald reasoning” mentioned in Section 6.4.2, and to substitute $\hat{\rho} = n_{\text{tot}}\rho$ for $\rho$ in the expression for the rms deviation in Eqn. 20. One obtains: $\hat{\sigma} = \sqrt{n_{\text{tot}}\rho(1 - \hat{\rho})}$ and it seems a simple step to the potentially disastrous “Wald interval” $\hat{\rho} \pm \hat{\sigma}$, i.e., $[\rho_1, \rho_2] = [\hat{\rho} - \hat{\sigma}, \hat{\rho} + \hat{\sigma}]$.

The Wald interval does not use the correct logic for frequentist confidence! In fact, $\hat{\sigma} = 0$ when $n_{\text{on}} = 0$ or $n_{\text{on}} = n_{\text{tot}}$.

Incredibly, the failure of the Wald interval when $n_{\text{on}} = 0$ (or $n_{\text{on}} = n_{\text{tot}}$) has been used as a foundational argument in favor of Bayesian intervals in at least four public HEP postings (one retracted) and one published astrophysics paper! Of all the misguided things that have been written about statistics (sometimes by me) in nominally scholarly writings, this is among most uninformed that I have seen. (Typically the authors were not informed about Bayesian statistics either, and thought that a prior uniform in $\rho$ was obvious, without having read the vast Bayesian literature on priors for a binomial parameter.)

Beware! Avoid the Wald interval except for “hallway estimates” — there is no reason to use it. And certainly do not make the silly claim that problems with the Wald interval point to foundational issues with confidence intervals. The Wald interval does not use “confidence” reasoning, and was already obsolete in 1927 as the Gaussian approximation to binomial confidence intervals; and by 1934 the exact intervals using confidence reasoning were published by C-P! They have no problem with the cases “fatal” to Wald intervals, $n_{\text{on}} = 0$ or $n_{\text{on}} = n_{\text{tot}}$, as can be easily verified.

6.5.4 HEP applications of confidence intervals for binomial parameter

As mentioned, the binomial model is directly relevant to efficiency calculations in the usual case where $n_{\text{on}}$ is not fixed by the experiment design but rather sampled.

Using a famous math identity, the binomial model is also directly applicable to confidence intervals for the ratio of Poisson means [46, 48]. Thus, it is applicable to statistical significance ($Z_{\text{Bi}}$) of an excess in a signal bin when a sideband is used to estimate the mean background. (See Cousins, Linnemann, and Tucker [49].) As discussed in our paper, one can even stretch the use of $Z_{\text{Bi}}$ (using a “rough correspondence”) to the problem of a signal bin when a Gaussian estimate of mean background exists.

6.6 Perceived problems with upper/lower limits and hence for central confidence intervals

For decades, issues with upper limits and central confidence intervals have been discussed in two prototype problems in HEP:
• Gaussian measurement resolution near a physical boundary (e.g., neutrino mass-squared is positive, but the sample \( x \) is negative);

• Poisson signal mean measurement when observed number of events is less than mean expected background (so that the naive “background-subtracted” mean is negative).

Many ideas have been put forward, and by 2002 the PDG RPP settled on three, which remains the case [12]. I have described some of this interesting history in a “virtual talk” [50] and in an arXiv post [51]. (See Section 14 in this paper.) In this section, I describe just one of these three ideas, namely using Neyman’s confidence interval construction, going beyond the common orderings of \( x \) discussed thus far (Section 6.2.1), to that advocated by Feldman and Cousins (F-C) [52]. (The other two ideas in the RPP are Bayesian upper limits and \( CL_s \) (Section 14.1.).)

6.7 Beyond upper/lower limits and central confidence intervals

Among the more general choices for ordering \( x \) in \( p(x|\mu) \), the most common in HEP is that based on a likelihood ratio (LR):

For each \( \mu \), order \( x_0 \) using the likelihood ratio \( \mathcal{L}(x_0|\mu)/\mathcal{L}(x_0|\mu_{\text{best-fit}}) \), where \( \mu_{\text{best-fit}} \) respects the physical boundaries of \( \mu \). This was advocated in HEP by Feldman and Cousins in 1998 [52]. In fact, as learned by F-C while their paper was in proof, the dual hypothesis test (Section 7.4) appeared in the hypothesis test section of the frequentist classic by “Kendall and Stuart” [53] long before and since. Unlike the orderings described above, the LR ordering is applicable in both 1D and multi-D for \( x \).

Recall from Section 4.1 that likelihood ratios as in F-C are independent of metric in \( x \) since the Jacobians cancel, so there is no issue there. In contrast, an alternative that might come to mind, namely ordering \( x \) by the probability density \( p(x|\mu) \), is not recommended. A change of metric from \( x \) to \( y(x) \) leads to a Jacobian \( |dy/dx| \) in \( p(y|\mu) = p(x|\mu)/|dy/dx| \) (as in Section 4.1). So ordering by \( p(y|\mu) \) is different than ordering by \( p(x|\mu) \), and so all that would follow from ordering by a pdf would depend on the arbitrary choice of metric.

In order to implement this more general ordering by likelihood ratios, we must go beyond finding the confidence interval endpoints \( \mu_1 \) and \( \mu_2 \) independently, and perform the construction of the whole interval at the same time, as in the next subsection.

6.8 Neyman’s Construction of Confidence Intervals

The general method for constructing “confidence intervals”, and the name, were invented by Jerzy Neyman in 1934-37. It takes a bit of time to sink in—given how often confidence intervals are misinterpreted, perhaps the argument is bit too ingenious! In particular, you should understand that the confidence level does not tell you “how confident you are that the unknown true value is in the specific interval you report”—only a subjective Bayesian credible interval has that property! Rather, as stated in Section 6.2, the confidence interval \([\mu_1, \mu_2]\) contains those values of \( \mu \) for which the observed \( x_0 \) is not “extreme”, according to the ordering principle chosen. In this section, we describe this construction in more detail and more generality. We begin with 1D data and one parameter \( \mu \).
Given a $p(x|\mu)$: For each value of $\mu$, one draws a horizontal acceptance interval $[x_1, x_2]$ such that

$$p(x \in [x_1, x_2]|\mu) = \text{C.L.} = 1 - \alpha,$$

as in Fig. 9(left). The “ordering principle” that was chosen for $x$ is used to well-define which values of $x$ are included.

Upon observing $x$ and obtaining the value $x_0$, one draws a vertical line through $x_0$, as in Fig. 9(right). The vertical confidence interval $[\mu_1, \mu_2]$ with confidence level C.L. = $1 - \alpha$ is the union of all values of $\mu$ for which the corresponding acceptance interval is intercepted by the vertical line, as in Fig. 9(bottom). (It need not be simply connected, as in highly nonlinear applications such as neutrino oscillations.)

*Important note:* $x$ and $\mu$ need not have the same range, units, or (in generalization to higher dimensions) dimensionality!

In fact, I think it is *much* easier to avoid confusion if $x$ and $\mu$ are qualitatively different. Louis Lyons gives the example where $x$ is the flux of solar neutrinos and $\mu$ is the temperature at the center of the sun. I like examples where $x$ and $\mu$ have different dimensions: Neyman’s original paper [42] has a 2D observation space and 1D parameter space; his figure was crucial for my own understanding of the construction.

### 6.9 Famous confusion re Gaussian $p(x|\mu)$ where $\mu$ is mass $\geq 0$

A prototype problem is the Gaussian model $p(x|\mu, \sigma)$ in Eqn. 10 in the case where $\mu$ corresponds to a quantity that is physically non-negative, e.g., a mass, a mass-squared, or an interaction cross section. Note that in this case negative values of $\mu$ do not exist in the model!

A particle’s mass-squared might be computed by measuring a particle’s energy-squared ($E^2$) with Gaussian resolution and also (independently) its momentum-squared ($p^2$) with Gaussian resolution. Then the observable $x$ corresponding to mass-squared could be computed from $E^2 - p^2$, with Gaussian resolution. If the true $m^2$ is zero or small compared to the resolution, then such a procedure can easily obtain a value of $x$ that is negative. There is *nothing anomalous* about negative $x$.

A key point that was a source of a lot of confusion historically in HEP, and which still trips up people, is the following: It is *crucial* to distinguish between the observed data $x$, which can be negative (no problem), and the model parameter $\mu$, for which negative values do not exist in the model. For parameter $\mu < 0$, $p(x|\mu)$ does not exist: You would not know how to simulate the physics of your detector response to negative mass!

The constraint $\mu \geq 0$ thus has *nothing* to do with a Bayesian prior pdf for $\mu$ (!!!) as sometimes mistakenly thought. The constraint is in the model, and hence in the likelihood $L(\mu)$, not in the prior pdf.

The confusion is encouraged since we often refer to $x$ as the “measured value of $\mu$”, and say that $x < 0$ is “unphysical”. This is a bad habit! The value $x$ is an observed sample from a Gaussian centered on $\mu$, with $\mu$ being “physical”.

Thus a proper Neyman construction graph for the case at hand has $x$ with *both arithmetic signs* but only non-negative $\mu \geq 0$. This is the case in the plot in Fig. 10(left), following that in F-C [52]. There was a lot of confusion in the early days when the vertical axis on
Figure 9: Steps in the Neyman construction, as described in the text. From Ref. [52].
Figure 10: (left) The Neyman construction for the nonnegative mean of a Gaussian with acceptance intervals shown in blue, as advocated in Ref. [52]. (right) The “confidence belt” obtained from the construction on the left, showing the envelope of the acceptance intervals, which are not drawn.

this plot was extended to non-physical values of $\mu$. Since the model does not exist there, it is a conceptual mistake to draw the acceptance intervals there (as some did).

For alternative methods for dealing with this situation, see Section 14.

6.10 Confidence belts

From the earliest days (as in the 1934 Clopper-Pearson paper [44]), the horizontal line segments of the acceptance intervals (such as in Fig. 10(left)) have been suppressed, and only their envelope, as in the black curves in Fig. 10(right), have been plotted. The black curves (and interior) are called a confidence belt.

I added the line segments for demonstrating the construction in the F-C paper after reading Neyman’s 1937 paper [42], in which his Fig. 1 has a couple planes with acceptance regions shown, and a 1D vertical line at the observed 2D point intercepting them. This practice in the F-C paper is fortunately spreading.

I had found other descriptions of the construction, showing only the belt, to be too obscure when I was trying to learn the construction. There would be statements that I found cryptic, such as “Notice that the confidence belt is constructed horizontally but read vertically.” This made sense to me only after I had understood the construction!
6.11 Confidence intervals and coverage

Do you recall how a vector is defined in an abstract math class? In math, one defines a vector space as a set with certain properties, and then the definition of a vector is “an element of a vector space”. A vector is not defined in isolation!

Similarly, whether constructed in practice by Neyman’s construction or some other technique, a confidence interval is defined to be “an element of a confidence set”, where the confidence set is a set of intervals defined to have the property of frequentist coverage under repeated sampling:

Let \( \mu_t \) be the unknown true value of \( \mu \). In repeated experiments, confidence intervals will have different endpoints \([\mu_1, \mu_2]\), since the endpoints are functions of the randomly sampled \( x \).

A little thought will convince you that a fraction C.L. = 1 – \( \alpha \) of intervals obtained from Neyman’s construction will contain (“cover”) the fixed but unknown \( \mu_t \). I.e.,

\[
P(\mu_t \in [\mu_1, \mu_2]) = \text{C.L.} = 1 - \alpha. \tag{23}
\]

This equation is the definition of frequentist coverage. In this (frequentist!) equation, \( \mu_t \) is fixed and unknown. The endpoints \( \mu_1, \mu_2 \) are the random variables (!). Coverage is a property of the set of confidence intervals, not of any one interval.

[Here is the “little thought” that explains why Neyman’s construction leads to coverage: For the unknown true value \( \mu_t \), the probability that \( x_0 \) is in its acceptance interval is C.L., by construction. When those \( x_0 \)’s are obtained, the vertical line will intercept \( \mu_t \)’s acceptance region, and so \( \mu_t \) be will be put into the confidence interval. Thus the coverage equation is satisfied.]

One of the complaints about confidence intervals is that the consumer often forgets (if he or she ever knew) that the random variables in Eqn. 23 are \( \mu_1 \) and \( \mu_2 \), and not \( \mu_t \); and that coverage is a property of the set, not of an individual interval! Please don’t forget! A lot of confusion might have been avoided if Neyman had chosen the names “coverage intervals” and “coverage level”! (Maybe we can have a summit meeting treaty where frequentists stop saying “confidence” and Bayesians stop saying “noninformative”!)

Note: It is true (in precisely the sense defined by the ordering principle used for \( x \) in the Neyman construction) that the confidence interval consists of those values of \( \mu \) for which the observed \( x_0 \) is among the C.L. least extreme values to be observed.

6.11.1 Over-coverage when observable \( x \) is discrete

A problem arises in Neyman’s construction when the observable \( x \) (or more generally, the test statistic) is discrete. This was already the case in the Clopper-Pearson paper. When constructing an acceptance interval, typically Eqn. 22 cannot be satisfied exactly. The traditional convention (still typically observed in HEP) is to include enough values of \( x \) so that the equality becomes “\( \geq \)”. This means that the coverage equation includes so-called over-coverage:

\[
P(\mu_t \in [\mu_1, \mu_2]) \geq \text{C.L.} = 1 - \alpha. \tag{24}
\]

For a discussion of this issue and various opinions about it, see Ref. [46] and references therein.


7 Frequentist (classical) hypothesis testing

At this point, we set aside confidence intervals for the moment and consider from the beginning the nominally different topic of hypothesis testing. In fact, we will soon find that in frequentists statistics, certain hypothesis tests will take us immediately back to confidence intervals. But first we consider the more general framework.

Frequentist hypothesis testing, often called “classical” hypothesis testing, was developed by J. Neyman and E. Pearson (N-P) in unfriendly competition with R.A. Fisher. Modern testing has a mix of ideas from both “schools”. Following the N-P approach [2, 54], we frame the discussion in terms of a null hypothesis \( H_0 \) (e.g., the Standard Model), and an alternative \( H_1 \) (e.g., some Beyond-SM model).

As in Section 6.1, \( x \) is a test statistic (function of the observed data) and \( \mu \) represents parameters. Then the model \( p(x|\mu) \) is different for \( H_0 \) and \( H_1 \), either because parameter \( \mu \) (often called \( \theta \) by statisticians) has a different value, or because \( p(x|\mu) \) itself is a different functional form, perhaps with additional parameters.

For the null hypothesis \( H_0 \), we order possible observations \( x \) from least extreme to most extreme, using an ordering principle (which can depend on \( H_1 \) as well). We choose a cutoff \( \alpha \) (smallish number).

We then “reject” \( H_0 \) if the observed \( x_0 \) is in the most extreme fraction \( \alpha \) of observations \( x \) (generated under \( H_0 \)). By construction:

\[
\alpha = \text{probability (with } x \text{ generated according to } H_0 \text{) of rejecting } H_0 \text{ when it is true, i.e., false discovery claim (Type I error). It is called the size or significance level of the test.}
\]

To quantity the performance of this test if \( H_1 \) is true, we further define:

\[
\beta = \text{probability (with } x \text{ generated according to } H_1 \text{) of not rejecting (“accepting”) } H_0 \text{ when it is false, i.e., not claiming a discovery when there is one (Type II error). The power of the test is defined as } 1 - \beta.
\]

Note: If the alternative \( H_1 \) is not specified, then \( \beta \) is not known and optimality cannot be well-defined. The test is then called a goodness-of-fit test of \( H_0 \), as discussed in Section 7.7.

There is tradeoff between Type I and Type II errors. Competing analysis algorithms (resulting in different test statistics) can be compared by looking at graphs of \( \beta \) vs \( \alpha \) at various \( \mu \), and at graphs of \( 1 - \beta \) vs \( \mu \) at various \( \alpha \) (power function). (See, e.g., Ref. [2], pp. 258, 262.) This is similar to comparing b-tagging efficiency for signal and background. It is equivalent to the ROC curve used on other fields.

Appendix A illustrates the tradeoff between \( \alpha \) and \( \beta \) with a toy example of spin discrimination of a new resonance.

7.1 The choice of Type I error probability \( \alpha \)

The choice of operating point on the \( \beta \) vs \( \alpha \) curve (or ROC curve) is a long discussion. (It is even longer when considered as the number \( N \) of events increases, so that both \( \alpha \) and \( \beta \) are reduced.) The N-P language of “accept” or “reject” \( H_0 \) should not be mistaken for a complete theory of decision-making: A decision on whether or not to declare discovery (falsifying \( H_0 \)) requires 2 more inputs:
• Prior belief in $H_0$ vs $H_1$. (Can affect choice of $\alpha$)

• Cost of Type I error (false discovery claim) vs cost of Type II error (missed discovery). (Can also affect choice of $\alpha$)

A one-size-fits-all criterion of $\alpha$ corresponding to $5\sigma$ is without foundation! For a discussion of this point, see Refs. [3, 55].

Considerations such as these for the choice of $\alpha$ typically depend on the context. Using the result of an experiment for a single test of a physics hypothesis is a very different context than repeatedly selecting candidate b-jets with a b-tagging algorithm as in Section 3.2. In the latter case, the tradeoff between $\beta$ vs $\alpha$ is usually determined by considerations downstream in the analysis.

7.2 Frequentist hypothesis testing: Simple hypotheses

In idealized cases that are sometimes reasonably well-approximated in HEP, a hypothesis may have no floating (unfixed) parameters. N-P called such hypotheses simple, in contrast to composite hypotheses that have unfixed parameters.

Examples in HEP where both $H_0$ and $H_1$ are truly simple are rare, but we do have a few examples where the quantity of interest is simple in both hypotheses, and the role of unfixed nuisance parameters does not badly spoil the “simplicity”. For example, the hypotheses $H_0$ vs $H_1$ might be:

• “jet originated from a quark” vs “jet originated from a gluon”, for a jet reconstructed in the detector

• spin-1 vs spin-2 for a new resonance in $\mu^+\mu^-$

• $J^P = 0^+$ vs $J^P = 0^-$ for the Higgs-like boson

A simplified, detailed illustration of the second test is in Appendix A, while an example of the latter test published by CMS is in Section 7.6.2. Of course, framing these tests in this way makes strong assumptions (in particular that one of the two hypotheses is true) that need to be revisited once data are in hand.

7.2.1 Testing Simple hypotheses: Neyman–Pearson lemma

If the Type I error probability $\alpha$ is specified in a test of simple hypothesis $H_0$ against simple hypothesis $H_1$, then the Type II error probability $\beta$ is minimized by ordering $x$ according to the likelihood ratio [54],

$$\lambda = \mathcal{L}(x|H_0)/\mathcal{L}(x|H_1).$$ (25)

One finds the cutoff $\lambda_{\text{cut},\alpha}$ for the desired $\alpha$ and rejects $H_0$ if $\lambda \leq \lambda_{\text{cut},\alpha}$. For a conceptual (but incomplete) outline of a proof, see the lecture of Kyle Cranmer [56] as well as Ref. [53] (p. 176). As mentioned, Appendix A has an example.

This “Neyman–Pearson lemma” applies only to a very special case: no fitted parameters, not even undetermined parameters of interest! But it has inspired many generalizations, and likelihood ratios are an oft-used component of both frequentist and Bayesian methods.
7.3 Nested hypothesis testing

In contrast to two disjoint simple hypotheses, it is common in HEP for \( H_0 \) to be *nested* in \( H_1 \). For example, commonly \( H_0 \) corresponds to the parameter \( \mu \) in \( H_1 \) being equal to a particular value \( \mu_0 \). (Typical values of \( \mu_0 \) are 0 or 1.) So we often consider:

\[ H_0: \mu = \mu_0 \text{ (the “point null”, or “sharp hypothesis”) vs} \]

\[ H_1: \mu \neq \mu_0 \text{ (the “continuous alternative”).} \]

Common examples are:

- Signal strength \( \mu \) of new physics: null \( \mu_0 = 0 \), alternative \( \mu > 0 \)
- \( H_0 \to \gamma\gamma \) before discovery of this decay, \( \mu = \) signal strength: null \( \mu_0 = 0 \), alternative \( \mu > 0 \)
- \( H_0 \to \gamma\gamma \) after discovery of this decay: \( \mu \) is the ratio of the signal strength to the SM prediction; null \( \mu_0 = 1 \) (i.e., SM prediction), alternative is any other \( \mu \neq \mu_0 \).

7.4 Nested hypothesis testing: Duality with intervals

In the classical frequentist formalism (but not the Bayesian formalism), the theory of these tests maps to that of confidence intervals! The argument is as follows.

1. Having observed data \( x_0 \), suppose the 90% C.L. confidence interval for \( \mu \) is \([\mu_1, \mu_2]\).
   This contains all values of \( \mu \) for which the observed \( x_0 \) is ranked in the least extreme 90% of possible outcomes \( x \) according to \( p(x|\mu) \) and the ordering principle in use.

2. With the same data \( x_0 \), suppose that we wish to test \( H_0 \) vs \( H_1 \) (as defined in Section 7.3) at Type I error probability \( \alpha = 10\% \). We reject \( H_0 \) if \( x_0 \) is ranked in the most extreme 10% of \( x \) according to \( p(x|\mu) \) and the ordering principle in use.

Comparing the two procedures, we see that we reject \( H_0 \) at \( \alpha = 10\% \) if and only if \( \mu_0 \) is outside the 90% C.L. confidence interval \([\mu_1, \mu_2]\).

(In this verbal description, I am implicitly assuming that \( x \) is continuous and that \( p(x|\mu) \) is a pdf that puts zero probability on a point \( x \) with measure zero. Thus I ignore any issues concerning endpoints of intervals.)

We conclude: *Given an ordering:* a test of \( H_0 \) vs \( H_1 \) at significance level \( \alpha \) is equivalent to asking: Is \( \mu_0 \) outside the confidence interval for \( \mu \) with C.L. = 1 - \( \alpha \)?

As Kendall and Stuart put it, “There is thus no need to derive optimum properties separately for tests and for intervals; there is a one-to-one correspondence between the problems as in the dictionary in Table 20.1” [53] (p. 175). The table mentioned maps the terminology that historically developed separately for intervals and for testing, e.g.,

\[ \alpha \leftrightarrow 1 - \text{C.L.} \]

Most powerful \( \leftrightarrow \) Uniformly most accurate

Equal-tailed tests \( \leftrightarrow \) central confidence intervals

Use of this duality is referred to as “inverting a test” to obtain confidence intervals, and vice versa.
7.5 Feldman-Cousins

As mentioned in Section 6.7, the “new” likelihood-ratio (LR) ordering principle that Gary Feldman and I advocated for confidence intervals in Ref. [52] turned out to be one and the same as the time-honored ordering (generalized to include nuisance parameters) described in Ref. [53] in the chapter of hypothesis testing using likelihood ratios. We had scoured statistics literature for precedents of “our” intervals without finding anything. But we over-looked the fact that we should also be scouring the literature on hypothesis tests, until Gary realized that, just in time to get a note added in proof. In fact, it was all on 1 1/4 pages of “Kendall and Stuart”, plus nuisance parameters! This led to rapid inclusion of the LR ordering in the PDG RPP, since the proposal suddenly had the weight of real statistics literature behind it.

7.6 Post-data p-values and Z-values

The above N-P theory is all a pre-data characterization of the hypothesis test. A deep issue is how to apply it after $x_0$ is known, i.e., post-data.

In N-P theory, $\alpha$ is specified in advance. Suppose after obtaining data, you notice that with $\alpha = 0.05$ previously specified, you reject $H_0$, but with $\alpha = 0.01$ previously specified, you accept $H_0$. In fact, you determine that with the data set in hand, $H_0$ would be rejected for $\alpha \geq 0.023$.

This interesting value has a name: After data are obtained, the $p$-value is the smallest value of $\alpha$ for which $H_0$ would be rejected, had that value been specified in advance.

This is numerically (if not philosophically) the same as the definition used e.g. by Fisher and often taught: “The $p$-value is the probability under $H_0$ of obtaining $x$ as extreme or more extreme than the observed $x_0$. “ [4] (p. 58). See also Ref. [2] (p. 299) and Ref. [12] (Section 39.3.2).

In HEP, a $p$-value is typically converted to a $Z$-value (unfortunately commonly called “the significance S”), which is the equivalent number of Gaussian standard deviations. E.g., for a one-tailed test in a search for an excess, $p$-value = $2.87 \times 10^{-7}$ corresponds to $Z = 5$.

Note that Gaussianity of the test statistic is typically not assumed when the $p$-value is computed; this conversion to equivalent Gaussian “number of sigma” is just for perceived ease of communication. This needs to be emphasized when communicating outside HEP, as I hear too often statisticians wondering about Gaussian assumptions, in effect making the conversion counter-productive (!).

Although these lectures are not “statistics in practice”, I mention ROOT commands for one-tailed conversions (improved version courtesy of Igor Volobouev):

```c++
  zvalue = -TMath::NormQuantile(pvalue)
pvalue = 0.5*TMath::Erfc(zvalue/sqrt(2.0))
```

In our usual one-tailed test convention, $p$-value > 0.5 corresponds to $Z < 0$.

7.6.1 Interpreting $p$-values and $Z$-values

In the example above, it is crucial to realize that that value of $\alpha$ equal to the $p$-value (0.023 in the example) was typically not specified in advance. So $p$-values do not correspond to Type I error probabilities of experiments reporting them.
The interpretation of $p$-values (and hence $Z$-values) is a long, contentious story—beware! They are widely bashed; I discuss why in Section 9. I also defend their use in HEP. (See for example my paper on the Jeffreys-Lindley Paradox [3].)

Whatever they are, $p$-values are not the probability that $H_0$ is true! This mis-interpretation of $p$-values is unfortunately so common as to be used as an argument against frequentist statistics. Please keep in mind:

- That $p$-values are calculated assuming that $H_0$ is true, so they can hardly tell you the probability that $H_0$ is true!
- That the calculation of the “probability that $H_0$ is true” requires prior(s) to invert the conditional probabilities, as in Section 3.3.

Please help educate press officers and journalists! (and physicists)!

### 7.6.2 Early CMS Higgs boson spin-parity test of $0^+$ vs. $0^-$

As noted at the beginning of Section 7.2, the test of $H_0$: $J^P = 0^+$ vs $H_1$: $J^P = 0^-$ for the Higgs-like boson is a case where the parameter of interest (parity $P$) has two discrete values of interest, and the role of the (many) unfixed nuisance parameters does not badly spoil this “simplicity” in practice. Thus the test statistic used is (twice the negative log of) the Neyman–Pearson likelihood ratio $\lambda$ (with nuisance parameters separately optimized for each $P$). An early result from CMS [57] is shown in Fig. 11. The pdf of the test statistic, obtained by simulation, is shown for each hypothesis.

The similarity with the spin discrimination example in Appendix A is evident; the principles are the same, but in the Higgs boson case the likelihood functions are more complicated and there are nuisance parameters. As such examples are fairly rare in HEP (compared to cases of a continuous alternative), there was a fair amount of discussion within CMS about how best to present the results post-data. CMS reported:

1. The observed value $\lambda = -2 \ln(L_{0^-}/L_{0^+}) = 5.5$, favoring $0^+$;
2. For a test of $H_0$: $0^-$, the $p$-value = 0.0072;
3. Reversing the role of the two hypotheses and testing $H_0$: $0^+$, the $p$-value = 0.7;
4. $CL_s = (0.0072)/(1 - 0.7) = 0.024$, “a more conservative value for judging whether the observed data are compatible with $0^-$.“ (See Section 14.1.)

Note that for each $p$-value calculation, the relevant tail probability is for the tail in the direction of the other hypothesis. The Bayes factor (Section D) for this test is similar to the observed value of $\lambda$ reported, as it differs only in the treatment of the nuisance parameters (marginalization rather than separate optimization).

Demortier and Lyons [58] discuss the two $p$-values in such a simple-vs-simple case, contrasting tail probabilities with the likelihood ratio. See also Fig. 4 of Ref. [59].
Figure 11: Figure and caption from the early CMS paper on a test of $J^P = 0^+ \text{ vs } J^P = 0^-$ for the Higgs-like boson [57].
7.6.3 Post-data choice of the C.L.

Section 7.4 describes how for a hypothesis test dual to intervals, the (pre-data) $\alpha$ corresponds to $1 - C.L.$ Then in Section 7.6, the (post-data) $p$-value is the smallest value of $\alpha$ for which $H_0 : \mu = \mu_0$ would be rejected. In light of the duality, the corresponding post-data quantity for intervals is “the largest value of the C.L. (or limiting value thereof) such that $\mu_0$ is not in the confidence interval for $\mu.$” This is clearly equal to one minus the $p$-value, but (remarkably to me) it seems not to have a standard name in the statistics literature. Thus I will call it the “critical C.L.” A more natural way to think about this critical value may be “the smallest value of the C.L. such that $\mu_0$ is in the confidence interval for $\mu.$” For people focused more on the interval aspect of the duality, the critical C.L. may seem a natural way to express a post-data result when a particular value $\mu_0$ is of interest. In fact, shortly after the F-C paper, the CDF collaboration [60] measured a quantity called $\sin 2\beta$ for which a key scientific question was whether $\sin 2\beta > 0$. They reported the critical value of C.L. (0.93) for which 0 was (just) included in the F-C interval (so that 0 was an endpoint of the interval). I was in a couple email exchanges regarding what this 0.93 number was, and how to interpret it (as people understood that it was not a pre-data coverage probability for the CDF interval). Eventually we all agreed (I think) that it had exactly the same status as a post-data $p$-value. Given the LR ordering used by F-C, a $p$-value associated with that ordering for the test of $\sin 2\beta = 0$ vs $\sin 2\beta > 0$ was simply $1 - 0.93 = 0.07$. Reporting the critical C.L. was dual to reporting that critical $\alpha$.

7.7 Classical frequentist goodness of fit (g.o.f.)

A more extended discussion of goodness of fit is in Appendix B.

If $H_0$ is specified but the alternative $H_1$ is not, then only the Type I error probability $\alpha$ can be calculated, since the Type II error probability $\beta$ depends on a $H_1$. A test with this feature is called a test for goodness-of-fit (to $H_0$). (Fisher called them significance tests. I leave it to others, e.g., Ref. [61], to try to explain his seemingly pathological opposition to explicit formulation of alternative hypotheses.) With no alternative specified, the question “Which test is best?” is thus ill-posed. Despite the popularity of tests with universal maps from test statistics to $\alpha$ (in particular $\chi^2$ and Kolmogorov tests), they may be ill-suited for many problems (i.e., they may have poor power $1 - \beta$ against relevant alternative $H_1$’s).

In 1D, the difficulty of the unbinned test question is exemplified by the following simple example: “Given 3 numbers (e.g. neutrino mixing angles) in $(0, 1)$, are they consistent with three calls to a random number generator that is uniform on $(0, 1)$?” Have fun with that! A plethora of possible tests in 1D are described in the book by D’Agostino and Stephens [62] (a must-read for those wanting to invent a new test).

As multi-D unbinned ML fits have proliferated in recent decades, there are increasing needs for multi-D unbinned g.o.f. tests. E.g., is it reasonable that 1000 events scattered in a 5D sample space have been drawn from a particular pdf (which may have parameters which were fit using an unbinned M.L. fit to those 1000 events)? Of course this is an ill-posed question, but we are looking for good omnibus tests. Then getting the null distribution of the test statistic from toy MC simulation (Section 13) is typically doable, it seems. One can follow an unbinned ML fit with a binned g.o.f. test such as $\chi^2$, but this brings in its own
issues. At a loss of power but increase in transparency, one can also perform tests on 1D or 2D distributions of the marginalized densities.

Appendix B has further discussion of g.o.f., based on my informal note [63].

8 Likelihood (ratio) intervals for 1 parameter

Recall from Part 1: the likelihood $L(\mu)$ is invariant under reparameterization from $\mu$ to $f(\mu)$:

$$L(\mu) = L(f(\mu)).$$

So likelihood ratios $L(\mu_1)/L(\mu_2)$ and log-likelihood differences $\ln L(\mu_1) - \ln L(\mu_2)$ are also invariant.

After using the maximum-likelihood method to obtain estimate $\hat{\mu}$ that maximizes either $L(\mu)$ or $L(f(\mu))$, one can obtain a likelihood interval $[\mu_1, \mu_2]$ as the union of all $\mu$ for which

$$2 \ln L(\hat{\mu}) - 2 \ln L(\mu) \leq Z^2,$$

for $Z$ real.

As sample size increases (under important regularity conditions) this interval approaches a central confidence interval with C.L. corresponding to $\pm Z$ Gaussian standard deviations. Section 9.3.2 of Ref. [2] has a heuristic argument why this might work; more rigorous discussions are in the literature on “asymptotic” (large sample size) approximations. (See Ref. [64]; Chapter 6 in Ref. [28]; and the discussions in Severini’s monograph devoted to likelihood methods [65].)

But! Regularity conditions, in particular the requirement that $\hat{\mu}$ not be on the boundary (which can also cause practical problems if it is close to a boundary), need to be carefully checked. If $\mu \geq 0$ on physical grounds, then $\hat{\mu} = 0$ requires care. (See, e.g., Ref. [66] and references therein.)

8.1 LR interval example: Gaussian pdf $p(x|\mu, \sigma)$ with $\sigma = 0.2\mu$

Recall from Section 6.4 the Gaussian pdf with $\sigma = 0.2\mu$. The likelihood function $L(\mu)$ for observed $x_0 = 10.0$ is plotted in Fig. 5, with a maximum at $\mu_{ML} = 9.63$. Fig. 12 is a plot of $-2\ln L(\mu)$, from which the likelihood ratio interval for $\mu$ at approximate 68% C.L. is $[\mu_1, \mu_2] = [8.10, 11.9]$. Compare with the exact confidence interval, $[8.33, 12.5]$.

8.2 Binomial likelihood-ratio interval example

Recall (Section 6.5) the example of $n_{\text{on}} = 3$ successes in $n_{\text{tot}} = 10$ trials, with $L(\rho)$ and $-2\ln L(\rho)$ plotted in Fig. 7. The minimum value of the latter is 2.64. Solving for solutions to $-2\ln L(\rho) = 2.64 + 1 = 3.64$, one obtains the likelihood-ratio interval $[\rho_1, \rho_2] = [0.17, 0.45]$. This can be compared to the Clopper-Pearson interval, $[\rho_1, \rho_2] = [0.14, 0.51]$, and the Wilson interval, $[\rho_1, \rho_2] = [0.18, 0.46]$.

8.3 Poisson likelihood-ratio interval example

Recall the plot of $L(\mu)$ in Fig. 2 for a Poisson process with $n = 3$ observed. Fig. 13 is a plot of $-2\ln L(\mu)$, from which the likelihood ratio interval at approximate 68% C.L. can
be similarly extracted, yielding $[\mu_1, \mu_2] = [1.58, 5.08]$. The central confidence interval is $[\mu_1, \mu_2] = [1.37, 5.92]$.

9 **Likelihood principle**

Recall the three methods of interval construction for binomial parameter $\rho$ upon observing $n_{on} = 3$ out of $n_{tot} = 10$ trials: Bayesian intervals as briefly outlined in Section 5, confidence intervals in Section 6.5, and LR intervals in Section 8.2. We can note that:

- For constructing Bayesian and likelihood intervals, $\text{Bi}(n_{on}|n_{tot}, \rho)$ is evaluated only at the observed value $n_{on} = 3$.
- For constructing confidence intervals we use, in addition, *probabilities for values of* $n_{on}$ *not observed*.

This distinction turns out to be a huge deal!

In both Bayesian methods and likelihood-ratio based methods, the probability (density) for obtaining the *data at hand* is used (via the likelihood function), *but probabilities for obtaining other data are not used*!

In contrast, in typical frequentist calculations (confidence intervals, $p$-values), one also uses probabilities of data that could have been observed but that were *not observed*.

The assertion that only the former is valid is captured by the

- **Likelihood Principle**: If two experiments yield likelihood functions that are proportional, then Your inferences from the two experiments should be identical.
There are various versions of the L.P., strong and weak forms, etc. See Ref. [53] and the book by Berger and Wolpert [67].

The L.P. is built into Bayesian inference (except e.g., when Jeffreys prior leads to violation). The L.P. is violated by $p$-values and confidence intervals. Jeffreys [15] (p. 385) still seems to be unsurpassed in his ironic criticism of tail probabilities, which include probabilities of data more extreme than that observed: “What the use of [the $p$-value] implies, therefore, is that a hypothesis that may be true may be rejected because it has not predicted observable results that have not occurred.”

Although practical experience indicates that the L.P. may be too restrictive, it is useful to keep in mind. When frequentist results “make no sense” or “are unphysical”, in my experience the underlying reason can be traced to a bad violation of the L.P.

### 9.1 Likelihood principle example #1: the “Karmen problem”

You expect background events sampled from a Poisson distribution with mean $b = 2.8$, assumed known precisely. For signal mean $\mu$, the total number of events $n$ is then sampled from a Poisson distribution with mean $\mu + b$. So $P(n) = (\mu + b)^n \exp(-\mu - b)/n!$.

Then suppose you observe no events at all! I.e., $n = 0$. (The numbers are taken from an important neutrino experiment [68].) Plugging in,

$$L(\mu) = (\mu + b)^0 \exp(-\mu - b)/0! = \exp(-\mu) \exp(-b)$$

Note that changing $b$ from 0 to 2.8 changes $L(\mu)$ only by the constant factor $\exp(-b)$. This gets renormalized away in any Bayesian calculation, and is irrelevant for likelihood ratios. So for zero events observed, likelihood-based inference about signal mean $\mu$ is independent
of expected $b$ when zero events are observed. (If the prior depends on $b$, as does the Jeffreys prior for this example in Section 5.3, then there is potentially an issue. But I do not see this used in HEP.)

For essentially all frequentist confidence interval constructions, the fact that $n = 0$ is less likely for $b = 2.8$ than for $b = 0$ results in narrower confidence intervals for $\mu$ as $b$ increases. This is a clear violation of the L.P.

### 9.2 Likelihood principle example #2: binomial stopping rule

This is famous example among statisticians, translated to HEP. You want to measure the efficiency $\epsilon$ of some trigger selection. You count until reaching $n_{\text{tot}} = 100$ zero-bias events, and note that of these, $m = 10$ passed the selection. The probability for $m$ is binomial with binomial parameter $\epsilon$:

$$\text{Bi}(m|n_{\text{tot}}, \epsilon) = \frac{n_{\text{tot}}!}{m!(n_{\text{tot}}-m)!}\epsilon^m(1-\epsilon)^{(n_{\text{tot}}-m)}$$

(28)

The point estimate is $\hat{\epsilon} = 10/100$, and we can compute the binomial confidence interval (Clopper-Pearson) for $\epsilon$. Also, plugging in the observed data, the likelihood function is

$$\mathcal{L}(\epsilon) = \frac{100!}{10!90!}\epsilon^{10}(1-\epsilon)^{90}$$

(29)

Suppose that your colleague counts zero-bias events until $m = 10$ have passed her trigger selection. She notes that this required $n_{\text{tot}} = 100$ minimum-bias events (a coincidence). Intuitively, the fraction 10/100 over-estimates her trigger’s $\epsilon$ because she stopped just upon reaching 10 passed events. Indeed an unbiased estimate of $\epsilon$ and confidence interval will be slightly different from the binomial case.

The relevant distribution here is (a version of) the negative binomial:

$$\text{NBi}(n_{\text{tot}}|m, \epsilon) = \frac{n_{\text{tot}}-1}{(m-1)!}\epsilon^m(1-\epsilon)^{(n_{\text{tot}}-m)}$$

(30)

Plugging in the observed data, her likelihood function is

$$\mathcal{L}(\epsilon) = \frac{99!}{9!90!}\epsilon^{10}(1-\epsilon)^{90}.$$  

(31)

So both you and your friend observed 10 successes out of 100 trials, but with different stopping rules. Your likelihood function is based on the binomial distribution. Your friend’s is based on the negative binomial distribution. The two likelihoods differ by (only!) a constant factor, so the (strong) LP says that inferences should be identical. In contrast, frequentist inferences that use probabilities of data not obtained result in different confidence intervals and $p$-values for the different stopping rules.

Amusing sidebar: The Jeffreys prior is indeed different for the two distributions, so use of Jeffreys prior violates (strong) L.P.
9.3 Stopping rule principle

The two efficiency measurements have different *stopping rules*: one stops after \( n_{\text{tot}} \) events, and the other stops after \( m \) events pass the trigger. Frequentist confidence intervals depend on the stopping rule; the likelihood function does not, except for an overall constant. So Bayesians will get the same answer in both cases, unless the *prior* depends on the stopping rule.

The strong L.P. implies, in this example, that the inference is independent of the stopping rule! This *irrelevance* has been elevated to the “Stopping Rule Principle”. (It is sometimes amusing to ask a recent Bayesian convert if they know that they just bought the Stopping Rule Principle.) Concepts that average/sum over the sample space, such as bias and tail probabilities, do not exist in the pure Bayesian framework.

A quote by L.J. (Jimmie) Savage (Ref. [69], p. 76), a prominent early subjective Bayesian advocate, is widely mentioned (as seen in Google hits, which can point you to a copy of the original “Savage forum” where you can read his original note):

“...I learned the stopping-rule principle from Professor Barnard, in conversation in the summer of 1952. Frankly, I then thought it a scandal that anyone in the profession could advance an idea so patently wrong, even as today I can scarcely believe that some people resist an idea so patently right.”

9.4 Likelihood principle discussion

We will not resolve this issue, but we should be aware of it. There is a lot more to the Likelihood Principle than I discuss here. See the book by Berger and Wolpert [67], but be prepared for the Stopping Rule Principle to set your head spinning. When frequentist confidence intervals from a Neyman construction badly violate the L.P., use great caution! And when Bayesian inferences badly violate frequentist coverage, again use great caution!

In these lectures I omitted the important (frequentist) concept of a “sufficient statistic”, due to Fisher. This is a way to describe data reduction without loss of relevant information. E.g., for testing a binomial parameter, one needs only the total numbers of successes and trials, and not the information on exactly which trials had successes. (See Ref. [53] for math definitions.) The “Sufficiency Principle” says (paraphrasing—there are strong and weak forms) that if the observed values of the sufficient statistic in two experiments are the same, then they constitute equivalent evidence for use in inference.

Birnbaum famously argued (1962) that the Conditionality Principle (Section 11.3) and the Sufficiency Principle imply the Likelihood Principle. Section 11.3 has a few more comments on this point.

Controversy continues. For a recent discussion and references, see Deborah Mayo’s 2014 detailed article [70] and references therein, with comments by six statisticians and rejoinder.

10 Summary of three ways to make intervals

Table 2 summarizes properties of the three ways discussed to make intervals. Only frequentist confidence intervals (Neyman’s construction or equivalent) can guarantee coverage. Only
Table 2: Summary of three ways to make intervals. The asterisk reminds us that the choice of prior might violate the likelihood principle.

| Requires prior pdf? | Bayesian credible | Frequentist confidence | Likelihood ratio |
|---------------------|-------------------|-------------------------|-----------------|
| Yes                 | No                | No                      | No              |
| Obeys Likelihood Principle? | Yes* | No | Yes |
| Random variable(s) in \( P(\mu_t \in [\mu_1, \mu_2]) = \text{C.L.} \) | \( \mu_t \) | \( \mu_1, \mu_2 \) | \( \mu_1, \mu_2 \) |
| (Over)Coverage guaranteed? | No | Yes | No |
| Provides \( P(\text{parameter}|\text{data}) \)? | Yes | No | No |

Table 3: 68 %C.L. confidence intervals for the mean of a Poisson distribution, based on the single observation \( n = 3 \), calculated by various methods.

| Method                     | Prior | Interval       | Length | Coverage? |
|----------------------------|-------|----------------|--------|-----------|
| Wald, \( n \pm \sqrt{n} \) | —     | (1.27, 4.73)   | 3.36   | no        |
| Garwood, Frequentist central | —     | (1.37, 5.92)   | 4.55   | yes       |
| Bayesian central           | 1     | (2.09, 5.92)   | 3.83   | no        |
| Bayesian central           | \( 1/\mu \) | (1.37, 4.64)   | 3.27   | no        |
| Bayesian central Jeffreys   | \( 1/\sqrt{\mu} \) | (1.72, 5.27)   | 3.55   | no        |
| Likelihood ratio           | —     | (1.58, 5.08)   | 3.50   | no        |

Bayesian and likelihood intervals are guaranteed to satisfy the likelihood principle (except when a prior such as Jeffreys’s prior violates it).

Table 3, inspired by Ref. [30], gives illustrative intervals for a specific Poisson case. It is of great historical and practical importance in HEP that the right endpoint of Bayesian central intervals with uniform prior is mathematically identical to that of the frequentist central confidence interval (5.92 in the example of \( n = 3 \), but true for any \( n \)). By the reasoning of Fig. 3, this identity applies to upper limits. In contrast, the prior \( 1/\mu \) is needed to obtain identity of the left endpoint of confidence intervals, and hence of lower limits (1.37 in the example, but true for any \( n \)).

The fact that our field is almost always concerned with upper (rather than lower) limits on Poisson means is responsible for the nearly ubiquitous use of the uniform prior (instead of the Jeffreys prior, for example); as noted in Section 5.7, the main use of the Bayesian machinery in HEP is as a technical device for generating frequentist inference, i.e., intervals that are (at least approximately) confidence intervals.

When known (fixed) background is added to the problem, the Bayesian intervals with uniform prior for \( \mu \) become conservative (over-cover), a feature that many are willing to accept in order to obey the likelihood principle (or perhaps for less explicitly stated reasons). (Even without background, frequentist intervals over-cover due to discreteness of \( n \), as discussed in Section 6.11.1.)
11 1D parameter space, 2D observation space

Until now we have considered 1D parameter space and 1D observation space. Adding a second observation adds surprising subtleties. As before, $\mu$ is a 1D parameter (often called $\theta$ by statisticians). An experiment has two observations, the set $\{x_1, x_2\}$. These could be:

- two samples from the same $p(x|\mu)$, or
- one sample each of two different quantities sampled from a joint density $p(x_1, x_2|\mu)$.

For frequentist confidence intervals for $\mu$, we proceed with a Neyman construction. Prior to the experiment, for each $\mu$, one uses an ordering principle on the sample space $(x_1, x_2)$ to select an acceptance region $A(\mu)$ in the sample space $(x_1, x_2)$ such that $P((x_1, x_2) \in A(\mu)) = \text{C.L.}$ (As mentioned in Section 6.8, this was the illustration in Neyman’s original paper.)

Upon performing the experiment and observing the values $\{x_{1,0}, x_{2,0}\}$, the confidence interval for $\mu$ at confidence level C.L. is the union of all values of $\mu$ for which the corresponding acceptance region $A(\mu)$ includes the observed data $\{x_{1,0}, x_{2,0}\}$.

The problem is thus reduced to choosing an ordering of the points $(x_1, x_2)$ in the sample space, in order to well-define $A(\mu)$, given a C.L. This turns out to be surprisingly subtle, exposing a further foundational issue.

11.1 Conditioning: Restricting the sample space used by frequentists

We now return to the point mentioned in Section 3.5 regarding the “whole space” of possibilities that is considered when computing probabilities.

In Neyman’s construction in the 2D sample space $(x_1, x_2)$, the probabilities $P((x_1, x_2) \in A(\mu))$ associated with each acceptance region $A(\mu)$ are unconditional probabilities with respect to the “whole” sample space of all possible values of $(x_1, x_2)$. In contrast, Bayesian inference is based on a single point in this sample space, the observed $(x_{1,0}, x_{2,0})$, per the Likelihood Principle. There can be a middle ground in frequentist inference, in which the probabilities $P((x_1, x_2) \in A(\mu))$ are conditional probabilities conditioned on a function of $(x_1, x_2)$, in effect restricting the sample space to a “recognizable subset” depending on the observed data.

Restricting the sample space in this way is known as conditioning. Here I discuss two famous examples:

- A somewhat artificial example of Welch [71] where the conditioning arises from the mathematical structure;
- A more physical example of Cox [72] where the argument for conditioning seems “obvious”.

52
11.1.1 Example of B.L. Welch (1939)

In this example, $x_1$ and $x_2$ are two samples from same $p(x|\mu)$, a rectangular pdf given by (Fig. 14)

$$p(x|\mu) = \begin{cases} 1, & \text{if } \mu - \frac{1}{2} \leq x \leq \mu + \frac{1}{2} \\ 0, & \text{otherwise.} \end{cases}$$  \hspace{1cm} (32)

The observed data is a set of two values $\{x_1, x_2\}$ sampled from this pdf. From these data, the point estimate for $\mu$ is the sample mean, $\hat{\mu} = \bar{x} = (x_1 + x_2)/2$. (Aside: if more than two samples are observed, the point estimate is the mean of the outermost two, not the whole sample mean; see Section E.0.1.)

What is a 68% C.L. central confidence interval for $\mu$? To perform a Neyman construction, for each $\mu$ we must define an acceptance region $A(\mu)$ containing 68% of the unit square $(x_1, x_2)$ centered on $\mu$, as in Fig. 15. Which 68% should one use? Centrality implies symmetry, but we need something else to rank points in the plane. The N-P Lemma suggests a likelihood ratio, but first let’s think about some examples of possible pairs $\{x_1, x_2\}$.

A “lucky” sample with $|x_1 - x_2|$ close to 1 is shown in Fig. 16(left): $L(\mu) = L_1(\mu) \times L_2(\mu)$ is very narrow. Is it thus reasonable to expect small uncertainty in $\hat{\mu}$?

An “unlucky” sample with $|x_1 - x_2|$ close to 0 is shown in Fig. 16(right): $L(\mu)$ has full width close to 1, as the second observation adds almost no useful information. Should we expect a 68% C.L. confidence interval for $\mu$ that is the same as for only one observation, i.e. with length 0.68?

Intuition says that a reasonable answer might be a confidence interval centered on $\hat{\mu}$, with a length that is 68% of the width of $\mathcal{L}$, i.e., the interval $\hat{\mu} \pm 0.34(1 - |x_1 - x_2|)$.

From this argument, it seems reasonable for the post-data uncertainty to depend on $|x_1 - x_2|$, which of course cannot be known in advance. This quantity $|x_1 - x_2|$ is a classic example of an ancillary statistic $A$: it has information on the uncertainty on the estimate of $\mu$, but no information on $\mu$ itself, because the distribution of $A$ does not depend on $\mu$. An idea dating to Fisher and before is to divide the full “unconditional” sample space into “recognizable subsets” (in this case having same or similar values of $A$), and calculate probabilities using the “relevant” subset rather than the whole space!

The (representative) diagonal lines in Fig. 17(left) show a partition of the full sample space into recognizable subsets.
Figure 15: The starting point for constructing confidence intervals in the Welch example: in the 2D data space centered on \((x_1 = \mu, x_2 = \mu)\) what should be the acceptance region \(A(\mu)\) containing 68% of the unit square? One should imagine a \(\mu\) axis perpendicular to the plane of the square, with such a square at each \(\mu\).

Figure 16: (left) A “lucky” set of observations \(\{x_1, x_2\}\) having small overlap of the likelihood functions, so that possible true \(\mu\) is localized. (right) an “unlucky” set of observations \(\{x_1, x_2\}\), for which the second observation adds little additional information.
space via the ancillary statistic $A = |x_1 - x_2|$. Within each partition, in Fig. 17(right), the shading shows a central 68% probability acceptance region (red fill). We are thus using conditional probabilities (still frequentist!) $p(x | A, \mu)$ in this Neyman construction, with desired probability 68% within each partition. (Aside: A set of measure zero has zero probability even if non-zero pdf, so in general, care is needed in conditioning on exact value of continuous $A$ in $p(x | A, \mu)$. This is not an issue here in this example.) The resulting $A(\mu)$ for the whole square fills 68% of the square, so there is correct unconditional probability as well.

Imagine a plane such as this for every $\mu$, and then obtaining the data $\{x_1, x_2\}$. The confidence interval for $\mu$ is then the union of all values of $\mu$ for which the observed data are in $A(\mu)$. A moment’s thought will confirm that this results in confidence intervals centered on $(x_1 + x_2)/2$, with a length that is 68% of $|x_1 - x_2|$, i.e., $\hat{\mu} \pm 0.34(1 - |x_1 - x_2|)$, as intuitively thought reasonable!

This construction is known as “conditioning” on the ancillary statistic $A$. In fact, it can be more simply stated: post-data, ignore the construction in the whole sample space for values of $A$ other than that observed, and proceed as if $A$ had been fixed, rather than randomly sampled!

Now the catch: one can find acceptance regions $A(\mu)$ that correspond to hypothesis tests with more power (lower Type 2 error probability $\beta$) in the unconditional sample space! A couple examples from the literature are shown in Fig. 18. The construction on the left results in 68% C.L. intervals with length independent of $|x_1 - x_2|$, namely $\hat{\mu} \pm 0.22$ at 68% C.L. They obtain 68% coverage in the unconditional sample space by having 100% coverage in the subspace where $|x_1 - x_2| \approx 1$ (narrow likelihood), while badly undercovering when $|x_1 \approx x_2|$. 
Welch’s 1939 paper argued \textit{against} conditioning because it is less powerful in the unconditional sample space! Neyman’s position is not completely clear but he also seems to have been against conditioning on ancillaries (which was Fisher’s idea) when it meant an overall loss of power [61, 73].

Most modern writers use Welch’s example as an “obvious” argument \textit{in favor} of conditioning, unless one is in an “industrial” setting where the unconditional ensemble is sampled repeatedly and the result for an individual sample is not of much interest.

\subsection{11.1.2 Efron example that is structurally similar to Welch example}

Brad Efron’s talk at PhyStat-2003 [8] included a similar example using the Cauchy distribution, where the ancillary statistic is the curvature of $L(\mu)$. He called the conditional answer “correct”.

\subsection{11.1.3 Cox two-measuring device example (1957)}

For measuring a mean $\mu$ with Gaussian resolution, one of two devices is selected randomly with equal probability:

Device #1 with $\sigma_1$

Device #2 with $\sigma_2 \ll \sigma_1$.

Then a single measurement sample is made with the chosen device.

In my notation, $x_1$ is the index (1 or 2) chosen randomly and specifying the device, and $x_2$ is the single sample from the selected Gaussian measurement. The total observed
data is then, as before, \( \{x_1, x_2\} \). But in this example, \( x_1 \) and \( x_2 \) are samples of two different quantities from the joint density \( p(x_1, x_2|\mu) \).

In Ref. [41] (p. 112) Luc Demortier gives a nice example in HEP: \( \mu \) is the mass of a decaying particle with probability \( p_h \) to decay hadronically (mass resolution \( \sigma_1 \)) and probability \( 1 - p_h \) to decay leptonically with mass resolution \( \sigma_2 \)). Thus the “measuring machine” chosen randomly is the detector used to measure the decay mode that is randomly chosen by quantum mechanics.

So \( \hat{\mu} = x_2 \). What is the confidence interval? The index \( x_1 \) is an ancillary statistic, and it is reasonable (obvious?) to condition on it. I.e., we report a confidence interval giving correct coverage in the \textit{subspace of measurements that used the same measuring device that we used}. So the 68\% C.L. confidence interval is:

\[ \hat{\mu} \pm \sigma_1 \text{ if Device #1 was randomly selected} \]
\[ \hat{\mu} \pm \sigma_2 \text{ if Device #2 was randomly selected} \]

Again it turns out that more powerful tests can be found. Demortier gives details on how the average length of intervals optimized in the unconditional sample space is shorter in the HEP example. Here I give Cox’s discussion.

If one is testing \( \mu = 0 \) vs \( \mu = \mu_1 \), with \( \mu_1 \) roughly the size of \( \sigma_1 \) (the larger \( \sigma \)), consider the following intervals: \( \hat{\mu} \pm (0.48) \sigma_1 \) if Device #1 used (covers true \( \mu \) in 37\% of uses), and \( \hat{\mu} \pm 5 \sigma_2 \) if Device #2 used (covers true \( \mu \) nearly 100\% of uses).

Then the true \( \mu \) is covered in \( (37/2 + 100/2)\% = 68\% \) of all intervals! The unconditional (full sample space) coverage is correct, but conditional coverage is not. Due to the smallness of \( \sigma_2 \), the average length of all intervals \textit{when averaging over the entire unconditional sample space} is smaller than for conditional intervals with independent coverage. One gives up power with Device #1 and uses it in Device #2.

Cox asserts: “If, however, our object is to say ‘what can we learn from the data that we have’, the unconditional test is surely no good.” [72] (p. 361) (See also Ref. [28] (pp. 47-48).)

### 11.2 Conditioning in HEP

A classic example is a \textit{measurement of the branching fraction of a particular decay mode} when the \textit{total} number of decays \( N \) can fluctuate because the experimental design is to run for a fixed length of time. Then \( N \) is an ancillary statistic. You perform an experiment and obtain \( N \) total decays, and then do a toy MC simulation (Section 13) of repetitions of the experiment. Do you let \( N \) fluctuate, or do you fix it to the value observed? It may seem that the toy MC should include your complete procedure, including fluctuations in \( N \).

But the above arguments would point toward \textit{conditioning on the value of the ancillary statistic actually obtained}. So your branching fraction measurement is binomial with trials \( N \). This was originally discussed in HEP by F. James and M. Roos [48]. For more complete discussion, see Ref. [46].

### 11.3 Conditioning and the likelihood principle

To summarize: conditioning on an ancillary statistic \( A \) means: Even though \( A \) was randomly sampled in the experimental procedure, after data are obtained, proceed as if \( A \) had been
fixed to the value observed. Ignore the rest of the sample space with all those other values of $A$ that you could have obtained, but did not.

The Welch and Cox (and Efron) examples reveal a real conflict between N-P optimization for power and conditioning to optimize relevance.

The assertion that inference should be conditioned on an ancillary in the Welch example (where it comes out of the math) is often called the “Conditionality Principle” (CP). Conditioning in the Cox example (a “mixture experiment” where the ancillary has physical meaning about which experiment was performed) is then called the “Weak Conditionality Principle” (WCP).

But note: in sufficiently complicated cases (for example if there is more than one ancillary statistic), the procedure is less clear. In many situations, ancillary statistics do not exist, and it is not at all clear how to restrict the “whole space” to the relevant part for frequentist coverage. For a comprehensive review of ancillary statistics and their applications, see Ref. [74].

The pure Bayesian answer is to collapse the whole sample space to the data observed, and refer only to the probability of the data observed, i.e., the likelihood principle discussed in Section 9. This is literally the ultimate extreme in conditioning, conditioning (in the continuous case) on a point of measure zero! (You can’t get any more “relevant”.) But the price is giving up coverage.

When there are “recognizable subsets” with varying coverage, Buehler [75] has discussed how a “conditional frequentist” can win bets against an “unconditional frequentist”. (See Refs. [50, 51].)

I emphasize conditioning not only for the practical issues, but also to explain that there are intermediate positions between the full unconditional frequentist philosophy and the Likelihood Principle of Section 9. A key point is that unconditional frequentist coverage is a pre-data assessment: the entire confidence belt is constructed independent of where the observation lies. Thus a big argument is whether unconditional coverage remains appropriate post-data, after one knows where one’s observed data lies in the sample space. When the “measurement uncertainty” depends strongly on where one’s data lies, then the arguments for conditioning seem strong. Whether or not one takes conditioning to the extreme and considers only the (measure-zero) subset of the sample space corresponding to the data observed is the issue of the Likelihood Principle [67].

It is not surprising that pure Bayesians argue for the importance of relevance of the inference, and criticize frequentists for the danger of irrelevance (and the difficulty of diagnostic of irrelevance). And it is not surprising that pure frequentists argue for the importance of a useful measure of “error rates”, in the sense of Type 1 and Type 2 errors, coverage, etc., which may at best be estimates if the L.P. is observed.

12 2D parameter space, multi-D observation space

We (finally) generalize to two parameters $\mu_1$ and $\mu_2$, with both true values unknown. (I hope that from context, there is no confusion from using the subscripts 1 and 2 to indicate different parameters, whereas in the 1D case above, they indicate the endpoints of a confidence interval on the single parameter $\mu$.) Let data $x$ be a multi-D vector, so the model is $p(x|\mu_1, \mu_2)$. The
observed vector value is $x_0$.

First consider the desire to obtain a 2D confidence/credible region in the parameter space $(\mu_1, \mu_2)$. All three methods discussed for intervals handle this in a straightforward (in principle) generalization. We mention the first two briefly and devote a subsection to the third:

**Bayesian:** Put the observed data vector $x_0$ into $p(x|\mu_1, \mu_2)$ to obtain the likelihood function $L(\mu_1, \mu_2)$. Multiply by the prior pdf $p(\mu_1, \mu_2)$ to obtain the 2D posterior pdf $p(\mu_1, \mu_2|x_0)$. Use the posterior pdf to obtain credible regions, etc., in $(\mu_1, \mu_2)$.

**Confidence intervals:** Perform a Neyman construction: Find acceptance regions $A(\mu_1, \mu_2)$ for $x$ as a function of $(\mu_1, \mu_2)$. The 2D confidence region is the union of all $(\mu_1, \mu_2)$ for which $x_0$ is in $A(\mu_1, \mu_2)$.

### 12.1 Likelihood regions in $\geq 2D$ parameter space

Recall the method for 1D confidence intervals, Eqn. 26. For a joint 2D likelihood region, first find the global maximum of $L(\mu_1, \mu_2)$, yielding point estimates $\hat{\mu}_1, \hat{\mu}_2$. Then find the 2D contour bounded by

$$2\Delta \ln L = 2 \ln L(\hat{\mu}_1, \hat{\mu}_2) - 2 \ln L(\mu_1, \mu_2) \leq C,$$

where $C$ comes from Wilks's Theorem, tabulated in the PDG RPP [12] (Table 39.2) for various C.L. and for various values of $m$, the dimensionality of the confidence region. Here we have the case $m = 2$, for which $C = 2.3$ for 68% C.L.

This region is an approximate confidence region, as sketched in Fig. 19. As in 1D, Wilks’s Theorem is an asymptotic (large $N$) result, with various “regularity conditions” to be satisfied. (Again see, e.g., Ref. [66] and references therein.)
12.2 Nuisance parameters

Frequently one is interested in considering one parameter at a time, irrespective of the value of other parameter(s). The parameter under consideration at the moment is called the "parameter of interest" and the other parameters (at that moment) are called "nuisance parameters". E.g., if $\mu_1$ is of interest and $\mu_2$ is a nuisance parameter, then ideally one seeks a 2D confidence region that is a vertical "stripe" in the $(\mu_1, \mu_2)$ plane as in Fig. 20(left); this allows the same 1D interval to be quoted for $\mu_1$, independent of $\mu_2$. Or, in different moment, $\mu_2$ may be of interest and $\mu_1$ is a nuisance parameter; then one seeks a horizontal stripe, as in Fig. 20(right). How can one construct these stripes?

Each of the three main classes of constructing intervals (Bayesian, Neyman confidence, likelihood ratio) has a "native" way to incorporate the uncertainty on the nuisance parameters, described in Sections 12.3–12.5. But this remains a topic of frontier statistics research.

12.2.1 Systematic uncertainties as nuisance parameters

Systematic uncertainties provide prototype examples of parameters that are frequently nuisance parameters, so I mention them briefly here. A typical measurement in HEP has many subsidiary measurements of quantities not of direct physics interest, but which enter into the calculation of the physics quantity of particular interest. E.g., if an absolute cross section is measured, one will have uncertainty in the integrated luminosity $L$, in the background level $b$, the efficiency $e$ of detecting the signal, etc. In HEP, we call these systematic uncertainties,
but statisticians (for the obvious reason) refer to $L$, $b$, and $e$ as *nuisance parameters*. For discussion of many of the issues with systematic uncertainties in HEP, see Refs. [76, 77, 78].

However, it is important to keep in mind is that whether or not a parameter is considered to be a nuisance parameter depends on context. For example, in measurements of Higgs boson couplings, the mass of the Higgs boson is typically regarded as a nuisance parameter. But clearly the mass of the Higgs boson can itself be the primary object of a measurement, in which case the couplings are the nuisance parameters.

### 12.3 Nuisance parameters I: Bayesian credible intervals

Construct a multi-D prior pdf $p(\text{parameters})$ for the space spanned by all parameters. Multiply by the likelihood function $L(\text{data} | \text{parameters})$ for the data obtained to obtained the multi-D posterior pdf. Integrate over the full subspace of all nuisance parameters (marginalization). Thus obtain the 1D posterior pdf for the parameter of interest. Further use of the posterior pdf is thus reduced to the case of no nuisance parameters.

*Problems:* The multi-D prior pdf is a problem for both subjective and non-subjective priors. In HEP there has been little use of the favored non-subjective priors (reference priors of Bernardo and Berger). The high-D integral can be a technical problem, more and more overcome by Markov Chain Monte Carlo.

As with all Bayesian analyses, how does one interpret probability if “default” priors are used, so that coherent subjective probability is not applicable?

#### 12.3.1 Priors for nuisance parameters

It used to be (unfortunately) common practice to express, say, a 50% systematic uncertainty on a positive quantity as a Gaussian with 50% rms. Then one “truncated” the Gaussian by not using non-positive values.

As mentioned in Section 5.11 but worth repeating, in Bayesian calculations, the interaction of a uniform prior for a Poisson mean and a “truncated Gaussian” for systematic uncertainty in efficiency leads to an integral that diverges if the truncation is at origin [38]. In evaluating the integral numerically, some people did not even notice!

*Recommendation:* Use lognormal or (certain) Gamma distributions instead of truncated Gaussian. Recipes are in my note [79].

### 12.4 Nuisance parameters II: Neyman construction

For each point in the subspace of nuisance parameters, treat them as fixed true values and perform a Neyman construction for multi-D confidence regions in the full space of all parameters. Project these regions onto the subspace of the parameter of interest.

*Problems:* Typically intractable and causes overcoverage, and therefore rarely attempted.

Tractability can sometimes be recovered by doing the construction in the lower dimensional space of the profile likelihood function, obtaining approximate coverage. (This is one way to interpret the Kendall and Stuart pages on the likelihood ratio test with nuisance parameters [53].)
Figure 21: Sketches for likelihood ratio regions. (left) The 2D confidence region from Fig. 19, when both parameters are of interest. (right) On the same scale, the 2D confidence region if $\mu_1$ is of interest and $\mu_2$ is a nuisance parameter, so that effectively one obtains a confidence interval for $\mu_1$ that is independent of $\mu_2$. The width of the stripe is smaller than the width of the extrema of the region on the left, since a smaller value of $C$ is used in Eqn. 33: the dashed contour on the right is inside the solid contour on the left. Both the left and the right shaded regions correspond to the same C.L.; the left region is relevant for joint inference on the pair of parameters, while the right region is relevant when only $\mu_1$ is of interest.

Problem: Not well-studied. Typically “elimination” is done in a way technically feasible, and the coverage studied with toy MC simulation (Section 13).

12.5 Nuisance parameters III: Likelihood ratio intervals

Many of us raised on MINUIT MINOS read the article by F. James, “Interpretation of the Shape of the Likelihood Function around Its Minimum,” [80]. Whereas the 2D region in Section 12.1 has $m = 2$ and hence $2\Delta \ln \mathcal{L} \leq 2.3$, for 1D intervals on $\mu_1$, we first make a 2D contour with the $m = 1$ value, $2\Delta \ln \mathcal{L} = 1$, as shown by the black dashed curve in Fig. 21(right). Then the extrema in $\mu_1$ of this curve correspond to the endpoints of the approximate confidence interval for $\mu_1$.

12.5.1 Profile likelihood function

At the Fermilab Confidence Limits Workshop in 2000, statistician Wolfgang Rolke expressed the construction in a different (but exactly equivalent) way [81, 82], as illustrated in Fig. 22
and paraphrased as follows:

- For each $\mu_1$, find the value $\hat{\mu}_2$ that minimizes $-2 \ln L(\mu_1, \hat{\mu}_2)$. Make a 1D plot vs $\mu_1$ of (twice the negative log of) this “profile likelihood function” $-2 \ln L_{\text{profile}}(\mu_1)$. Use the $m = 1$ threshold on $-2 \ln L_{\text{profile}}(\mu_1)$, i.e., Eqn. 26, to obtain intervals at the desired C.L.

The interval one obtains in Fig. 22 is the exact same interval as obtained by “MINOS” in Fig. 21(right). Can you see why? Since 2000, the “profile” statistical terminology has permeated HEP. The “hat-hat” notation (stacked circumflex accents) is also used by “Kendall and Stuart” [53] in the generalized hypothesis test that is dual to the intervals of Feldman and Cousins. See also Ref. [66].

**Warning:** Combining profile likelihoods from two experiments is unreliable. Apply profiling after combining the full likelihoods [83].

**Problems with profile likelihood:**

Coverage is not guaranteed, particularly with small sample size. By using the best-fit value of the nuisance parameters corresponding to each value of the parameter of interest, this has an (undeserved?) reputation for underestimating the true uncertainties.

In Poisson problems, the profile likelihood (MINUIT MINOS) gives surprisingly good performance in many problems. See Rolke, et al. [82].

In some cases (for example when there are spikes in $L$), marginalization may give better frequentist performance, I have heard. For small sample sizes, there is no theorem to tell us whether profiling or marginalization of nuisance parameters will give better frequentist coverage for the parameter of interest.
12.6 Not eliminating a nuisance parameter: the “raster scan”

In the 2D example of Figure 21, the right side is an attempt to “eliminate” the nuisance parameter \( \mu_2 \) by obtaining an interval estimate for \( \mu_1 \) that is independent of \( \mu_2 \). However, it may be that it is preferable simply to quote a 1D interval estimate for \( \mu_1 \) as a function of assumed true values for \( \mu_2 \). In a toy neutrino oscillation example, Feldman and Cousins [52] contrasted their unified approach with this method, which they referred to as a “raster scan”, in analogy with the way old televisions drew lines across the screen.

As an example, I am reminded that before the top quark mass was known, other measurements (and theoretical predictions) were typically given as a function of the unknown top quark mass, with no attempt to “eliminate” it (for example by putting a Bayesian prior pdf on it and integrating it out). In the search for the Higgs boson and ultimately the discovery, its unknown mass was a nuisance parameter that was also treated by raster scan: all the plots of upper limits on cross section, as well as \( p \)-values testing the background-only hypothesis, are given as a function of mass.

When to use a raster scan is a matter of judgment; for some useful considerations and detailed explanations, see Ref. [84].

12.7 Hybrid techniques: Introduction to pragmatism

Given the difficulties with all three classes of interval estimation, especially when incorporating nuisance parameters, it is common in HEP to relax foundational rigor and:

• Treat nuisance parameters in a Bayesian way (marginalization) while treating the parameter of interest in a frequentist way. Virgil Highland and I were early advocates of this for the luminosity uncertainty in upper limit calculation [85]. At PhyStat 2005 at Oxford, Kyle Cranmer revealed problems when used for background mean in a 5\( \sigma \) discovery context [86]. For a review of the background case and connection to George Box’s semi-Bayesian “prior predictive \( p \)-value”, see Cousins, Linnemann, and Tucker [49].

• Or, treat nuisance parameters by profile likelihood while treating parameter of interest another way,

• Or, use the Bayesian framework (even without the priors recommended by statisticians), but evaluate the frequentist performance [24]. In effect (as in profile likelihood) one gets approximate coverage while respecting the L.P. In fact, the statistics literature has attempts to find prior pdfs that lead to posterior pdfs with good frequentist coverage: probability matching priors. At lowest order in 1D, the matching prior is the Jeffreys prior! [87].

12.8 A couple looks at the literature on nuisance parameters

In the mid-2000s, Luc Demortier and I both looked in the statistics literature regarding nuisance parameters. I thought that my note was fairly thorough until I read his! Our writeups:
• R.D. Cousins, “Treatment of Nuisance Parameters in High Energy Physics, and Possible Justifications and Improvements in the Statistics Literature,” presented at the PhyStat 2005 at Oxford [88] with response by statistician Nancy Reid [89].

• Luc Demortier, “P Values: What They Are and How to Use Them,” [90]. See also Luc’s scholarly Chapter 4 on interval estimation in Ref. [41].

12.9 HEP “State of the art” for dealing with nuisance parameters

All three main classes of methods are commonly used on the parameter of interest. In addition:

• Both marginalization and profiling are commonly used to treat nuisance parameters.

• Many people have the good practice of checking coverage.

• Too little attention is given to priors, in my opinion. But the flat prior for Poisson mean is “safe” (from frequentist point of view) for upper limits (only!).

A serious analysis using any of the main methods requires coding up the model $p(x|\mu)$. (It is needed at $x = x_0$ to obtain the likelihood function, and at other $x$ as well for confidence intervals.) Doing this (once!) with the RooFit [91] modeling language gives access to RooStats [92] techniques for all three classes of calculations, and one can mix/match nuisance parameter treatments.

13 Evaluation of coverage with toy MC simulation

For a single parameter of interest $\mu$, one typically reports the confidence interval $[\mu_1, \mu_2]$ at some C.L. after elimination of nuisance parameters by some approximate method and construction of intervals perhaps involving more approximations. It is important to check that the approximations in the whole procedure have not materially altered the claimed coverage, defined in Eqn. 23. Typically the performance is evaluated with a simplified MC simulation, referred to as “toy Monte Carlo simulation”. First I describe the most thorough evaluation (very CPU intensive), and then some approximations.

In frequentist statistics, the true values of all parameters are typically fixed but unknown. A complete, rigorous check of coverage considers a fine multi-D grid of all parameters, and for each multi-D point in the grid, generates an ensemble of toy MC pseudo-experiments, runs the full analysis procedure, and finds the fraction of intervals covering the $\mu_t$ of interest that was used for that ensemble. I.e., one calculates $P(\mu_t \in [\mu_1, \mu_2])$, and compares to C.L.

Thus a thorough check of frequentist coverage includes:

1. Fix all parameters (of interest and nuisance) to a single set of true values. For this set,
   (a) Loop over “pseudo-experiments”
   (b) For each pseudo-experiment, loop over events, generating each event with toy data generated from the statistical model with parameters set equal to the fixed set.
(c) Perform the same analysis on the toy events in the pseudo-experiment as was
done for the real data.

(d) Find that fraction of the pseudo-experiments for which parameter(s) of interest
are included in stated confidence intervals or regions.

2. **Repeat for various other fixed sets of all parameters**, ideally a fine grid.

*But...* the ideal of a fine grid is usually impractical. So the issue is what selection of “var-
ious other fixed sets” is adequate. Obviously one should check coverage for the set of true
values set equal to the global best-fit values. Just as obviously, this may not be adequate.
Some exploration is needed, particularly in directions where the uncertainty on a parameter
depends strongly on the parameter value. One can start by varying a few critical parameters
by one or two standard deviations, trying parameters near boundary/ies, and seeing how
stable coverage is.

A Bayesian-inspired approach is to calculate a weighted average of coverage over a neigh-
borhood of parameter sets for the nuisance parameters. This requires a choice of multi-D
prior. Instead of fixing the true values of nuisance parameters during the toy MC simulation,
one samples the true parameters from the posterior pdf of the nuisance parameters.

Numerous studies have been done for elimination of nuisance parameters in the test
statistic (typically a likelihood ratio), many concluding that results are relatively insensitive
to profiling vs marginalization, so that choice can be made based on CPU time. See for
example John Conway’s talk and writeup at PhyStat-2011 [93]. It seems that the method
for treating nuisance parameters in the toy MC generation of events may be more important
than the treatment choice in test statistic: with poor treatment in the test statistic, one may
lose statistical power but still calculate coverage correctly, while poor treatment in the toy
MC generation may lead to incorrect coverage calculation.

## 14 Downward fluctuations in searches for excesses

As mentioned in Section 6.6 and discussed in more detail in Section 6.9, a key problem that
has been a driver of the development of special methods for upper limits in HEP is the situa-
tion where there is Gaussian measurement resolution near a physical boundary. Specifically,
in the Gaussian model \( p(x|\mu, \sigma) \) in Eqn. 10, \( \mu \) may be a quantity that is physically non-
negative, e.g., a mass, a mass-squared, or an interaction cross section. Recall (Section 6.9)
that in this case negative values of the parameter \( \mu \) do not exist in the model, but that
negative values of the observation \( x \) do exist in the sample space.

The traditional Neyman construction of frequentist one-sided 95% C.L. upper limits, for
\( \alpha = 1 - \text{C.L.} = 5\% \), is shown in Fig. 23. As the observation \( x_0 \) becomes increasingly negative,
the standard frequentist upper limit (obtained by drawing a vertical line at observed \( x_0 \))
becomes small, and then for \( x_0 < -1.64\sigma \), the upper limit is the *null set*!

Some people prefer to extend the construction to negative \( \mu \), which is a bad idea in my
opinion, since the model does not exist there (!); this leads to a different description of the
issue, so-called “unphysical” upper limits.

In any case, one should report enough information so that the consumer can make
interval estimates by any desired method. This would include the observed \( x \) (not constrained

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Figure 23: The traditional frequentist construction for one-sided upper limits at 95% C.L., for a Gaussian measurement with unit rms. A vertical line drawn through observed $x_0$, for $x_0 < -1.64\sigma$, intersects no acceptance intervals, resulting in an empty-set confidence interval.

to positive values) and the model $p(x|\mu)$. Such information is also essential for combining results of different experiments.

This was an acute issue 20–30 years ago in experiments to measure the $\bar{\nu}_e$ mass (actually the mass-squared) in tritium $\beta$ decay: several observed $x_0 < 0$. (With neutrino mixing, $\bar{\nu}_e$ is presumably not a mass eigenstate, but one still speaks loosely of its mass, which is actually an expectation value.) At the time (and still today, unfortunately), $x_0$ was referred to as the “measured value”, or point estimate $\hat{m}_e^2$. The resulting confusion and resolutions make a very long story; see my “virtual talk”, “Bayes, Fisher, Neyman, Neutrino Masses, and the LHC” [50] and arXiv post [51]. (These also contain an introduction to “Buehler’s betting game”, related to conditioning.)

The confidence intervals proposed by F-C and described in Section 6.9 are just one of the three proposed ways to deal with this issue that have been widely adopted. The other two are Bayesian with uniform prior (for the quantity with Gaussian resolution), and the $CL_s$ criterion of the next subsection.

14.1 $CL_s$

The unfortunately named $CL_s$ is the traditional frequentist one-tailed $p$-value for upper limits divided by another tail probability (associated with the alternative hypothesis), i.e., by a number less than 1. The limits are thus (intentionally) conservative. A brief definition in good notation is in the PDG RPP [12] (Eqn. 39.78, Section 39.4.2.4). $CL_s$ is a generalization of an earlier result by Günter Zech [94] that considered the case of Poisson distribution with
background and applied a non-standard form of conditioning on an inequality. The rationale is further described by Alex Read in the early papers [95, 96]; an implementation with further commentary is described by Tom Junk [97].

What is new (non-standard statistics) in $CL_s$ is combining two $p$-values into one quantity. (This is referred to as a “modification” to the usual frequentist $p$-value.) The combination (equivalent to a non-standard form of conditioning) is designed to avoid rejecting $H_0$ when the data are similarly incompatible with $H_1$. This situation can arise when an experiment has little sensitivity for distinguishing $H_0$ from $H_1$.

There is no established foundation in the statistics literature for this as far as I know. In fact, the two uncombined $p$-values are considered to be the (irreducible) post-data “evidence” for simple-vs-simple hypothesis testing in a philosophical monograph by Bill Thompson [98] (p. 108). Clearly, with both $p$-values at hand, as with the Higgs spin-parity example in Section 7.6.2, the consumer has the complete information regarding post-data tail probabilities.

(Ofer Vitells has unearthed a suggestion in a 1961 paper by Birnbaum [99] (p. 434) that combines the pre-data Type I and Type II errors rates $\alpha$ and $\beta$ into one quantity in the identical manner, i.e., $\alpha/(1-\beta)$; Birnbaum’s motivation was that this quantity equals the likelihood ratio in a very special case where the test statistic is the single binary digit “reject $H_0$” or “do not reject $H_0$” (rather than the full likelihood ratio). But this seems to be obscure to modern statisticians, and Birnbaum’s last paper [100] examined both $\alpha$ and $1-\beta$ (the usual “power”), not just the combination $\alpha/(1-\beta)$, in defining his “confidence concept”.)

In any case, the $CL_s$ quantity does have properties that many find to be attractive. In particular, for the two simple prototype problems (Poisson with known mean background, and the bounded Gaussian problem), the results are numerically identical to the Bayesian answers with uniform prior, and hence the likelihood principle is respected. These Bayesian interval estimates over-cover from a frequentist point, which is not considered to be as bad as under-coverage. (Regarding the uniform priors, for both these models negative $\mu$ does not exist in the model, so it is incorrect to speak of the prior being zero for negative $\mu$, as in Section 6.9)

The step of combining the two $p$-values into one quantity is called “the $CL_s$ criterion” in (most) CMS papers. Unfortunately, the calculation of the $p$-values themselves, typically using a likelihood-ratio test statistic, is sometimes called the “$CL_s$ method” in HEP. But these $p$-values themselves have long existed in the statistics literature and should be designated that way (and not denoted with equally unfortunate names that the original papers of $CL_s$ use for them).

The many issues of $p$-values are of course inherited by $CL_s$, namely:

- What specific likelihood ratio is used in the test statistic;
- How nuisance parameters are treated (marginalization, profiling);
- What ensembles are used for “toy MC” simulation used to get the distribution of the test statistic under $H_0$ (e.g. no Higgs) and $H_1$ (e.g. SM with Higgs).

LEP, Tevatron, and LHC Higgs experimenters differed in the choices made (!).
15 ATLAS and CMS Conventions

For many years, ATLAS and CMS physicists have collaborated on statistics tools (the RooStats [92] software), and attempted to have some coherence in methods, so that results could be compared, and (when worth the effort) combined.

A key development was the paper by Cowan, Cranmer, Gross and Vitells (CCGV) [66] that extends asymptotic formulas to various cases where Wilks’s theorem is not valid.

As the CCGV asymptotic formulas correspond to the “fully frequentist” treatment of nuisance parameters, for consistency we tended to use that treatment in many cases at small \( N \) as well. Toy MC simulation is thus performed in an approximate frequentist manner in which the underlying parametric distribution of the data is known up to one or more parameters, and sampling is performed from that distribution after substituting estimates for the parameter(s). (This is known as the parametric bootstrap [101].)

For upper limits, there was a lot of discussion among CMS and ATLAS physicists in the early LHC days without convergence, with the result that the two experiments’ physics coordinators in 2010 decreed that \( C_{LS} \) (Section 14.1) be used in most cases.

The ATLAS/CMS Higgs boson results followed these trends. A jointly written description is, “Procedure for the LHC Higgs boson search combination in Summer 2011” [102].

Many issues were further discussed and described in the ATLAS-CMS combination papers for mass [103] and couplings [104]. In particular, a lot of attention was paid to correlations. In the last couple years, Feldman-Cousins [52] starts to be used in some analyses, without my pushing. (Initially some at the LHC were very opposed, evidently because it could return a two-sided interval not including zero when they insisted on a strict upper limit.)

16 My advocacy for \( \geq 10 \) years

Have in place tools to allow computation of results using a variety of recipes, for problems up to intermediate complexity:

- Bayesian with analysis of sensitivity to prior
- Profile likelihood ratio (MINUIT MINOS)
- Frequentist construction with approximate treatment of nuisance parameters
- Other “favorites” such as \( C_{LS} \) (an HEP invention).

The community can (and should) then demand that a result shown with one’s preferred method also be shown with the other methods, and sampling properties studied.

When the methods all agree, we are in asymptotic Nirvana (idyllic state). When methods disagree, we are reminded that the results are answers to different questions, and we learn something! E.g.:

- Bayesian methods can have poor frequentist properties
- Frequentist methods can badly violate Likelihood Principle.
In fact, the community reached the point of having the tools in place (RooStats [92]) by the time of the Higgs boson discovery, and they have continued to be improved. What is not as far along is the “demands” of the community, in my opinion. I would prefer that it be more common for papers to compare explicitly the chosen method with other methods, as is sometimes done.

17 Unsound statements you can now avoid

- “It makes no sense to talk about the probability density of a constant of nature.”
- “Frequentist confidence intervals for efficiency measurements don’t work when all trials give successes.”
- “We used a uniform prior because this introduces the least bias.”
- “We used a uniform positive prior as a function of the parameter of interest.”
- “A noninformative prior probability density does not contain any information.”
- “The total number of events could fluctuate in our experiment, so obviously our toy Monte Carlo simulation should let the number of events fluctuate.”
- “We used Delta-likelihood contours so there was no Gaussian approximation.”
- “A five-sigma departure from the SM constitutes a discovery.”
- “The confidence level tells you how much confidence one has that the true value is in the confidence interval.”
- “We used the tail area under the likelihood function to measure the significance.”
- “Statistics is obvious, so I prefer not to read the literature and just figure it out for myself!”

A Details of spin discrimination example of simple-vs-simple hypothesis test

Ref. [105] describes an enlightening toy example with simple hypotheses. The setup is the observation of a new resonance with a mass of 1.5 TeV in the dilepton final state at the LHC (unfortunately optimistic thus far). We consider here the case of just two simple hypotheses for the spin of the new resonance, either a spin-1 vector boson or a spin-2 graviton. In order to avoid confusion between subscripts and spin values, the hypotheses are called $H_A$ and $H_B$.

The distinguishing observable is the so-called Collins-Soper angle $\theta^{\ast}_{CS}$, which is a useful approximation to the angle in the CM frame between the incoming quark and the outgoing $\mu^-$. Figure 24 shows the simulated distributions of $\cos \theta^{\ast}_{CS}$ for the two spin hypotheses. The
Figure 24: Histograms of $\cos \theta_{CS}^*$ of individual events from the generated (dashed) and accepted (solid) samples of spin-1 $Z'$ (left) and spin-2 $G^*$ (right) for 1.5 TeV mass. From Ref. [105].

As dictated by the Neyman–Pearson lemma (Section 7.2.1), the optimal test statistic for distinguishing the two hypotheses is the likelihood ratio

$$\lambda = \frac{L(H_A)}{L(H_B)},$$

from which one usually considers the monotonic function $-2 \ln \lambda$. For a data set with $N$ events indexed by $i$, $\lambda$ is the product of event likelihood ratios, so that $-2 \ln \lambda$ is the sum of the individual event quantities,

$$-2 \ln \lambda = \sum_{i}^{N} -2 \ln \left( \frac{p(\cos \theta_{CS,i}^*|H_A)}{p(\cos \theta_{CS,i}^*|H_B)} \right).$$

Figure 25(left) and right are histograms of the individual terms in the sum, with events on the left simulated according to $H_A$ as in Figure 24(left), and events on the right simulated according to $H_B$, as in Figure 24(right).

We then consider data sets (“experiments”) that each contain a sample of $N$ events from the distributions in Figure 25, with the values summed as in Eqn. 35. Figure 26 shows on the left the distribution for 10,000 simulated experiments, each with $N = 50$, and on the right for $N = 200$. We see the dramatic effect of the central limit theorem, which says that each histogram of sums tends to Gaussian in spite of the highly non-Gaussian distribution of the addends from Fig. 25; and that furthermore the mean and rms of each are correctly related to those in Fig. 25.
Figure 25: Histograms of $-2 \ln \lambda = 2 \ln \mathcal{L}(H_A) - 2 \ln \mathcal{L}(H_B)$ for individual events from the accepted samples generated according to $H_A$ (spin-1) and $H_B$ (spin-2) for a 1.5 TeV resonance. From Ref. [105].

Figure 26: Histograms of $-2 \ln \lambda$ for simulated experiments with 1.5 TeV dilepton mass, each of which is a sum of $N$ values of $-2 \ln \lambda$ from spin-1 and spin-2 events in Fig. 25, for $N = 50$ (left) and $N = 200$ (right) events per experiment. The superimposed Gaussian curves have means fixed at a factor of $N$ greater than that of the events in Fig. 25, and rms deviations a factor of $\sqrt{N}$ greater. From Ref. [105].
Recalling the prescriptions in Sections 7 and 7.2.1, to perform a N-P hypothesis test of $H_A$, one finds the cutoff $\lambda_{\text{cut}, \alpha}$ for the desired Type I error probability $\alpha$ and rejects $H_A$ if $\lambda \leq \lambda_{\text{cut}, \alpha}$. The Type II error probability $\beta$ then follows. Both of these error probabilities are easily obtained from the histograms in Fig. 26 and plotted as a function of $-2 \ln \lambda_{\text{cut}, \alpha}$, in Fig.27(left), for $N = 50$. One can also plot $\beta$ vs $\alpha$ as in Fig. 27(right) for $N = 50$. As noted in Section 7.1, the choice of operating point on the $\beta$ vs $\alpha$ curve (or equivalent ROC curve) requires multiple considerations.

**B Further discussion of goodness of fit**

As introduced in Section 7.7, a goodness-of-fit (g.o.f.) test is generally defined as a test of the null hypothesis (typically composite, i.e., having adjustable parameters) when an alternative hypothesis has not been explicitly specified. In a typical example, one has observed data $\vec{x}$, and the null hypothesis $H_0$ is that $\vec{x}$ is a random sample from a specific probability density function (pdf) $p_0(\vec{x}; \vec{\mu})$; here $\vec{\mu}$ indicates parameters that are typically not specified in advance, but rather set to their “best-fit” values. A g.o.f. test is then used to test $H_0$. As noted in Section 4, the given pdf $p_0$ is often called “the model” (short for “the statistical model”). In spite of the issues raised in this note, g.o.f. tests constitute an important step in data analysis; in fact the discussion here indicates that using more than one g.o.f. test is advisable.

The most common g.o.f. test is surely the chisquare g.o.f. test used in introductory lab classes, either for measurements of dependent variables $x_i$ as a function of an independent variable (say current vs. voltage), or for binned data. As analyses with unbinned likelihood functions have become commonplace in HEP, the use of unbinned g.o.f. tests has increased as well. For unbinned measurements in one dimension (1D), the Kolmogorov-Smirnov (K-
Figure 28: Scatter plot shown by Joe Incandela at the CMS talk on the discovery of the Higgs-like boson. For Higgs to $ZZ^*$ candidates in the four-lepton final state, the horizontal axis is the mass of the higher-mass pair ($Z_1$), while the vertical axis is the mass of the lower-mass pair ($Z_2$). The large dots are the 10 events in data. The gray shading, peaking in the region around (90 GeV,30 GeV), is the expected pdf for a SM Higgs with mass of 126 GeV.

S) test is commonly used, probably because it has been readily available in HEP software packages (CERNLib and ROOT) for decades, and (like the chi-square test) the interpretation of the test statistic is asymptotically independent of the null hypothesis model $p_0$. However, as this note emphasizes, other tests may be more appropriate than the K-S test (for example when one is interested in departures from $p_0$ in the tails).

For g.o.f. tests of unbinned data in more than one dimension, there are no conventions in HEP, in spite of sporadic work in the last 25 years or more. An example of a potential application arose in the $ZZ^*$ Higgs discovery channel, in which the events were expected to have one $Z$ nearly on mass shell and the other off-shell. The CMS data presented at the discovery talk on 4 July 2012 included Figure 28, a scatter plot of the invariant mass of the lower-mass pair vs the higher-mass pair. In this case, the null hypothesis $p_0$ could be taken as SM Higgs production and decay, for which the pdf is shown in gray shading. To the eye there seemed to be fewer on-shell Z's than expected. This was noted and presumed to be a statistical fluctuation (borne out when more data was obtained). As far as I know, no unbinned 2D g.o.f. test of $p_0$ was attempted. One can imagine that such tests might be useful for future discovery plots in low-statistics regions.

As noted above, in common g.o.f. tests the model $p_0$ has parameters that are adjusted to obtain the “best fit”, in which case the g.o.f. test is performed using the best-fit parameters.
In such a case, it is important keep in mind that the g.o.f. test is a test of the complete model including the best-fit adjustable parameters. This is distinct from the separate inference problems of “measuring” the parameters and uncertainties on them (known to statisticians as point estimation and interval estimation, respectively).

B.1 Relevance of Neyman–Pearson Lemma to g.o.f. tests

In approaching the theory of g.o.f. tests, it is useful to recall the Neyman–Pearson (N-P) theory of hypothesis testing, as discussed in Section 7. The N-P theory provides the language in which the limitations of g.o.f. tests become clear. Recalling in particular the testing of simple hypothesis $H_0$ vs simple hypothesis $H_1$ in Section 7.2.1, for a given $\alpha$, $\beta$ is minimized if the test statistic $T$ is the likelihood ratio $\lambda$ in Eqn. 25 that depends explicitly on $H_1$. By definition, in a g.o.f. test $H_1$ has not been specified. Thus the problem of choosing a “best” $T$ for a g.o.f. test of $H_0$ is not well-posed! There typically exist many possible choices for $T$ in a g.o.f. test. Some may be particularly popular (e.g. the ubiquitous chi-square g.o.f. test), but that does not mean that they are “best” in any general sense.

In fact, it follows from the Neyman–Pearson Lemma that for any choice of $T$ used for a g.o.f. test, that choice will tend to have high power against some alternative $H_1$ if it happens that $T$ is approximately monotonic with the likelihood ratio $\lambda = \mathcal{L}(H_0)/\mathcal{L}(H_1)$, while the choice is vulnerable to having poor power against alternative hypotheses from which $T$ bears no relationship to $\lambda$. Thus a choice of g.o.f. test statistic $T$ picks out alternatives to $H_0$ (sometimes called directions of deviations from $H_0$) for which $T$ has higher discrimination power. This is true whether or not one is aware of it!

Although the strict superiority of $\lambda$ as test statistic $T$ no longer holds with composite hypotheses, the lesson remains that the choice of $T$ defines directions of high discrimination power.

B.2 Prototype problem: test of uniform density on (0,1)

A prototype g.o.f. test is the following: suppose that $\vec{y}$ consists of a set of $N$ numbers $\{y_i\}$ between 0 and 1, and you want to test the hypothesis that they were obtained by sampling $N$ times from a uniform density on (0,1). While this may seem to be an artificial special case (useful for testing the validity of a pseudorandom number generator), in fact many models can be re-cast into this form without loss of generality by using the probability integral transform of Section 4.3. That is, we can consider the more general null hypothesis $H_0$ as the model in which each number $x_i$ in the set of $N$ numbers $\{x_i\}$ is an independent random sample from a general pdf $p(x)$ defined in the domain $a < x < b$, with $x$ continuous. Then the probability integral transform of Eqn. 15 defines $y(x)$ such that $p(y)$ is uniform on (0,1). Thus without loss of generality, the g.o.f. test of the null hypothesis $H_0$ for the model $p(x)$ is re-cast as the hypothesis that the set $\{y_i\} = \{y(x_i)\}$ is a random sample from the uniform density on (0,1). (If $x$ is discrete, there are complications which are discussed in some of the cited papers.)

Since $1-y$ is also uniform on (0,1), typically some other consideration (such as the distribution of $x$ under a different $p$) dictates if one end of the interval is of more interest than the other.
Over the last century, a plethora of tests have been invented to test for uniformity of $\vec{y}$ on (0,1), and hence test for $\vec{x}$ drawn from any given continuous $p_0(x)$. The book by D’Agostino and Stephens [62] contains a comprehensive discussion. The more recent article by Marhuenda et al. [106] defines and compares a plethora of tests against standard sets of parameterized alternatives (higher or lower density near 0 or 1, or both, etc.). Subsets of tests in common use in HEP are discussed by F. James [2], and a few are implemented in ROOT.

B.2.1 Tests based on the empirical distribution function

The most widely used methods in HEP are based on the cumulative distribution function (CDF) and empirical distribution function (EDF). While in science “distribution” is often used synonymously with probability density function (pdf), in statistics “distribution function” is often short for cumulative distribution function, which is an integral of a pdf. Often $f(x)$ is used for a pdf, and upper case $F(x)$ is used for its CDF:

$$F(x) = \int_{-\infty}^{x} f(x')dx'. \quad (36)$$

Given $N$ observed values $x_i$ as above, the EDF is

$$F_N(x) = \frac{\text{number of observed values } \leq x}{N}. \quad (37)$$

Thus $F_N(x)$ is an increasing piecewise-constant function, starting from 0 for $x$ less than the smallest observed $x_i$, increasing by $1/N$ at every observed value, and obtaining unity above the highest observed value of $x_i$.

If the observed $\vec{x}$ is drawn from $p_0(x)$, then we expect the EDF $F_N(x)$ to be similar to the CDF calculated from $p_0(x)$, which we call $F_0(x)$. A variety of g.o.f. tests are thus based on various definitions of the “distance” between $F_0(x)$ and $F_N(x)$. These tests include, for example, the Kolmogorov-Smirnov test (based on extremum of $|F_0(x) - F_N(x)|$), and the Cramér-von Mises family based on integrals weighted by a function $w(x)$ of the squared difference:

$$N \int_{-\infty}^{+\infty} (F_0(x) - F_N(x))^2 w(x)dF(x). \quad (38)$$

The unweighted case (i.e. $w(x) = 1$) corresponds to the classic Cramér-von Mises statistic. The weight function $w(x)$ can be chosen to give more power against certain deviations. For example, the Anderson-Darling (AD) test is designed to have more power against deviations at both ends of the distribution, with a weight function

$$w(x) = \frac{1}{F(x)(1 - F(x))}. \quad (39)$$

Since departures from assumed Gaussianity are often in the tails, AD is reputed to be useful for testing Gaussianity, as well as being generally useful. There are also versions that emphasize only one tail [62]. On the other hand, both the Kolmogorov-Smirnov family and the Cramér-von Mises family have variations that make the endpoints not special by posing the problem on a circle.
Keeping in mind the probability integral transform and the fact that Eqn. 38 is defined in terms of \( dF(x) \) rather than \( dx \), one can see that the distribution of such test statistics under the null hypothesis does not depend on the specific form \( p_0 \) in the null. Such tests are called distribution-free and are popular since standard tables can be computed and used. Nowadays, with the ability to simulate data sets and obtain the null distribution directly, it can be worth exploring the use of more powerful tests that do not have this property.

B.2.2 Other families of tests of uniformity on \((0,1)\)

Refs. [62, 106] describe multiple classes of tests in addition to those based on the EDF. These include tests based on the “ordering statistics”, i.e., on the ordered set of the observed points \( y_i \) (testing mean values of \( i \)th points, moments of differences \( y_j - y_i \), etc.). Among the many tests, one can attempt to choose “omnibus” tests that perform reasonably well against a number of different alternatives. The conclusion of Ref. [106] is that a member of the class of tests called “Neyman smooth tests” is unique in being in the top-10 most powerful tests for all the alternatives that they considered.

Neyman smooth tests and more general “smooth” tests seem to have had little use in HEP thus far, in spite of popularity in the statistics literature [107, 108]. They are tests where the alternative hypothesis is constructed by fitting the data to a sum of Legendre polynomials. (The variant that Ref. [106] studies uses Schwarz’s Bayesian information criterion [109] to choose the degree of polynomials.) This spirit of using the data to construct the alternative hypothesis used in a likelihood ratio (or asymptotic equivalent) is similar to that of the saturated model discussed below for binned data. Recently, a real-world example using the Neyman smooth test in X-ray astronomy was published by astrophysicists collaborating with statistician Algeri and her student Zhang [110]. Grosso et al. [111] have investigated a further generalization that uses machine learning to construct an alternative model that is used in a likelihood ratio.

B.3 Chissquare g.o.f. and variants

As noted above, Neyman and Pearson taught us that (even for simple hypotheses) the best test of the null hypothesis depends on the alternative, and hence there is no universally best g.o.f. test. Nonetheless, the ubiquity of the chisquare g.o.f. test attests to its utility, at least for picking up certain departures from the null. In its usual form for uncorrelated Gaussian (normal) distributed data, one has

\[
\chi^2 = \sum_i \frac{(d_i - f_i)^2}{\sigma_i^2},
\]

where \( d_i \pm \sigma_i \) is the \( i \)th measured data point with rms deviation \( \sigma_i \) (each assumed to be a known constant), and \( f_i \) is the model prediction (perhaps with parameters) to be compared with \( d_i \). (If \( \sigma_i \) is not a known constant at each \( i \), but depends on the unknown true value of the model at \( i \), then there are subtleties beyond the scope of this note.) Since the test statistic \( \chi^2 \) is a function of the random data, it is itself a random variable, and in unbounded Gaussian applications it has a probability density function [12] which is itself also frequently called
chisquare. The potentially confusing ambiguity in multiple meanings is usually resolvable by context. This could also be avoided by using another name, such as $S^2$ or $Q^2$ for the left hand side of Eqn. 40, but I yield to common practice in this note.

In HEP, we can also encounter situations in which the so-called “regularity conditions” are not met, so that the distribution of the test statistic in Eqn. 40 is not a chisquare function; two common cases are when the true or best-fit values of parameters are on the boundary (physical constraint such as non-negativity), and when there are issues with degrees of freedom not being well-defined. Again, these issues are beyond the scope of this note.

More information regarding the chisquare test, including the generalization of Eqn. 40 to include correlations, is in the PDG RPP [12].

B.3.1 Gaussian chisquare g.o.f. is a likelihood ratio using the saturated model

For the same data and model as above, the likelihood for the null hypothesis $H_0$ is:

$$L(H_0) = \prod_i \frac{1}{\sqrt{2\pi\sigma_i^2}} \exp\left(-\frac{(d_i - f_i)^2}{2\sigma_i^2}\right).$$  \hspace{1cm} (41)

It is sometimes said that $-2\ln L$ is equal to $\chi^2$; this is clearly not correct since the former quantity has extra constant terms. Understanding how the extra terms “disappear” in the g.o.f. test (from the point of view of N-P testing) is enlightening.

Given only the null hypothesis and the data, one can use the data to invent an alternative hypothesis for which the model $f_i$ is equal to the data $d_i$ at every measured value! Such a model, which typically needs as many parameters as there are data points, is called a saturated model [112].

For the Gaussian data above, the saturated model sets $f_i = d_i$, so that the likelihood of the alternative hypothesis $H_1$ (the saturated model) is (since $\exp(0) = 1$)

$$L(H_1) = \prod_i \frac{1}{\sqrt{2\pi\sigma_i^2}}.$$  \hspace{1cm} (42)

Inspired by Eqn. 25, we consider the ratio of the two likelihoods above, i.e,

$$\lambda = L(H_0)/L(H_1) = \prod_i \exp\left(-\frac{(d_i - f_i)^2}{2\sigma_i^2}\right),$$  \hspace{1cm} (43)

and thus

$$\chi^2 = -2\ln \lambda.$$  \hspace{1cm} (44)

From this point of view, the constants in $-2\ln L$ were not just ignored; they were canceled when a ratio was formed. (There are other paths to the chisquare expression not as relevant to this note.) Since the saturated model does not depend on the parameters of the original model, the maximum of $\lambda$ is of course at those parameters that maximize the original $L(H_0)$.

B.3.2 Pearson’s chisquare for binned histograms

The original chisquare variable is that of Karl Pearson in 1900, designed for histograms (“frequency tables”) with multinomial-distributed bin contents, and defined as

$$\chi^2 = \sum_i \frac{(d_i - f_i)^2}{f_i}.$$  \hspace{1cm} (45)
(In a multinomial histogram, the total number of events is fixed by design, so there is one fewer independent bin content than in Poisson data.) This is very similar to Eqn. 40, since in multinomial and Poisson data, \( f_i \) can be a proxy for \( \sigma_i^2 \).

**B.3.3 Use of saturated model to construct improved chisquare g.o.f. for binned histograms**

In 1983, Baker and Cousins [113] reviewed construction of likelihood ratios as in Eqn. 25 using saturated models for testing g.o.f. for Poisson and multinomial data in histograms. (They did not call them saturated models, instead citing a 1928 paper by Neyman and Pearson.) By that time, it had been widely noted that using a Poisson likelihood model for fitting typical HEP histograms cured a defect of fits using Pearson’s chisquare, namely that the area under the fitted curve was not equal to the observed number of events. It was less well known how to construct a g.o.f. test consistent with such a likelihood fit. For histograms with independent Poisson-distributed bin contents \( d_i \), the result for the g.o.f. test statistic,

\[
-2 \ln \lambda = 2 \sum_i f_i - d_i + d_i \ln(d_i/f_i),
\]

was called \( \chi^2_{\lambda,p} \) since asymptotically its pdf tends to the chisquare distribution. This Poisson form is mentioned in the PDG’s Review of Particle Properties [12]; some time ago it was decided that it is best just to denote it by \( -2 \ln \lambda \) as some felt that calling it \( \chi^2 \) might encourage people to forget that it only asymptotically follows the \( \chi^2 \) distribution (and only if conditions are satisfied). As noted in the Baker-Cousins paper, probably the safest thing to do is to study the distribution by Monte Carlo.

Heinrich [114] has studied the distribution and moments of \( \lambda \) for small statistics, and makes the point that for the asymptotic formulas to be valid, the contents of all bins must each be large. More generally, how to bin data is another complex problem since binning discards information on the location of events within the bin, and suppresses the ability to observe high-frequency components. Thus the robustness of results (or lack thereof) to the binning chosen should be understood and communicated.

**B.3.4 Tests complementary to the chisquare g.o.f. test**

The tests based on chisquare or asymptotic equivalents discard all or most of the information on the ordering of the deviations as well as the signs of the deviations. Hence they can easily miss a trend in the deviations that is obvious to the eye (e.g., all deviations of the same sign, or a trend due to a slope not present in the null hypothesis). Thus, authors such James [2] suggest complementing the chisquare test with a “runs test”, often called the Wald-Wolfowitz runs test. Performing more than one g.o.f. test raises the issue of whether or not the results can be combined into one overall g.o.f. summary. Doing so might be useful in some contexts, but one should be aware that combining p-values is itself fraught with ambiguity, as discussed in Ref. [115].
B.4 Caution against absolute likelihood as g.o.f. test statistic

Occasionally one finds the recommendation to use as a g.o.f. test statistic the absolute likelihood at its maximum, as opposed to a ratio of likelihood maxima; typically Monte Carlo simulation is recommended as the way to get the null distribution of the test statistic. Although this might at first seem plausible, it is a flawed concept: unlike the likelihood ratio, such a g.o.f. statistic is without foundation, and power can vary arbitrarily with the metric. Simple examples can make clear that the value of the likelihood at its maximum must be compared to something. For example, for Poisson counts, the probability of observing 100 events when $\mu = 100.0$ is much less than the probability of observing 1 event when $\mu = 1.0$, even though in both cases the data perfectly fit the theory. For binned data, the saturated model provides the reference of the largest value that the likelihood can be for that data (for any model), and hence provides a reasonable normalization for the maximum observed for a more constraining model.

Heinrich [116] discusses the pitfalls of using the absolute likelihood as a g.o.f. statistic. For unbinned likelihoods, which are common in HEP, the problem is exacerbated. One might hope that one could just take binned g.o.f. in the limit of small bins, but the answer depends on the way the limit is taken, i.e., in which metric the bin boundaries are equally spaced.

B.5 Discussion

From the above, it is clear that, for “g.o.f. test” defined in its purest form of no specified alternative, there is no unique “best” g.o.f. test. Therefore trying several can give some indication of how well the chosen statistics model approximates reality, and in which directions departures might be suspected (heavier tails, skewness, etc.). It is therefore useful to be aware of directions against one would like to have power, and to choose g.o.f. tests appropriately; simple toy MC simulations, such as those in the cited references, can help in this regard. For a g.o.f. test for unbinned data in one dimension, one has a variety of tests to choose among [62, 106], depending on roughly what sort of alternatives one wants power against. A recent monograph is by Thas [108]. If, on the other hand, there is a specific alternative of interest, then typically one leaves the world of generic g.o.f. tests and gains power by constructing alternative-specific likelihood ratio tests (as in the Higgs searches).

Generalization of these g.o.f. tests to higher dimensions, as in Fig. 28, remains a topic of research. Some comparisons were made by Aslan and Zech at Durham in 2002 [117], including their proposed energy test [118]. Williams [119] has provided a more recent review, including work by Cuadras and Fortiana (first pointed out to me by Ilya Narsky) that is closely related to the energy test. Williams also discusses the close relationship between g.o.f. tests and two-sample tests, which are beyond the scope of this note. One can of course resort to binning the data for g.o.f. tests even if the parameters are fit with an unbinned likelihood; in this case as noted above the robustness with respect to the binning chosen needs to be understood.
C Look-elsewhere effect

In these lectures, I did not have time for the important (and increasingly mandatory) calculation of the LEE. A starting point for self-study is the discussion by Louis Lyons, “Comments on ‘Look Elsewhere Effect’ ” [120]. See also Section 9.2 of my paper on the Jeffreys-Lindley Paradox [3].

An important paper for practical calculations, and also for qualitative insight, is by Eilam Gross and Ofer Vitells, “Trial factors for the look elsewhere effect in high energy physics,” [121].

D Bayesian hypothesis testing (model selection)

As mentioned very briefly in Sections 5, 5.11, and 10, the duality used in frequentist hypothesis testing (Section 7.4) is not used in Bayesian statistics. The usual methods follow Chapter 5 of Harold Jeffreys’s book [15]: Bayes’s Theorem is applied to the models themselves after integrating out all parameters, including the parameter of interest! This is typically presented by Bayesian advocates as “logical” and therefore simple to use, with great benefits such as automatic “Occam’s razor” penalizing less predictive models, etc.

In fact, Bayesian model selection is full of subtleties, and even for the experts, it can be a “can of worms” (James Berger [31], Rejoinder, p. 459). As just one indication, Jeffreys and followers use different priors for integrating out parameter(s) in model selection than for the same parameter(s) in parameter estimation. Here I mainly just say: Beware! There are posted/published applications in HEP that are silly (by Bayesian standards). As mentioned in Section 5.11, a pseudo-Bayes example in PRL provoked me to write a Comment [40] that has some references to useful Bayesian literature.

The dependence on prior probabilities for the models themselves can be factored out, leading to a “Bayes factor” that is the ratio of posterior odds to prior odds. However, the Bayes factor still depends on prior pdfs for parameters in the models, and this leads to direct sensitivity to the prior pdf for a parameter that is in one model but not in the other. For testing $H_0: \mu = \mu_0$ vs $H_1: \mu \neq \mu_0$, improper priors for $\mu$ that work fine for estimation become a disaster. Adding a cut-off to make them proper just gives (typically arbitrary) cutoff dependence.

In the asymptotic limit of lots of data, your answers in a test of a point null vs a continuous alternative (either the probability $H_0$ is true, or also the Bayes factor) remain directly proportional to the prior pdf for the parameter of interest. This is totally different behavior compared to Bayesian interval estimation, where the effect of a prior typically becomes negligible as the likelihood function becomes narrowly peaked at large $N$.

For a review and comparison to $p$-values in the discovery of Higgs boson, see my paper, “The Jeffreys-Lindley Paradox and Discovery Criteria in High Energy Physics” [3]. As mentioned in Section 5.11, see also Chapter 12 by Harrison Prosper in Ref. [41].
E  Point estimation

Most of this paper is about intervals; I have do not say much about what to quote as the “measured value” (typically using the MLE by default). Statisticians call this the “point estimate”. There is a huge literature on point estimation; see e.g. Chapters 7 and 8 in Ref. [2].

If you are well-grounded in interval estimation, one approach is to use that machinery to get a point estimate. E.g., one might take the mid-point of (say) your 68% C.L. central interval. But a better approach is probably to let the C.L. go to 0, so that your interval gets shorter and shorter, and use the limiting point. For both the LR ordering for confidence intervals (F-C), and for likelihood ratio intervals, this results in the maximum likelihood estimate.

To give an idea of how rich the subject is, I show a few interesting things from Ref. [2].

E.0.1  Point estimation: Traditional desiderata

- Consistency: Estimate converges toward true value as number of observations $N$ increases
- Unbiasedness: Expectation value of estimate is equal to the true value. (Bias and consistency are independent properties; see Fig. 7.2 in Ref. [2].)
- Efficiency: Estimate has minimum variance
- Minimum loss of information: (technical definition)
- Robustness: Insensitivity to departures from the assumed distribution

One can add:
- Simplicity: transparent and understandable
- Minimum computer time: still relevant in online applications, less relevant otherwise
- Minimum loss of physicist’s time (how much weight to put on this?)

These desired properties can be impossible to achieve simultaneously. How to choose? A thorough analysis requires further input: what are the costs of not incorporating various desiderata? Then formal decision theory can be used to choose estimator.

In practice in HEP, maximum likelihood estimates are often used (even though they are typically not unbiased). Typically the MLE is consistent and has other excellent asymptotic properties (e.g., estimate is asymptotically normal). For finite $N$, the MLE works well in the so-called exponential family that includes binomial, Poisson, and Gaussian. As noted in Section 4.2, the MLE is invariant under reparameterization. (This means that if it is unbiased in one metric, it is typically biased in other metrics, as discussed in Ref. [10], Section 5.3.1.)
E.0.2 Alternatives to the arithmetic mean when model is non-Gaussian

Fred James [2] (pp. 209 ff) has a very illuminating discussion of the MLEs for a diverse set of pdfs, representing long tails, short tails, and in between. If \( p(x|\mu) = f(x - \mu) \), where \( f \) is some pdf, then \( \mu \) is called a location parameter. Some common examples of pdfs were \( \mu \) is a location parameter are:

- Normal: \( p \sim \exp\left(-\frac{(x - \mu)^2}{2\sigma^2}\right) \)
- Uniform: \( p = \text{constant for } |x - \mu| < a; \ p = 0 \text{ otherwise} \)
- Cauchy: \( p \sim \frac{1}{a^2 + (x - \mu)^2} \)
- Double exponential: \( p \sim \exp\left(-a|x - \mu|\right) \)

These examples are all symmetric about \( \mu \): \( p(\mu + y) = p(\mu - y) \)

Suppose you are given \( N=11 \) values of \( x \) randomly sampled from \( p(x|\mu) \). What estimator (function of the 11 values) gives you the “best” estimate of \( \mu \)? If by “best” you mean minimum variance, it is the M.L. estimate, resulting in a different formula for each of the above cases! Three of the four are special cases of \( L^p \), the estimator that minimizes the sum over the observations of \( |x_i - \mu|^p \). Different values of \( p \) put different emphasis on observations in the tails.

Only for the normal pdf is the MLE equal to the arithmetic mean, obtained by the familiar least-squares technique (\( p = 2 \)). Can you guess what the MLE is for the uniform and the exponential cases? (For the Cauchy pdf, with its long tails, the arithmetic mean is particularly useless; see also discussion by Efron [8]).

If the true distribution departs from that assumed, then the estimate of location is no longer optimal. Sensitivity is in the tails! See the nice discussion of asymptotic variance and robustness in Ref. [2] (pp. 211 ff).

Acknowledgments

Thanks to many in HEP (Frederick James, Gary Feldman, Louis Lyons, Luc Demortier, and numerous others) from whom I learned... and to many statisticians that Louis invited to PhyStat meetings. For Bayesian statistics that was especially Jim Berger (multiple times) and Michael Goldstein, and more recently, David van Dyk (multiple times). Thanks also to CMS Statistics Committee (Olaf Behnke et al., including Igor Volobouev, who pointed to Refs. [106, 108]) for many discussions and comments on earlier versions of the slides and writeup... and to the authors of numerous papers from which I learned, including early (1980s) Bayesian papers by Harrison Prosper... Thanks also to Diego Tonelli of the LHCb experiment for encouragement to update the slides in 2017 and for comments on an earlier version.

This work was partially supported by the U.S. Department of Energy under Award Number DE–SC0009937.
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