

# Probability and Statistical Inference \*

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## Abstract

These lectures introduce key concepts in probability and statistical inference at a level suitable for graduate students in particle physics. Our goal is to paint as vivid a picture as possible of the concepts covered.

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## I. LECTURE 1 - PROBABILITY THEORY, PART I

Sir Harold Jeffreys [1] begins his book, *Theory of Probability*, with these words

“The fundamental problem of scientific progress, and a fundamental one of everyday life, is that of learning from experience.”

In everyday life, we learn from experience in a way that is still deeply mysterious. However, in scientific research the learning is more readily formalized: we collect data in a systematic way about some aspect of the world and, from these data, infer something of interest using more or less formal methods. Probability theory is useful at all stages.

Given its central role in statistical inference, we believe it is helpful to have a clear understanding of what probability is and how that notion arose. Accordingly, these lectures are divided into two parts: Lectures 1 and 2 cover probability theory, while Lectures 3 and 4 deal with statistical inference. In the first lecture, we begin with a sketch of the history of probability. This is followed by a discussion of the elements of deductive and inductive reasoning, ending with a discussion of some elementary aspects of probability theory.

### A. Historical Note

The theory of probability arose from the ancient and popular pastime of gambling. One of the earliest references to chance, and to the woes of gambling, occurs in the cautionary tale of *King Nala* from the epic poem *Mahabharata* [2]. King Nala lost his kingdom in a gambling contest and was reduced to working for King Bhargasuri as a chariot-driver. One day, while on a journey with the king, Nala boasted of his mastery of horses. The king did not take too kindly to such boasting and reminded Nala that no man knows everything. To make his point, the king made a quick estimate of the number of fruit on a nearby tree, the extraordinary accuracy of which was verified by Nala, who counted the fruit one by one. Nala pleaded with the king to divulge the method that yielded such an astonishingly accurate estimate. The king replied:

“Know that I am a knower of the secret of the dice and therefore adept in the art of enumeration.”

In the end, the king relented and told Nala the secret. It would seem from this tale that some notions of chance were understood, at least by some, in ancient times. However, probability theory as a recognizable mathematical discipline was established only centuries later.

In 1654, the French nobleman, Chevalier de Méré, complained to Blaise Pascal that the rules of arithmetic must be faulty. His reason: the observation that his two methods of placing bets, using dice, did not work equally well, contrary to his expectation. He would bet on the basis of obtaining at least one 6 in 4 throws of a single die, or, at least one double 6 in 24 throws of two dice. Pascal worked out the probabilities and showed that the first outcome was indeed slightly more probable than the second. Thus was born the mathematical theory of probability.

By the late 17th century, probability was interpreted in several ways:

- as the fraction of favorable outcomes in a set of outcomes considered *equally likely*,
- as a measure of *uncertain knowledge* of outcomes,
- as a physical *tendency* in things that exhibit chance.

James Bernoulli (1654–1705) labored hard to make sense of these different aspects of probability, but, dissatisfied with his labors, he chose not to publish his results. Happily, however, in 1713, his nephew Nicholas Bernoulli published *Ars Conjectandi* (*The Art of Conjecture*), James Bernoulli's famous treatise on probability. This book contains the proof of an important result, namely, the **weak law of large numbers**, which we discuss later in this lecture. Some decades later, the English cleric Thomas Bayes (1702–1761) read (via a proxy!) the following paper before the Royal Society, on 23 December, 1763: *An Essay towards solving a Problem in the Doctrine of Chances*. This paper is notable for at least two reasons. Firstly, in it, a proof is given of a special case of what became known as Bayes' theorem. Secondly, this paper makes explicit use of probability as a measure of uncertain knowledge about something, in this case, uncertain knowledge of the value of a probability! The ideas of Bayes, and probability theory, in general, were brought to great heights by Pierre Simon de Laplace (1749–1827) in his book of 1812 entitled: *Théorie Analytique des Probabilités*. In it, amongst other things, one finds the general form of Bayes' theorem. One also finds results that soon became controversial; indeed, that became the object of ridicule. Laplace made extensive use of Bayes' theorem, sometimes in ways that yielded odd results. From

one of his results (the *law of succession*) one would conclude that a 9-year old boy has a lesser chance of reaching the age of 10 than does a 99-year old man to reach the age of 100. The logician George Boole was particularly scornful of Laplace's use of Bayes' theorem. In the Bayes-Laplace view of probability, the foundation of the **Bayesian approach** to statistical inference, probability is construed as a measure of the *plausibility* of an assertion. For example, Bayes and Laplace would have had no difficulty with the assertion "There is a 60% chance of rain tomorrow".

For Boole and other mathematicians and philosophers, however, the notion of probability as a measure of uncertain knowledge, or the plausibility, of the truth of an assertion seemed metaphysical and therefore unscientific. They therefore sought a different interpretational foundation for the theory of probability, grounded, as they perceived it, more firmly in experience. As a result of the critiques of the Bayes-Laplace methods, and the growing "ideology of the objective" in the natural sciences [3], these methods fell into disfavor. This was not only because of discomfort with the inherent subjectivity of the probabilities manipulated by Bayes and Laplace, but because of the seemingly arbitrary manner in which they assigned certain probabilities. To excise such alleged defects in the theory of probability a different approach was developed, which, at the start of the 20th century, became the foundation of what has come to be known as the **frequentist approach** to statistical inference. The newer approach, which comprises the body of statistical ideas with which most physicists are familiar, is closely associated with the names of Sir Ronald Aylmer Fisher (1890–1962), Jerzy Neyman, Pearson, Cramer, Rao, Mahalanobis, von Mises and Kolmogorov, to name but a few [4]. The frequentist approach is typically presented as if it were a single coherent school of thought. In fact, however, within this approach views differed, sometimes sharply. Indeed, the sharpest disagreements were between Jerzy Neyman and Ronald Fisher, the two principal architects of the frequentist approach.

Fisher and Neyman, along with the other frequentists, did, however, agree on one crucial point: probability is to interpreted not as a measure of plausibility, or uncertain knowledge, or **degree of belief**, but rather as the **relative frequency** with which something happens, or will happen [5]. From the frequentist point of view, statements such as "There is a 60% chance of rain tomorrow" are devoid of empirical content. Why? Because it is not possible to repeat the day that is tomorrow and count how often it rained. By contrast, the statement "There is a 60% chance of rain on days named March 7th" is judged meaningful because

such days repeat and we can, therefore, assess by enumeration the relative frequency with which it rains on days so named.

The frequentist viewpoint took hold in the physical sciences and became the norm in particle physics [6]. Indeed, that viewpoint is so entrenched in our field that, until fairly recently, it was hardly recognized that one has a choice about how to conduct statistical inferences. However, during the latter half of the 20th century the methods of Bayes and Laplace have undergone a renaissance initiated, in large measure, by Sir Harold Jeffreys [1] (1891–1989) and vigorously developed by like-minded physicists and mathematicians, notably Cox, de Finetti, Lindley, Savage and Jaynes [7, 8, 9, 10]. Moreover, after a somewhat slow start, beginning with a few papers in the 1980s [11, 12, 13] a similar renaissance is underway in particle physics [14].

## B. Reasoning

“Probability theory is nothing but common sense reduced to calculation.”

— Laplace, 1819

Aristotle, who lived around 350 BC, was one of the first thinkers to attempt a formalization of reasoning. He noticed that on those rare occasions when we reason correctly we did so according to rules that can be reduced to the syllogisms:

	<b>modus ponens</b> (ponere=affirm)	<b>modus tollens</b> (tollere=deny)
Major premise	If $A$ is TRUE, then $B$ is TRUE	If $A$ is TRUE, then $B$ is TRUE
Minor premise	$A$ is TRUE	$B$ is FALSE
Conclusion	Therefore, $B$ is TRUE	Therefore, $A$ is FALSE

In addition, if the statement  $A$  is TRUE then its negation, written as  $\overline{A}$ , is, of necessity, FALSE. The statement  $A$  is said to contradict  $\overline{A}$ . A simple mnemonic for the syllogisms are the set of symbolic expressions:

	<b>modus ponens</b>	<b>modus tollens</b>
Major premise	$AB = A$	$AB = A$
Minor premise	$A = 1$	$B = 0$
Conclusion	$B = 1$	$A = 0$

The symbols  $A$ ,  $B$ , 1, 0, and their negations,  $\bar{A}$ ,  $\bar{B}$ ,  $\bar{1}$  and  $\bar{0}$ , are variously referred to as events, statements, assertions, or **propositions**. The symbol 1 represents a proposition that is always TRUE; the symbol 0, its negation, is always FALSE.

Here is a simple example. Let  $A = \textit{She finished school}$  and let  $B = \textit{She is educated}$ . Our major premise is: If *She finished school* is TRUE then *She is educated* is TRUE. Suppose that our minor premise is *She finished school* is TRUE. We may, as a matter of logic, conclude that *She is educated* is TRUE. On the other hand, however, if the proposition  $B$  is TRUE, that is, *She is educated* it does *not* follow that  $A$  is TRUE, that is, that *She finished school*. She may be educated because she is self-taught! Conversely, if  $A$  is FALSE, that is, *She finished school* is FALSE, we cannot logically conclude that  $B$  is FALSE, that is, *She is educated* is FALSE. But, if *She is educated* is, in fact, FALSE then we can conclude that *She finished school* is FALSE.

These logical arguments can be readily constructed using the symbolic expressions and noting that if  $B$  is set to 1 (that is, to the proposition that is always TRUE) in  $AB = A$  we get  $A = A$  and we are no wiser about the truth or falsity of  $A$ . Likewise, if  $A = 0$ , that is,  $A$  is FALSE, then the truth or falsity of  $B$  cannot be ascertained.

Deductive reasoning, as we have just sketched, is extremely powerful; witness the immense scope and power of mathematics. However, to learn from experience we need a way to reason as it were “backwards”, that is, to reason *inductively*. In the example above, suppose it is true that *She is educated*. We acknowledge the possibility that we could be wrong, but, it is certainly *plausible* that if *She is educated* is, in fact, true this renders the proposition *She finished school* more likely. The methods of Bayes and Laplace can be viewed as a formalization of this mode of **plausible reasoning**. Indeed, the Bayes-Laplace theory, and its subsequent developments by Sir Harold Jeffreys, Cox, Jaynes and others, can be viewed as an extension of logic to include truth values that lie between FALSE and TRUE. Moreover, if one makes the idealization that truth values can be represented by real numbers in the interval  $[0, 1]$ , it can be shown that these numbers satisfy the axioms of probability and, as

such, are a quantitative measure of the plausibility of propositions. These arguments assign a quantitative meaning to the weaker syllogisms:

Major premise	If $A$ is TRUE, then $B$ is TRUE	If $A$ is TRUE, then $B$ is TRUE
Minor premise	$B$ is TRUE	$A$ is FALSE
Conclusion	Therefore, $A$ is more plausible	Therefore, $B$ is less plausible.

### C. Probability Calculus

The theory of probability can be founded in many different ways. One way, is to regard probability as a *function* with range  $[0,1]$ , defined on sets of events or propositions. But in order speak of sets of propositions, we need to know how they are to be manipulated; that is, we need an algebra of propositions. The appropriate algebra, **Boolean algebra**, was invented by George Boole (1854). If  $A, B, C, 1, 0$  and their negations are propositions, and  $+$  and  $\cdot$  are binary operations then, one form of the axioms—the **Huntington axioms**—is

Commutativity law	$A + 0 = A$	$A \cdot 1 = A$
	$A + \bar{A} = 1$	$A \cdot \bar{A} = 0$
	$A \cdot B = B \cdot A$	$A + B = B + A$
Distributivity law	$A \cdot (B + C) = A \cdot B + A \cdot C$	$A + B \cdot C = (A + B) \cdot (A + C)$

Usually, we drop the “ $\cdot$ ” operator in expressions to simplify the notation. From these axioms the theorems of Boolean algebra can be deduced as logical consequences.

**Exercise:** Prove the theorems below.

Idempotency law	$A + 1 = 1$	$A0 = 0$
	$\bar{0} = 1$	$\bar{1} = 0$
	$A + AB = A$	$A(A + B) = A$
	$AA = A$	$A + A = A$
Associativity law	$A(BC) = (AB)C$	$A + (B + C) = (A + B) + C$
de Morgan’s laws	$\overline{AB} = \bar{A} + \bar{B}$	$\overline{A + B} = \bar{A}\bar{B}$ .

Consider the propositions  $A, B, A+B$  and  $AB$ , to each of which we (somehow) have assigned

the numbers  $P(A)$ ,  $P(B)$ ,  $P(A + B)$  and  $P(AB)$ . The axioms of probability specify how these numbers are related. Let  $A$  and  $B$  be the propositions  $A = \textit{It will rain today}$  and  $B = \textit{It is the rainy season}$ , respectively. The probability of  $A$  given  $B$ , written thus  $P(A|B)$ , that is, the probability it will rain today *given* that it is the rainy season, is defined by

$$P(A|B) \equiv \frac{P(AB)}{P(B)}. \quad (1.1)$$

The number  $P(A|B)$  is called the **conditional probability** of  $A$  given  $B$ . Note that  $P(B)$  is the probability of  $B$  *without* restriction, while  $P(A|B)$  is the probability of  $A$  when we *restrict* to the circumstance in which  $B$  is true. Strictly speaking, there is a restriction on  $B$  also;  $B$  is true given some other more encompassing circumstance  $C$ . Probabilities are always context-dependent numbers. There is no such thing as the probability to create a  $t\bar{t}$  pair; there is, however, the probability to create a  $t\bar{t}$  *given* some particular set of conditions. Therefore, we should, in principle, always make the conditioning explicit and write every probability in the form  $P(A|C)$ . In practice, if the conditioning is clear we may drop it from the notation.

The other set of probability axioms can be taken to be the **product rule**

$$\begin{aligned} P(AB|C) &= P(B|AC)P(A|C), \\ &= P(A|BC)P(B|C), \end{aligned} \quad (1.3)$$

and the **sum rule**

$$P(A|C) + P(\bar{A}|C) = 1, \quad (1.4)$$

and the conventions

$$\begin{aligned} P(1|C) &= 1, \\ P(0|C) &= 0. \end{aligned} \quad (1.6)$$

As an illustration of the use of the rules given above we prove a theorem that relates

$P(A + B|C)$  to  $P(A|C)$  and  $P(B|C)$ . We need merely to apply the above rules repeatedly:

$$\begin{aligned}
P(A + B|C) &= 1 - P(\overline{A + B}|C) \\
&= 1 - P(\overline{A}\overline{B}|C) \\
&= 1 - P(\overline{B}|\overline{A}C)P(\overline{A}|C) \\
&= 1 - [1 - P(B|\overline{A}C)]P(\overline{A}|C) \\
&= 1 - P(\overline{A}|C) + P(B|\overline{A}C)P(\overline{A}|C) \\
&= P(A|C) + P(B|\overline{A}C)P(\overline{A}|C) \\
&= P(A|C) + P(\overline{A}B|C) \\
&= P(A|C) + P(\overline{A}|BC)P(B|C) \\
&= P(A|C) + [1 - P(A|BC)]P(B|C) \\
&= P(A|C) + P(B|C) - P(A|BC)P(B|C) \\
P(A + B|C) &= P(A|C) + P(B|C) - P(AB|C). \tag{1.8}
\end{aligned}$$

The Huntington axioms seem intuitively reasonable, but the product and sum rules, Eqs. (1.3) and (1.4), seem less so. Remarkably, these rules can be derived from the more primitive axioms:

- **Axiom 1)** Plausibilities  $q$  can be represented by real numbers.
- **Axiom 2)** The plausibilities  $q(B)$  and  $q(A|B)$  of a proposition  $B$  and that of another  $A$  *given* the first determine the plausibility  $q(AB)$  of the joint proposition  $AB$ ; that is,  $q(AB)$  is some function of  $q(B)$  and  $q(A|B)$ .
- **Axiom 3)** The plausibility  $q(A)$  of a proposition  $A$  determines the plausibility  $q(\overline{A})$  of its converse  $\overline{A}$ .

This was first done by the physicist, R.T. Cox [7], in 1946, who showed that plausibilities or degrees of belief follow rules that are isomorphic to those of probability and thus provide a **subjective interpretation** of the latter. Moreover, well before Cox's theorem, James Bernoulli, who, along with his contemporaries, regarded the subjective interpretation of probability as self-evidently sensible [3], proved a theorem that provides a link between relative frequency and the abstraction we call probability.

#### D. Objective Interpretation

In the **objective interpretation**, probability is interpreted as the relative frequency with which something happens, or could happen. Let  $n$  be the number of experiments or **trials**; for example, this could be the number of proton-proton collisions at the LHC. Let  $k$  be the number of *successes*; for example, it could be the count in a given mass bin of Higgs boson events. The relative frequency of successes is

$$\frac{k}{n}. \tag{1.9}$$

It is a matter of experience that as  $n$  grows ever larger the relative frequency  $k/n$  settles down to a number, call it  $p$ , whose natural interpretation is the probability of a success. Unfortunately, this interpretation is not quite as straightforward as it seems. Any theory of probability that *defines* the latter as the limit of  $k/n$  must contend with the following possibility. It is possible that on every trial we get a success, or a failure, or we alternate between the two *ad infinitum*. It is important, therefore, to be precise about what is meant by the *limit* of the (rational) number  $k/n$ . The correct statement, first noted by James Bernoulli (1703), is the **weak law of large numbers**, mentioned briefly above. This theorem states that

$$\lim_{n \rightarrow \infty} \Pr\left[\left|\frac{k}{n} - p\right| > \epsilon\right] = 0, \tag{1.10}$$

for any real number  $\epsilon > 0$ . That is, as the number of trials goes to infinity, the *probability*  $\Pr[*]$ , that the relative frequency  $k/n$  differs from the *probability*  $p$  by more than  $\epsilon$ , becomes vanishingly small.

The implied recursion in this theorem is conceptually problematic. If, indeed, probability is to be defined as *nothing more* than the limit of a relative frequency, then the two probabilities that occur in Bernoulli's theorem must both be limits of relative frequencies. The second probability  $p$  in the theorem may legitimately be viewed as the "limit" of the relative frequency  $k/n$ . However, to define the first probability  $\Pr[*]$  requires a *second* application of Bernoulli's theorem. But that second application will specify yet another  $\Pr[*]$ , which must itself be defined in terms of a limit, and so it goes. It would seem that we cannot avoid being ensnared in an infinite hierarchy of infinite sequences of trials. Moreover, never, in practice, do we ever conduct infinite sequences of trials and therefore the limit, as it true of all limits, is an abstraction.

## E. Subjective Interpretation

We can avoid the infinite hierarchy of trials if we are prepared to interpret the first probability in Bernoulli's theorem differently from the second. If we interpret the first as a measure of plausibility then the theorem is a statement about the plausibility of the proposition  $\lim_{n \rightarrow \infty} k/n = p$ . Bernoulli's theorem, as he himself interpreted it, declares that it is plausible to the point of certainty that  $k/n \rightarrow p$  as the number of trials grows without limit. The import of this theorem, and Bernoulli's interpretation of it, is that probability as relative frequency is a *derived* notion pertaining to a special class of circumstances, namely, those in which one can entertain, in principle, performing *identically* repeated trials in which the relative frequency converges, in the precise manner of Bernoulli's theorem, to some number  $p$ , which, because it satisfies the axioms of probability, we are at liberty to call a probability. The Standard Model is an example of a physical theory that can predict the limiting numbers  $p$  for the kind of identically repeated trials performed in high energy physics experiments.

The position advocated here is that probability is an abstraction that can be usefully interpreted in at least two different ways: as the limit of a relative frequency and as a degree of belief. Moreover, the first is best understood in terms of the second.

## F. Bayes' Theorem

In 1763, Thomas Bayes published a paper in which a special case of a theorem, that bears his name, appeared. Bayes' theorem

$$P(B_k|AC) = \frac{P(A|B_kC)P(B_k|C)}{\sum_i P(A|B_iC)P(B_i|C)}, \quad (1.11)$$

where  $A$ ,  $B_k$  and  $C$  are propositions, is a direct consequence of the product rule, Eq. (1.3), of probability theory. Consider two propositions  $A$  and  $B$ . They are said to be *mutually exclusive* if the truth of one denies the truth of the other, that is:  $P(AB|C) = 0$ . In that case, from the theorem we proved earlier, we conclude that

$$P(A + B|C) = P(A|C) + P(B|C), \quad (1.12)$$

which is easily generalized to any number of mutually exclusive propositions. A set of mutually exclusive propositions  $B_k$  is said to be *exhaustive* if their probabilities sum to

unity:

$$\sum_k P(B_k|C) = 1. \quad (1.13)$$

Let  $B_1$  and  $B_2$  be exhaustive propositions. Consider the propositions  $AB_1$  and  $AB_2$ . From the product rule, we can write

$$P(AB_1) = P(B_1|A)P(A), \quad (1.15)$$

$$P(AB_2) = P(B_2|A)P(A). \quad (1.16)$$

Now add the two equations

$$P(AB_1) + P(AB_2) = [P(B_1|A) + P(B_2|A)] P(A), \quad (1.18)$$

$$= P(A). \quad (1.19)$$

This summation over exhaustive propositions is called **marginalization**, and is an extremely important operation in probability calculations. If  $B_k D_j$  are a set of mutually exclusive and exhaustive joint propositions, then we can write Bayes' theorem as

$$P(B_k D_j | AC) = \frac{P(A | B_k D_j C) P(B_k D_j | C)}{\sum_{i,l} P(A | B_i D_l C) P(B_i D_l | C)}. \quad (1.20)$$

**Exercise:** Prove this form of Bayes' theorem.

Bayes' theorem is, of necessity, true irrespective of how probabilities are interpreted. Consider the following example. A calorimeter shower arises either from an electron ( $e$ ) or from a jet ( $j$ ). Some fraction of the energy of the incident object is deposited in the electromagnetic calorimeter, often referred to as the "em-fraction". We impose the requirement  $f \equiv \text{em-fraction} > 0.6$  and assume:

$$P(f|e) = 0.90 \quad \text{Pr}[\text{electron to pass cut}],$$

$$P(f|j) = 0.05 \quad \text{Pr}[\text{jet to pass cut}],$$

$$P(e) = 0.15 \quad \text{Pr}[\text{electron}],$$

$$P(j) = 0.85 \quad \text{Pr}[\text{jet}].$$

We wish to compute  $P(e|f)$ , the probability that the shower was caused by an electron, given that the em-fraction exceeds 0.6. Applying Bayes' theorem we get

$$\begin{aligned} P(e|f) &= \frac{P(f|e)P(e)}{P(f|e)P(e) + P(f|j)P(j)}, \\ &= \frac{0.90 \times 0.15}{0.9 \times 0.15 + 0.05 \times 0.85}, \\ &= 0.76. \end{aligned} \tag{1.22}$$

We conclude that there is a 76% probability that the shower is caused by an electron. This calculation is correct whether or not the probabilities are regarded as relative frequencies or degrees of belief.

## II. LECTURE 2 - PROBABILITY THEORY, PART II

### A. Probability Distributions

#### 1. Random Variables

Statisticians make a distinction between a **random variable**  $\mathbf{X}$  and its value  $\mathbf{x}$ . A random variable can be thought of as a map  $X$ ,

$$X : \Omega \rightarrow \mathbb{R}, \quad (2.1)$$

between a set of possible **events** or **outcomes**  $\Omega = \{\omega_1, \dots, \omega_N\}$  and the set of reals  $\mathbb{R}$ . The map  $X$  assigns a real number  $x = X(\omega)$ , called the value of the random variable, to every outcome  $\omega \in \Omega$ . The height of persons who pass you in the street is an example of a random variable. Its possible events are the people who can pass you and its value is the height of a person. Since the outcome is random so too is the value of the random variable. Note, however, that in spite of the name the map  $X$  itself is generally not random! Rather it is the set  $\Omega$  of possible outcomes that possesses the (rather mysterious) quality called **randomness**. One can think of that property as a manifestation of a **randomizing agent** whose job it is to pick an outcome from the set of possibilities, according to a rule that is not readily discernable. The randomizing agent, however, need not be governed by chance! Consider the set of possible outcomes  $\Omega = \{0, \dots, 9\}$  and the function  $X$  that maps this set to the subset  $\{0, \dots, 9\} \in \mathbb{R}$ . There exists a random variable  $X$  whose value is the next decimal digit of  $\pi$ , starting, say, from the first. The digits of  $\pi$  do not occur by chance even though they form an excellent random sequence. The same is true of, so-called, pseudo-random number generators, which provide sufficiently random sequences of real numbers—indispensable in Monte Carlo-based calculations, even though, again, the randomizing agent is not governed by chance; indeed, it is strictly deterministic. Usually, a random variable is denoted by an upper case symbol, while one of its values is denoted by the corresponding lower case symbol. Thus, if  $\mathbf{X}$  is a random variable then  $\mathbf{x}$  denotes one of its values. However, for simplicity we shall not use this convention, but refer to both with the same symbol.

## 2. Properties

In general, we are most interested in propositions involving real numbers of the form  $x \in (x_1, x_2)$ . When  $x$  is continuous,  $P(x)$ , is called a **probability distribution function**, while its derivative

$$f(x) = \frac{dP(x)}{dx}, \quad (2.2)$$

(assuming it exists) is called a **probability density function**. Notice that probabilities, being pure numbers, are dimensionless, whereas densities have dimensions  $x^{-1}$ . Note, also, that from the definition, Eq. (2.2),

$$dP(x) = f(x) dx, \quad (2.3)$$

and

$$P(x) = \int dP(x), \quad (2.5)$$

$$= \int f(x) dx. \quad (2.6)$$

Given a probability distribution function  $P(x)$ , its **moments**  $m_r(z)$  about a value  $z$  is defined by

$$m_r(z) = \int (x - z)^r dP(x), \quad (2.8)$$

$$= \int (x - z)^r f(x) dx. \quad (2.9)$$

Of particular importance are the first moment about zero and the second moment about the first. The first moment about zero,  $m_1(0)$ , is called the **mean** and is often denoted by the symbol  $\mu$ . The second moment about the first, that is about the mean,  $m_2(\mu)$ , is called the **variance** of the distribution. Its square-root, often denoted by the symbol  $\sigma$ , is the **standard deviation**, which is one measure of the width of the distribution. The **mode** of a probability density  $f(x)$  is the value of  $x$  at which the density is a maximum. Finally, the **median** of a distribution is the value of  $x$  that divides it into two equal parts. The median is generally most meaningful if  $x$  is a 1-dimensional variable. Note, that if the density  $f(x)$  is symmetrical about the mode, its mode, mean and median coincide.

## 3. Common Densities and Distributions

Below we list the most commonly encountered densities and distributions, while in Fig. 1

Uniform( $x, a, b$ )	$1/(b - a)$	$x \in [a, b]$
Binomial( $x, n, p$ )	$\binom{n}{x} p^x (1 - p)^{n-x}$	$x \in [0, 1, \dots, n]$
Poisson( $x, a$ )	$a^x \exp(-a)/x!$	$x \in [0, 1, \dots]$
Gaussian( $x, \mu, \sigma$ )	$\exp[-(x - \mu)^2/2\sigma^2]/\sigma\sqrt{2\pi}$	$x \in (-\infty, +\infty)$
Chisq( $x, n$ )	$x^{n/2-1} \exp(-x/2)/2^{n/2}\Gamma(n/2)$	$x \in [0, +\infty)$
Gamma( $x, a, b$ )	$x^{b-1} a^b \exp(-ax)/\Gamma(b)$	$x \in [0, +\infty)$
Exp( $x, a$ )	$a \exp(-ax)$	$x \in [0, +\infty)$

we show examples of a few of them.

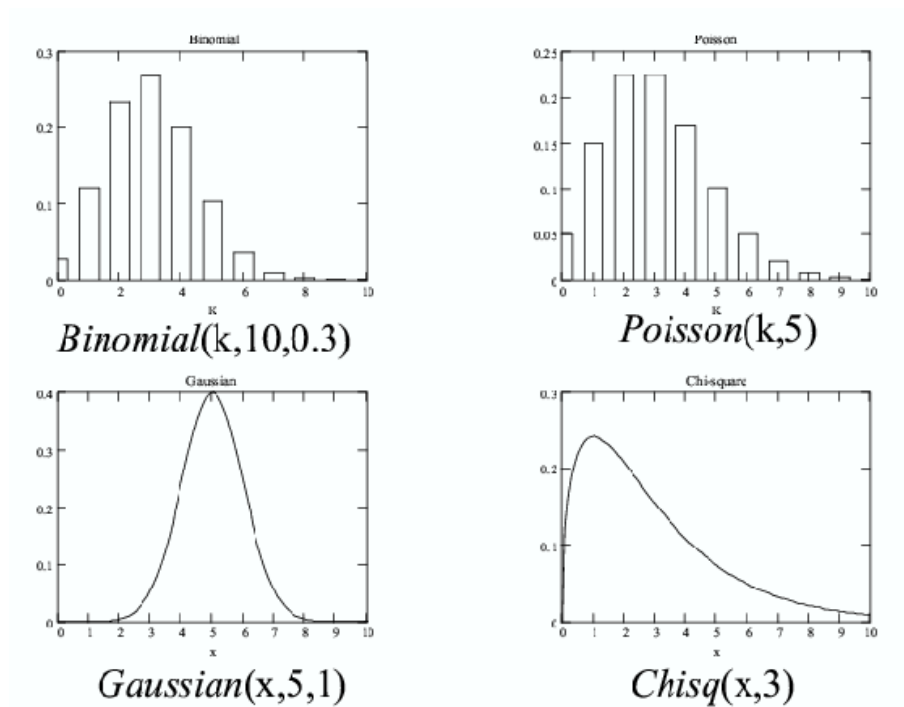


FIG. 1: Examples of the most commonly used distributions in particle physics.

**Exercise:** Calculate the mean and variance of each density, listed above.

## B. The Binomial Distribution

A **Bernoulli** trial is one with only two outcomes, success ( $S$ ) or failure ( $F$ ). Particle physicists conduct almost perfect Bernoulli trials in which every collision, say between a

proton and a proton at the Large Hadron Collider, creates ( $S$ ), or does not create ( $F$ ), an event of interest. A success could be, for example, the creation of a Higgs boson event. Typically, we are interested in the probability  $P(k|n)$  of  $k$  successes given  $n$  trials, or some function thereof. Our task is to calculate this probability, from first principles. Even if one is of the opinion that relative frequency is the only legitimate scientific way to think about probability, in practice it is exceedingly difficult, if not impossible, to make headway, *from first principles*, using this interpretation alone. Instead, we reproduce here an interesting result about Bernoulli trials, due Bruno de Finetti [8], following the presentation given by Heath and Sudderth[15] and Caves [16].

Suppose we have observed a sequence of Bernoulli trials  $S_{k,n} = x_1, \dots, x_n$ , with  $k$  successes in  $n$  trials. We assume that these are the *only* data of which we have knowledge. We note that the probability we wish to calculate,  $P(k|n)$ , makes no reference to the particular sequence at hand. But, to compute  $P(k|n)$ , we must, nevertheless, be able to assign a probability to a sequence of trials, a problem that, in general, is extremely difficult. However, given some crucial assumptions the problem can be solved.

We assume that the details of the particular sequence observed are unimportant and that the only thing that matters is the total number of successes  $k$  in the  $n$  trials we have conducted. We are therefore led to consider, not just the sequence we have observed, but the set of all sequences of length  $n$  with  $k$  successes, of which the one we observed is a particular instance. Denote by  $P(S_{k,n,j})$  the probability of the  $j^{\text{th}}$  sequence  $S_{k,n,j}$ . de Finetti [8] argues that the probabilities we assign, *at this stage*, must *of necessity* be subjective. They are subjective in that they are based on what we believe to be reasonable probability assignments, given the objective information at hand, namely, the observed sequence of trials and their outcomes. The probabilities we assign may be informed by predictions from, say, the Standard Model or some theory beyond it, but we do not know *at this stage* whether or not the predictions are correct. After all, the trials are being conducted precisely for the purpose of testing these predictions.

What then is the probability of  $k$  successes in  $n$  trials, regardless of the sequence? The answer, according to the rules of probability theory, is to add up all the probabilities  $P(S_{k,n,j})$ ,

$$P(k|n) = \sum_j P(S_{k,n,j}), \tag{2.10}$$

that is, to marginalize over all the details that are deemed irrelevant; in this case, propositions of the form: the  $j^{\text{th}}$  sequence is  $x_1, \dots, x_n$ . Unfortunately, we can go no further unless we are prepared to introduce more assumptions. We shall make two more assumptions. The first is that the order of trials is irrelevant; more precisely, we assume that the probability of a sequence of trials is symmetric with respect to all permutations of the order of trials. Each sequence,  $S_{k,n,j}$ , becomes, in effect, indistinguishable. Since they are indistinguishable we have no reason to favor one sequence over another. In the absence of reasons to do otherwise it would be rational to assign, to each sequence, the *same* probability. Since there are  $\binom{n}{k}$  indistinguishable sequences, the probability of  $k$  successes in  $n$  trials, regardless of the sequence, is

$$P(k|n) = \binom{n}{k} P(S_{k,n}), \quad (2.11)$$

where  $S_{k,n}$  can be any one of the sequences  $S_{k,n,j}$ . The second assumption is that the sequence  $S_{k,n}$  can be embedded in one or more *arbitrarily long* sequences  $S_{r,m}$  of  $r$  successes in  $m \geq n$  trials in the following way

$$P(S_{k,n}) = \sum_{r=0}^m P(S_{k,n}|S_{r,m}) P(S_{r,m}). \quad (2.12)$$

Sequences that satisfy both of these assumptions are said to be **exchangeable**. The probabilities  $P(S_{r,m})$  must still be freely assigned by us and, at present, there is nothing more about them that can be said. However, the exchangeability assumption yields a unique assessment of  $P(S_{k,n}|S_{r,m})$ , to which we now turn.

By assumption, all successes are indistinguishable, as are all failures. Therefore, the probability  $P(S_{k,n}|S_{r,m})$  of  $k$  successes and  $n - k$  failures in  $n$  trials *given* that they are embedded in a sequence of  $r$  successes and  $m - r$  failures, in  $m$  trials, is akin to drawing, *without replacement*,  $k$  red balls and  $n - k$  white balls out of a box containing  $r$  red balls plus  $m - r$  white balls. Since the sequences are indistinguishable, and that consequently the order of trials is irrelevant, we can consider *any* convenient sequence to compute  $P(S_{k,n}|S_{r,m})$ , such as the one in which we get  $k$  successes (red balls) followed by  $n - k$  failures (white balls). Noting that we start with a box containing  $m$  balls of which  $r$  are red, the probability to draw  $k$  red balls is the product of  $k$  fractions

$$\left(\frac{r}{m}\right) \left(\frac{r-1}{m-1}\right) \cdots \left(\frac{r-(k-1)}{m-(k-1)}\right) = \frac{r!}{(r-k)!} / \frac{m!}{(m-k)!}, \quad (2.13)$$

while the probability to draw  $n - k$  white balls from the remaining  $m - k$  balls of which  $m - r$  are white is the product of  $n - k$  fractions

$$\begin{aligned} \left(\frac{m-r}{m-k}\right) \left(\frac{m-r-1}{m-k-1}\right) \cdots \left(\frac{m-r-(n-k-1)}{m-k-(n-k-1)}\right) &= \frac{(m-r)!}{(m-r-(n-k))!} \\ &/ \frac{(m-k)!}{(m-n)!}, \end{aligned} \quad (2.15)$$

which yields

$$P(S_{k,n}|S_{r,m}) = \frac{r!}{(r-k)!} \frac{(m-r)!}{(m-r-(n-k))!} / \frac{m!}{(m-n)!}. \quad (2.16)$$

We can write Eq. (2.12) as an integral

$$P(S_{k,n}) = \int_0^1 P(S_{k,n}|S_{zm,m}) \pi_m(z) dz, \quad (2.17)$$

where

$$\pi_m(z) \equiv \sum_{r=0}^m P(S_{zm,m}) \delta(z - r/m), \quad (2.18)$$

and  $r/m$  is the observed relative frequency of success. By assumption, we can make the sequences  $S_{r,m}$  arbitrarily long. When we do so,  $P(S_{k,n}|S_{zm,m}) \rightarrow z^k(1-z)^{n-k}$  as  $m \rightarrow \infty$  and the functions  $\pi_m(z)$  coalesce into a continuous density  $\pi(z)$ . Putting together the pieces we obtain de Finetti's Representation Theorem

$$P(k|n) = \int_0^1 \text{Binomial}(k, n, z) \pi(z) dz, \quad (2.19)$$

for Bernoulli trials. This remarkable result shows that for exchangeable sequences of trials the probability  $P(k|n)$  of  $k$  successes in  $n$  trials is a binomial distribution weighted by a density,  $\pi(z)$ . What exactly is  $\pi(z)$ ? It is simply the probability *we* have assigned to every sequence, characterized by the relative frequency  $z$ . In other words,  $\pi(z)$  encodes *our* assessment of the likely value of the relative frequency *in an infinite sequence of trials*. If we knew, or we wished to act as if we knew, or we have a prediction, that the relative frequency is  $p$ , then we would set  $\pi(z) = \delta(z - p)$ , in which case Eq. (2.19) reduces to the binomial distribution.

The important point to take away from this is that we have arrived at the binomial distribution starting with *subjective* assessments of the probability of sequences of trials and the powerful assumption of exchangeability.

### C. The Poisson Distribution

From the discussion above, it would seem that the binomial distribution is the appropriate one to describe a typical high energy physics **counting experiment**. However, it is more usual to take note of the fact that the probability of a success  $p \ll 1$ . Given  $n$  trials, the average number of successes is  $a = pn$ . If we write Binomial( $k, n, p$ ) in terms of  $a = pn$  and take the limit  $n \rightarrow \infty$ , while keeping  $a$  constant, it will tend towards Poisson( $k, a$ ). Given that the probabilities  $p$  are typically very small, in practice it is the Poisson distribution that is used to describe the number of events observed or the count in a given bin of a histogram.

**Exercise:** Show that Binomial( $k, n, p$ )  $\rightarrow$  Poisson( $k, a$ ) in the limit  $p = a/n \rightarrow 0$ .

Another interesting way to understand the Poisson distribution is as the outcome of a particular **stochastic process**, which, roughly speaking, is a system that evolves through *random* changes of state. Suppose that at time  $t + \Delta t$  we have recorded  $k$  counts. In a Poisson process one assumes that the probability to get a single count in the short time interval  $(t, t + \Delta t)$  is given by  $q\Delta t$ . Since this probability is small, we can arrive at  $k$  counts at time  $t + \Delta t$  in *at most* two ways:

1. we had  $k$  counts at time  $t$  and recorded none in  $(t, t + \Delta t)$ ,
2. we had  $k - 1$  counts at time  $t$  and recorded 1 count in  $(t, t + \Delta t)$ .

Let

$$P_k(t + \Delta t) = \text{be the probability that the count is } k \text{ at time } t + \Delta t, \quad (2.21)$$

$$P_k(t) = \text{be the probability that the count is } k \text{ at time } t, \quad (2.22)$$

$$P_{k-1}(t) = \text{be the probability that the count is } k - 1 \text{ at time } t, \quad (2.23)$$

$$q\Delta t = \text{be the probability of recording a } \textit{single} \text{ count in } (t, t + \Delta t). \quad (2.24)$$

Given the two possible state changes from time  $t$  to time  $t + \Delta t$  we deduce that the probabilities are related by the **finite difference equation**

$$P_k(t + \Delta t) = (1 - q\Delta t) P_k(t) + q\Delta t P_{k-1}(t), \quad (2.25)$$

which can be re-expressed as

$$\frac{P_k(t + \Delta t) - P_k(t)}{\Delta t} = -qP_k(t) + qP_{k-1}(t). \quad (2.26)$$

In the limit  $\Delta t \rightarrow 0$ , we obtain the differential equation

$$\frac{dP_k(t)}{dt} = -qP_k(t) + qP_{k-1}(t), \quad (2.27)$$

which is a simple example of a **birth - death equation**. (See Ref. [17] for another example involving Poisson processes.) The first term on the right-hand side describes the “death” rate, while the second term describes the “birth” rate. Such equations describe the probability of a given “population” size at time  $t$ .

**Exercise:** Solve Eq. (2.27) and show that  $P_k(t) = \text{Poisson}(k, qt)$ , for  $q = \text{constant}$ .

**Exercise:** Repeat the calculation with  $q(t) = \exp(-t/\tau)/\tau$ .

#### D. The Gaussian Distribution

The Gaussian distribution, also known as the **normal distribution**, is the most important distribution in applied probability, principally because of the **Central Limit Theorem**, which roughly states that

*All reasonable distributions become Gaussian in the limit of large numbers.*

This is true, in particular, for the Poisson distribution. This is a result of practical importance in that it is the basis of  $\chi^2$  methods to fit functions to histograms and in the associated goodness-of-fit tests (see Lecture 4). To illustrate this theorem, first write  $\text{Poisson}(k, a)$  as  $\exp[\ln \text{Poisson}(a + x, a)]$ , in which we have set  $k = a + x$ , and then allow  $k \rightarrow \infty$ . By using the approximation

$$\begin{aligned} \ln \text{Poisson}(k, a) &= k \ln a - a - \ln k!, \\ &\approx k \ln a - a - k \ln k + k - \ln \sqrt{2\pi k}, \end{aligned} \quad (2.29)$$

$$(2.30)$$

one can show that the Poisson distribution becomes Gaussian when the counts become large.

**Exercise:** Show that  $\text{Poisson}(k, a) \rightarrow \text{Gaussian}(k, a, \sqrt{a})$ .

### E. The $\chi^2$ Distribution

The  $\chi^2$  distribution is closely related to the Gaussian. Indeed, if  $x_i \sim \text{Gaussian}(x_i, \mu_i, \sigma_i)$ , where  $\mu_i$  and  $\sigma_i$  are known constants, then the quantity  $z = \sum_{i=1}^n (x_i - \mu_i)^2 / \sigma_i^2$  has a  $\chi^2$  density with  $n$  degrees of freedom [18]. An instructive way to compute the density of  $z$  is to use the intuitively clear formula [19]

$$f(z) = \int \delta(z - h(x)) dP(x), \quad (2.31)$$

where  $h(*)$  is some function of  $x$ , for example,  $h(x) = \sum_{i=1}^n (x_i - \mu_i)^2 / \sigma_i^2$ . The formula states that the density  $f(z)$  is given by the sum of the probabilities  $dP(x) = \prod_{i=1}^n f(x_i) dx_i$  over all values of  $x_i$  consistent with the constraint  $z = h(x)$ . By using the integral representation of the  $\delta$ -function,

$$\delta(x) = \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{i\omega x} d\omega, \quad (2.32)$$

we can write  $f(z)$  as the Fourier integral

$$f'(z) = \frac{1}{2\pi i} \int_{-\infty}^{\infty} e^{i\omega z} F(\omega) d\omega, \quad (2.33)$$

of the complex function

$$F(\omega) = i \int e^{-i\omega h(x)} dP(x). \quad (2.34)$$

If the exponential function in Eq. (2.34) can be factorized into a product of terms, each depending on a single variable  $x_i$ , it may be possible to calculate  $F(\omega)$  explicitly. This happens to be the case for the function  $h(x) = \sum_{i=1}^n (x_i - \mu_i)^2 / \sigma_i^2$ . For this case, we can write

$$F(\omega) = i \int dx_1 \text{Gaussian}(x_1, \mu_1, \sigma_1) \cdots \int dx_n \text{Gaussian}(x_n, \mu_n, \sigma_n) e^{-i\omega h(x)}, \quad (2.35)$$

which factorizes into a product of  $n$  1-dimensional integrals, each of the same form. Using the result  $\int_{-\infty}^{\infty} \exp[-(x - \mu)^2 / 2\sigma^2] = \sigma\sqrt{2\pi}$ , one finds

$$F(\omega) = \frac{i}{(1 + 2i\omega)^{n/2}}, \quad (2.36)$$

which, from Eq. (2.33), yields  $z \sim \text{Chisq}(z, n)$ .

**Exercise:** Give a complete derivation of this result. Hint: use contour integration.

For a more complex example of such a calculation, see Ref. [20].

1. *A Brief Word on Fitting*

The quadratic form  $Q = \sum_{i=1}^n (x_i - \mu_i)^2 / \sigma_i^2$  is commonly used to fit a function  $\mu(\theta_1, \dots, \theta_P)$ , with  $P$  parameters  $\theta_k$ ,  $k = 1, \dots, P$ , to a histogram of  $n$  bins, with count  $k_i$  in bin  $i$ . If the counts are large enough (say  $k > 10$ ), and if the variances  $\sigma_i^2$  are accurately known, then  $Q \sim \text{Chisq}(Q, n - P)$  approximately. However, even if either, or both, conditions are not met  $Q$  can still be used to perform a fit, but its density will not be  $\chi^2$ , in general. Its actual density, however, can be estimated by Monte Carlo simulation. The density of  $Q$  is typically used to test goodness-of-fit (see Lecture 4).

### III. LECTURE 3 - STATISTICAL INFERENCE, PART I

#### A. Descriptive Statistics

One of the very first tasks in the analysis of data is to characterize the data using a few numerical summaries. A **statistic** is any function of the data sample  $\mathbf{x} = x_1, \dots, x_n$ . They can be as simple as the **sample average**,

$$\bar{x} = \frac{1}{n} \sum_{i=1}^n x_i, \quad (3.1)$$

and the **mean squared error** (MSE),

$$\text{MSE} = \frac{1}{n} \sum_{i=1}^n (x_i - \bar{x})^2, \quad (3.2)$$

or as complex as the output of a full-blown analysis program. These summaries provide a useful compression of the data, making it easier to gain some understanding of the main features.

#### B. Ensemble Averaging

In principle, before any serious analysis is undertaken a thorough exploration of the behaviour of the proposed analysis method should be conducted. This forms part of the **experimental design** phase of an experiment. Such studies usually appear in Technical Design Reports (TDR). The goal, in principle, is to ascertain, *a priori*, which analysis method is best, in some agreed upon manner, with the intention of applying the best method to the data when they are available. In practice, however, such studies are done before, during, and after analyses of data. And often one decides, after the fact, which of several analyses merit seeing the light of day. Whatever the motivation, and stage of the analysis, there is broad agreement that it is crucial to study the behaviour of methods on an **ensemble** of artificial data samples, usually created by Monte Carlo simulation. These studies are often referred to as **ensemble tests**. As a simple illustration, we discuss the ensemble behaviour of a few simple statistics.

In general, each sample  $\mathbf{x} = x_1, \dots, x_n$  within the ensemble will yield a different value for the average, Eq. (3.1). Intuitively, we expect these averages to be closer to the mean of the

distribution, from which the data have been generated, than the individual data  $x_1, \dots, x_n$  that comprise each average. Given some measure of “closeness” to the mean it would be natural to compute its average value over the ensemble; that is, to perform an **ensemble average**, denoted by the symbol  $\langle \dots \rangle$ , of the closeness measure. Consider first the ensemble average of the sample average, Eq. (3.1),

$$\begin{aligned} \langle \bar{x} \rangle &= \left\langle \frac{1}{n} \sum_{i=1}^n x_i \right\rangle, \\ &= \frac{1}{n} \sum_{i=1}^n \langle x_i \rangle, \\ &= \frac{1}{n} n \mu, \\ &= \mu. \end{aligned} \tag{3.4}$$

We have assumed that the  $x_i$  are identically distributed, in which case  $\langle x_i \rangle = \mu$ , and that the **bias**,

$$b \equiv \langle x \rangle - \mu, \tag{3.5}$$

is zero. Take as our measure of closeness to the mean  $\mu$  the square of

$$\Delta \bar{x} = \frac{1}{n} \sum_{i=1}^n \Delta x_i, \tag{3.6}$$

where the **error**,  $\Delta x_i = x_i - \mu$ . Squaring both sides, and taking the ensemble average, yields

$$\langle \Delta \bar{x}^2 \rangle = \frac{1}{n^2} \sum_{i=1}^n \sum_{j=1}^n \text{Cov}(x_i, x_j), \tag{3.7}$$

where  $\text{Cov}(x_i, x_j) \equiv \langle \Delta x_i \Delta x_j \rangle$  is called the **covariance matrix**. If this matrix is diagonal, the data are said to be **uncorrelated**. However, this does *not* necessarily imply that they are independent; that is, that the probability distribution  $P(x)$ , generating the samples, is of the form  $dP(x) = \prod_{i=1}^n f(x_i) dx_i$ . If the  $x_i$  are independent in this sense then they are of necessity uncorrelated, but the converse is not true; uncorrelated data may, or may not, be independent. The diagonal elements  $\text{Var}(x_i) \equiv \langle \Delta x_i^2 \rangle$ , which can be written as  $\text{Var}(x_i) = \langle x_i^2 \rangle - \langle x_i \rangle^2$ , are the **variances**. Note that the MSE, Eq. (3.2), the bias and the variance are related as follows

$$\text{MSE} = b^2 + \text{Var}(x). \tag{3.8}$$

The common practice is to use ensembles whose samples are independent and therefore uncorrelated. However, for practical reasons it may be necessary to use an ensemble in which the correlation between samples is not quite zero. This will be the case in an ensemble in which the samples are generated by a **bootstrap** method [21]. In a bootstrap method one draws many samples of size  $n$  from a population  $x_1, \dots, x_m$  of size  $m \geq n$ . Each sample is created by drawing elements  $x_i$ , one at a time — at random and *with replacement*, from the finite population. Since the samples are drawn with replacement, they will in general have elements  $x_i$  that are common. Consequently, any statistic calculated from them will be correlated across the ensemble. In particular, the sample averages will be correlated. In the following we shall assume this to be the case.

We can re-write  $\langle \Delta \bar{x}^2 \rangle$  as follows

$$\begin{aligned}
 \langle \Delta \bar{x}^2 \rangle &= \frac{1}{n^2} \sum_{i=1}^n \sum_{j=1}^n \langle \Delta x_i \Delta x_j \rangle, \\
 &= \frac{1}{n^2} \sum_{i=1}^n \langle \Delta x_i^2 \rangle + \frac{1}{n^2} \sum_{i=1}^n \sum_{j \neq i}^n \langle \Delta x_i \Delta x_j \rangle, \\
 &= \frac{\sigma^2}{n} + \frac{1}{n^2} \sum_{i=1}^n \sum_{j \neq i}^n \langle \Delta x_i \Delta x_j \rangle, \tag{3.10}
 \end{aligned}$$

assuming zero bias and variance  $\sigma^2 = \langle \Delta x_i^2 \rangle$ . If the samples are uncorrelated then the cross-terms in Eq. (3.10) average to zero and we obtain the well-known result that the variance of the average,  $\bar{x}$ , is smaller by a factor  $n$  than the variance of  $x$ , confirming that the average is indeed closer to the mean  $\mu$  than is  $x$ . Suppose, however, that the cross-terms do not vanish and each is given by  $\langle \Delta x_i \Delta x_j \rangle = \rho \sigma^2$ , where  $\rho \in (-1, +1)$  is the **correlation coefficient**. For this simple case we find

$$\langle \Delta \bar{x}^2 \rangle = \frac{\sigma^2}{n} [1 + (n-1)\rho]. \tag{3.11}$$

As expected, correlated samples yield less precise averages. And, unlike averages from uncorrelated samples, increasing the sample size  $n$  indefinitely does not help since according to Eq. (3.11) the variance of the average has a lower bound of  $\rho \sigma$ .

### C. Estimators

As noted in Lecture 1, our goal as scientists is to learn from experience by conducting carefully controlled experiments that yield data from which we can *infer* something interesting

about the system under investigation. Given a **data-set**  $\mathbf{x} = \{x_1, \dots, x_N\}$ , a mathematical model  $M$ , characterized by the parameters  $\theta$ , and the associated probability  $P(\mathbf{x}|\theta)$  we use statistical inference to decide the best values to assign to the parameters  $\theta$ . If we have several models  $M_1, M_2 \dots$  then we may, in addition, wish to decide which one is best. This, of course, presupposes that we know what we mean by *best*. The mapping  $\{x_1, \dots, x_N\} \rightarrow \{\theta_1, \dots, \theta_M\}$  from our data-set to the parameters, or to the set of models, is an example of a **decision function**, which will be denoted by the symbol  $d$ . Suppose that our model depends upon a single parameter  $\theta$ . Denote by  $\hat{\theta}$  any **estimate** thereof. If the decision function is such that  $\hat{\theta} = d(\mathbf{x})$  then the function  $d$  is called an **estimator** for  $\theta$ . One can think of the estimator as a program, which when data are entered into it outputs estimates. The estimator could be as simple as an averaging operation or as complex as several full-scale analysis program.

#### D. Loss and Risk

To choose a decision function we need a way to quantify the quality of the associated decisions. In general, every decision, especially bad ones, entail some loss. The loss can be quantified with a **loss function**,  $\mathcal{L}(\theta, d)$ , which depends on both the decision function and the parameter being estimated. The idea of a loss function is useful in both frequentist and Bayesian analysis. However, the two approaches use the loss function differently:

- **Frequentist:** In making *inferences* data we could have observed are as relevant as data observed.
- **Bayesian:** In making *inferences*, only the data observed are relevant.

Accordingly, in the frequentist approach we consider the loss pertaining to every data-set which could have been observed, as well as the loss pertaining to the data actually obtained. In the Bayesian theory, on the other hand, all possible hypotheses must be considered in light of the data-set actually obtained.

In either case, the desire to average the loss function in some way motivates the definition of a new function

$$\mathcal{R} = \langle \mathcal{L}(\theta, d) \rangle_*, \tag{3.12}$$

called the **risk function**, where the subscript  $*$  denotes averaging with respect to either  $\mathbf{x}$  or  $\theta$ . In one case, the averaging is done with respect to all possible data-sets  $\mathbf{x}$  for fixed  $\theta$  (frequentist), while in the other the averaging is done with respect to all possible  $\theta$  for fixed  $\mathbf{x}$  (Bayesian). In the frequentist approach, the risk function is an ordinary function of the parameter  $\theta$  but a functional of the decision function  $d$ ; that is, it depends on the set of all possible values of  $d$ . In the Bayesian approach, the risk function is a functional of  $\theta$ . However, it is generally not regarded as a function of  $\mathbf{x}$  because the data are considered to be constants.

It should not be construed from the above that Bayesians do not care about data-sets that could have been observed. On the contrary, it is absolutely essential during the *design* of an experiment, or of an analysis, to consider what could be observed in order to conduct the best possible experiment or the most effective analysis. In the Bayesian approach, however, when the time comes to make inferences only the data actually acquired are deemed relevant.

### E. Risk Minimization

A statistical analysis can be viewed as a procedure that minimizes a risk function in order to arrive at an optimal decision, usually an optimal decision about the value of a parameter or a model. In particle physics, one often speaks of “optimizing an analysis”. What we are doing, without being explicit about it, is minimizing *some* unstated risk function. If the risk function is known then, in principle, an optimal decision can be had with respect to the underlying loss function. However, in many circumstances although the loss function is known, since we choose it, the risk function is not. In these cases, we must make do with an estimate of the risk function, the most common of which is given by

$$\mathcal{R}_{\text{emp}} = \frac{1}{n} \sum_{i=1}^n \mathcal{L}(\theta, f(\mathbf{x}_i, \omega)), \quad (3.13)$$

where  $f(\mathbf{x}_i, \omega)$  is a suitably parameterized function, with parameters  $\omega$  and data  $\mathbf{x}_i$ , that one hopes is flexible enough to include a good approximation to the optimal decision function  $d$ , say at the point  $\omega = \omega_0$ . The function  $\mathcal{R}_{\text{emp}}$  is called the **empirical risk function**. Its minimization, to obtain an approximation to the optimal decision function  $d$ , is a widely used strategy in data analysis, encompassing everything from curve-fitting to the training of sophisticated learning machines.. The strategy is referred to as **empirical risk mini-**

**mization.**

The most important mathematical property of empirical risk, and the property that makes it useful in practice is that the function  $f(\mathbf{x}_i, \omega_0)$ , found by minimizing the empirical risk, is expected to converge to the optimal decision function  $d(\mathbf{x})$  as the sample size  $n$  goes to infinity, provided that the function  $f(\mathbf{x}, \omega)$  is sufficiently flexible and the minimization algorithm is effective at finding the minimum.

## F. The Bayesian Approach

The Bayesian approach to statistical inference is firmly grounded in the subjective interpretation of probability. Whereas the frequentist approach deals only with the distributional properties of data, that is, with statements of the form

$$P(Data|Theory), \tag{3.14}$$

the Bayesian approach admits, in addition, statements of the form

$$P(Theory|Data), \tag{3.15}$$

that is, the probability that a given *Theory* is true, in light of evidence provided by *Data*. This is precisely the kind of statement that most physicists would wish to make. The connection between the two probabilities, Eqs. (3.14) and (3.15), is given by Bayes' theorem, Eq. (1.20),

$$P(Theory|Data) = P(Data|Theory) P(Theory)/P(Data). \tag{3.16}$$

The probability  $P(Theory)$  is called the **prior probability**. It encodes what we believe we know about the *Theory* independently of the *Data*. The probability  $P(Data|Theory)$  is sometimes referred to, loosely, as the **likelihood**, while the probability  $P(Theory|Data)$  is called the **posterior probability**. More correctly, the likelihood is a function  $\propto P(Data|Theory)$ . Viewed this way, it is not a probability.

The power of the Bayesian approach is due in large measure to the fact that one can speak, meaningfully, of the probability of a theory, or of an hypothesis. Moreover, since *Theory* can be anything whatsoever one anticipates that the domain of applicability of Bayesian reasoning is considerable larger than that of a theory where the notion of the probability of an hypothesis is absent, as is the case in the frequentist approach. However, this enormous

conceptual gain comes at a price. In order to arrive at a posterior probability the price to be paid is the specification of a prior probability for the *Theory*, independently of the *Data*. There is simply no way around this if one wishes to adhere to the rules of probability theory.

In many applications in high energy physics we are interested in propositions of the form  $\theta \in (a, b)$ , that is, a parameter has a value within some continuous set. Let

$$P(\mathbf{x}|\theta, \lambda) = \int_{\Omega} f(\mathbf{z}|\theta, \lambda) d\mathbf{z}, \quad (3.17)$$

be the probability assigned to the data-set  $\mathbf{x}$ , contained in a neighborhood  $\Omega$  of  $\mathbf{x}$ , and let  $\theta$  and  $\lambda$  be the parameters of the model currently under consideration. Perhaps  $\theta$  is the parameter of interest, say the mass of the Higgs boson, while  $\lambda$  represents parameters such as the mean background rate and the jet energy scale. It could even represent purely theoretical parameters, such as the renormalization and factorization scales. All such parameters, which are not of intrinsic interest, are referred to as **nuisance parameters**.

If  $P(\theta, \lambda) = \pi(\theta, \lambda) d\theta d\lambda$  is the prior probability assigned to the proposition that  $\theta$  and  $\lambda$  have certain values — where  $\pi(\theta, \lambda)$  is the **prior density**, we can write Bayes' theorem as

$$\begin{aligned} P(\theta, \lambda|\mathbf{x}) &= \frac{P(\mathbf{x}|\theta, \lambda) P(\theta, \lambda)}{\int_{\theta, \lambda} P(\mathbf{x}|\theta, \lambda) P(\theta, \lambda)}, \\ &= f(\theta, \lambda|\mathbf{x}) d\theta, \end{aligned} \quad (3.19)$$

which in terms of densities becomes

$$f(\theta, \lambda|\mathbf{x}) = \frac{f(\mathbf{x}|\theta, \lambda) \pi(\theta, \lambda)}{\int d\theta \int d\lambda f(\mathbf{x}|\theta, \lambda) \pi(\theta, \lambda)}. \quad (3.20)$$

Since the nuisance parameters  $\lambda$  are not of interest we need a way to get rid of them in order to say something useful about the parameter that is. This is technically difficult in the frequentist approach, but straightforward in principle in the Bayesian approach: one “merely” integrates them out of the problem

$$f(\theta|\mathbf{x}) = \int f(\theta, \lambda|\mathbf{x}) d\lambda. \quad (3.21)$$

The quotation about the word merely is appropriate because it may be difficult, in practice, to perform what are often high-dimensional integrals. That being said, the posterior density, Eq. (3.21), is an elegant encapsulation of all that we know about the parameter  $\theta$ , given the data we have acquired and the prior knowledge encoded in the prior density  $\pi(\theta, \lambda)$ .

## G. The Likelihood Principle

The posterior density,  $f(\theta|\mathbf{x})$  — the final result of our inference about  $\theta$ , displays a very important philosophical, and practical, difference between the frequentist and Bayesian approaches that we have alluded to, namely, that in a Bayesian analysis

an inference depends only on the data observed,

a principle that is referred to as the **likelihood principle**, not to be confused with the method of maximum likelihood. Clearly, to base an *inference* on an ensemble of possible data-sets is to be sharply at odds with the likelihood principle. Consequently, the principle is at odds with a host of standard frequentist practice. Since these methods are still firmly entrenched, one is naturally led to ask: is the likelihood principle sensible? Certainly, this was Jeffreys [1] opinion. Ironically, even Fisher — a forceful critic of all things Bayesian — was an advocate of the likelihood principle. Indeed, Fisher was extremely critical of what he regarded as the “extreme frequentism” advocated by Neyman. A further irony is that, according to a theorem due to Birnbaum [22], the likelihood principle follows from ideas that many frequentist statisticians consider unimpeachable.

## H. Parameter Estimation

The posterior probability is a complete statement of the results of an inference. However, particular summaries are often of direct interest. Having finally arrived at a posterior density for the Higgs boson mass, what we want, of course, is a single mass estimate plus some idea of how well the mass has been measured. In some circumstances, it may be useful to take the mean of the posterior density as an estimate of the parameter of interest. However, the mean is not the only possibility. One way to formalize the construction of estimates is through loss functions, which we discussed in general terms in Sect. III D and which we discuss in more detail below.

In the Bayesian approach it is natural to speak of our *knowledge* being uncertain, in particular, our knowledge of the value of a parameter. Moreover, the uncertainty in our knowledge is measured not by the expected scatter of estimates over an ensemble, as would be the case in a frequentist analysis, but rather by some measure of the width of the posterior

density, which, in accordance with the likelihood principle, depends only on the observed data.

As noted above, a loss function is a way to measure the quality of a decision. A typical decision is: given a data-set  $\mathbf{x}$  decide that the estimate of  $\theta$  is  $\hat{\theta} = d(\mathbf{x})$ , where  $d(\mathbf{x})$  is a special kind of decision function called an estimator. To illustrate these ideas, we consider two commonly used loss functions.

### 1. Quadratic Loss

The quadratic loss, introduced earlier, is

$$\mathcal{L}(\theta, d) = (\theta - d)^2. \quad (3.22)$$

Earlier, we also introduced the average loss, that is, the risk function. In the frequentist theory, the averaging is done with respect to an ensemble of possible data-sets  $\mathbf{x}$ . In the Bayesian theory, one averages over all possible propositions about the value of  $\theta$ , constrained by the fact that we have obtained a specific data-set. Therefore, we are led to consider the risk function

$$\begin{aligned} \mathcal{R}(\mathbf{x}) &= \langle \mathcal{L}(\theta, d) \rangle_{\theta}, \\ &= \int \mathcal{L}(\theta, d) f(\theta|\mathbf{x}) d\theta, \end{aligned} \quad (3.24)$$

that is,

$$\mathcal{R}(\mathbf{x}) = \int (\theta - d)^2 f(\theta|\mathbf{x}) d\theta, \quad (3.25)$$

for the quadratic loss, where  $f(\theta|\mathbf{x})$  is the posterior density. The best estimator is declared to be that which minimizes the risk

$$\begin{aligned} D_d \mathcal{R}(\mathbf{x}) &= D_d \int \mathcal{L}(\theta, d) f(\theta|\mathbf{x}) d\theta, \\ &= \int D_d \mathcal{L}(\theta, d) f(\theta|\mathbf{x}) d\theta, \\ &= 0. \end{aligned} \quad (3.27)$$

To simplify the notation, we use the symbol  $D_d$  to represent the derivative with respect to  $d$ . (Also, being physicists, we naturally assume that the derivative and integral operators commute.) After minimization, we obtain the intuitively pleasing result

$$\hat{\theta} = d(\mathbf{x}) = \int \theta f(\theta|\mathbf{x}) d\theta. \quad (3.28)$$

In words:

The optimal estimate with respect to a quadratic loss is the mean of the posterior density.

## 2. Absolute Loss

The absolute loss, defined by

$$\mathcal{L}(\theta, d) = |\theta - d|, \quad (3.29)$$

is used when one wishes to be more tolerant of deviations from the mean. Estimates based on the absolute loss are less sensitive to the tails of the posterior density and in that sense are more robust than those based on the quadratic loss. As before, we obtain the estimator  $d$  by minimizing the risk

$$\mathcal{R}(\mathbf{x}) = \int |\theta - d| f(\theta|\mathbf{x}) d\theta. \quad (3.30)$$

Differentiating with respect to the function  $d$  yields

$$\begin{aligned} D_d \mathcal{R}(\mathbf{x}) &= 0 \\ &= \int D_d |\theta - d| f(\theta|\mathbf{x}) d\theta \\ &= - \int \frac{\theta - d}{|\theta - d|} f(\theta|\mathbf{x}) d\theta, \end{aligned} \quad (3.32)$$

that is,

$$\int_{\theta < d} f(\theta|\mathbf{x}) d\theta = \int_{\theta > d} f(\theta|\mathbf{x}) d\theta, \quad (3.33)$$

which shows that the optimal estimator  $d$ , using the absolute loss, is the **median** of the posterior density.

## 3. Uncertainty

The uncertainty in our knowledge of a parameter is quantified by some measure of the width of the posterior density. One such measure is the variance

$$\text{Var}(\theta) = \langle \theta^2 \rangle - \langle \theta \rangle^2. \quad (3.34)$$

Another is a **credible interval**,  $[l(\mathbf{x}), u(\mathbf{x})]$ , referred to also as a Bayesian interval, obtained from the formulae

$$\int_{\theta \leq l(\mathbf{x})} f(\theta|\mathbf{x})d\theta = \alpha_L \quad (3.35)$$

and

$$\int_{\theta \geq u(\mathbf{x})} f(\theta|\mathbf{x})d\theta = \alpha_R, \quad (3.36)$$

where  $\alpha_L$  and  $\alpha_R$  as chosen so that  $\beta = 1 - \alpha_L - \alpha_R$ , where  $\beta$  is the desired probability, that is, degree of belief, to be assigned to the specified interval. The interpretation of credible intervals is direct:  $\beta$  is the probability that the proposition  $\theta \in [l(\mathbf{x}), u(\mathbf{x})]$  is true.

## I. Combining Results

In the frequentist approach the results from different experiments are combined using a weighted average. However, more generally, results can be combined using Bayes' theorem. Let  $f(\mathbf{x}_k|\theta, \lambda, \alpha_k)$  be the likelihood for experiment  $k$ , where  $\theta$  is the parameter of interest and  $\lambda$  represents any nuisance parameters that are common to all experiments — this could be, for example, a measured cross section used by all experiments — and  $\alpha_k$  represents nuisance parameters specific to experiment  $k$ . Ideally, for each experiment the **marginal likelihood**,

$$f(\mathbf{x}|\theta, \lambda) = \int f(\mathbf{x}|\theta, \lambda, \alpha_k) \pi(\alpha_k) d\alpha_k, \quad (3.37)$$

would be reported, that is, the likelihood function marginalized with respect to the nuisance parameters  $\alpha_k$  specific to the experiment. We do not marginalize, at this stage, with respect to  $\lambda$  because these parameters are common across experiments. The function  $\pi(\alpha_k)$  is the prior density for  $\alpha_k$ . In writing Eq. (3.37), we have implicitly factorized the full prior density  $\pi(\theta, \lambda, \alpha_k)$  as follows

$$\pi(\theta, \lambda, \alpha_k) = \pi(\theta, \lambda|\alpha_k) \pi(\alpha_k). \quad (3.38)$$

We shall assume that for every experiment, whose results are to be combined, the prior density  $\pi(\theta, \lambda|\alpha_k)$  is independent of  $\alpha_k$ , in which case we may write

$$\pi(\theta, \lambda, \alpha_k) = \pi(\theta, \lambda) \pi(\alpha_k). \quad (3.39)$$

Given this assumption, each experimental group, if it wishes, can produce an inference about  $\theta$  and  $\lambda$  by supplying a prior density  $\pi(\theta, \lambda)$ . This observation provides the clue about how

to combine results. The prior density  $\pi(\theta, \lambda)$  for a given experiment is simply the posterior density  $f(\theta, \lambda|\mathbf{x})$  from another. Therefore, by recursively combining the results from  $K$  experiments we obtain the overall posterior density

$$f(\theta, \lambda|\mathbf{x}_1, \dots, \mathbf{x}_K) = \frac{f(\mathbf{x}_1|\theta, \lambda) \cdots f(\mathbf{x}_K|\theta, \lambda)\pi(\theta, \lambda)}{\int d\theta \int d\lambda f(\mathbf{x}_1|\theta, \lambda) \cdots f(\mathbf{x}_K|\theta, \lambda)\pi(\theta, \lambda)}. \quad (3.40)$$

This is proportional to the product of the joint likelihood function for the combined results and a prior density for  $\theta$  and  $\lambda$ . This method will yield estimates that converge to the true value as more and more experiments are combined, provided that the result from each experiment is **consistent**. By consistent we mean that the estimates from an experiment would converge to the true value, as more and more data are acquired in that experiment, with a probability that approaches unity. Note that a consistent estimator need not be unbiased. However, by definition, its bias vanishes in the limit of large data-sets.

## J. Model Selection

Suppose we have a set of competing models  $M$ , which may depend upon different sets of parameters  $\theta_M$  and we wish to pick the one that fits the data best. Given some prior information and a data-set  $\mathbf{x}$ , how should one make this decision? This is the problem of **hypothesis testing** or **model selection**.

Our first task is to assign a probability density,  $f(\mathbf{x}|\theta_M, M)$ , to our data-set given a model  $M$  and hypotheses about the values of the corresponding parameters  $\theta_M$ . We must also assign a prior density  $\pi(\theta_M, M)$ . Then write down Bayes' theorem

$$f(\theta_M, M|\mathbf{x}) = \frac{f(\mathbf{x}|\theta_M, M) \pi(\theta_M, M)}{\sum_M \int f(\mathbf{x}|\theta_M, M) \pi(\theta_M, M) d\theta_M}. \quad (3.41)$$

The function  $f(\theta_M, M|\mathbf{x})$  represents the probability density of the proposition:  $M$  is the true model and it has parameter values  $\theta_M$ .

It is very important to understand that the probability densities  $f(\theta_M, M|\mathbf{x})$  are conditioned on the set of models considered, *so far*. “Best model” in this context simply means the best of the current set. Should another model be added to the set, the probabilities assigned to different models would, in general, change. Therefore,  $f(\theta_M, M|\mathbf{x})$  cannot be construed as an absolute measure of the validity of a model. But it *is* a measure of the *conditional* validity of a model: it provides a way to *compare* models within a given set

in light of what we know. If a rational thinker had to choose a single model she would opt for the model with the highest posterior probability. But, should she acquire further pertinent information, that information, via Bayes' theorem, could cause her to change her mind about which model is currently best.

Finally, we can marginalize  $f(\theta_M, M|\mathbf{x})$  with respect to  $\theta_M$  to obtain  $P(M|\mathbf{x})$ , the probability of model  $M$ . This is potentially very useful if each model, within the set, are identical, except for the value of a single parameter  $\alpha$ . For example,  $M$  could label models that differ by an assumed value for the mass of the Higgs boson. We then have a way to estimate that parameter:

$$\hat{\alpha} = \sum_M \alpha_M P(M|\mathbf{x}), \quad (3.42)$$

and its associated uncertainty

$$\sigma_\alpha^2 = \sum_M (\alpha_M - \hat{\alpha})^2 P(M|\mathbf{x}). \quad (3.43)$$

## K. Optimal Event Selection

Before we can measure something, we must find it. Therefore, a basic task of data analysis is to separate signal from background. Given a set of discriminating variables, the traditional method combines a judicious use of common sense, physical intuition, and trial and error to separate signal from background. However, much of the energy devoted to this can be better spent elsewhere since the task of finding the optimal separation between signal and background is a well-defined mathematical problem whose solution is known.

It helps to think about the problem geometrically. Suppose we have found  $n$  variables that we consider useful for separating signal from background. The  $n$  variables can be thought of as a point in an  $n$ -dimensional space, sometimes referred to as **feature space**. Presumably, by construction, the signal tends to cluster in one part of this space while the background tends to occupy a different region. However, inevitably, there will be some overlap between the signal and background densities. The problem to be solved is to find the boundary that separates optimally signal from background. Traditionally, one does the simplest thing: one constructs a boundary from planes that are perpendicular to the axes, where each plane corresponds to a cut on a specific variable. However, in general, the optimal boundary cannot be built from such intersecting planes; in general, it will be a curved surface.

The problem of finding this surface, however, is indeterminate until we have specified what we mean by optimal. A generally accepted definition of an optimal boundary is one that minimizes the probability to misclassify events. For the moment, we shall suppose that we know the signal and background densities,  $f(\mathbf{x}|S)$  and  $f(\mathbf{x}|B)$ , respectively. Let us further assume that we know the signal and background prior probabilities  $P(S)$  and  $P(B)$ . These prior probabilities are not controversial:  $P(S)$  is just the chance to pick a signal event without regard to its feature vector  $\mathbf{x}$ , and likewise for  $P(B)$ . Since the event must be either signal or background it must be the case that  $P(S) + P(B) = 1$ . The probability to misclassify a signal event, with feature vector  $\mathbf{x}$ , is just the probability for signal events to land on the background side of the optimal boundary, or for a background event to land in the signal region. For simplicity, we consider a one dimensional problem, with the boundary, say, at  $x = x_0$ . The probability  $E_S$  to misclassify a signal event is

$$E_S(x_0) = P(S) \int h(x_0 - x) f(x|S) dx, \quad (3.44)$$

where  $h(z)$  is the Heaviside step function, defined by  $h(z) = 1$  if  $z > 0$  and zero otherwise. The probability to misclassify the background is, likewise, the probability for the background to land on the signal side,

$$E_B(x_0) = P(B) \int h(x - x_0) f(x|B) dx. \quad (3.45)$$

Hence, the probability to misclassify events, that is, the **error rate**, regardless of whether they are signal or background, is the sum

$$E(x_0) = E_S(x_0) + r E_B(x_0), \quad (3.46)$$

where  $r$  is a weight that allows for the possibility that we may wish to weight the background more (or less) than the signal. We now minimize  $E(x_0)$  with respect to the choice of boundary, that is, we set  $D_{x_0} = 0$  and obtain

$$P(S) \int \delta(x_0 - x) f(x|S) dx + P(B) \int \delta(x - x_0) f(x|B) dx = 0. \quad (3.47)$$

The derivative has conveniently converted the step functions into delta functions, thereby rendering the integrals trivial, yielding the result

$$r(x_0) = \frac{f(x_0|S)P(S)}{f(x_0|B)P(B)}. \quad (3.48)$$

The function  $r(\ast)$  is called the **Bayes discriminant** because of its intimate connection with Bayes' theorem,

$$P(S|x) = \frac{r}{1+r} = \frac{f(x|S)P(S)}{f(x|S)P(S) + f(x|B)P(B)}. \quad (3.49)$$

The  $n$ -dimensional generalization of this has the same Bayesian form. (See Ref. [23] for an interesting derivation of this result.) The posterior probability  $p(S|\mathbf{x})$  is precisely that needed for event classification. It is the probability that an event characterized by the vector  $\mathbf{x}$  is of the signal class. By using this probability we have succeeded in mapping the original  $n$ -dimensional problem into a more tractable one-dimensional one.

This is all very well, but there is a serious practical problem. Rarely do we have analytical expressions for the signal and background densities  $f(\mathbf{x}|S)$  and  $f(\mathbf{x}|B)$ . We seem, alas, to have achieved a pyrrhic victory! Happily, however, many methods exist that provide good approximations to the posterior probability. In particular, it has been shown that, under suitable circumstances, neural networks [24] compute a direct approximation to the probability  $p(S|\mathbf{x})$ .

## L. Prior Probabilities

So far, we have skirted over a potentially serious difficulty of the Bayesian approach; to solve an inference problem we must assign two quantities, a prior and a likelihood. There is broad agreement within physical sciences about the use of a Poisson distributions to model counting experiments. However, even amongst those who agree that prior probabilities are necessary, there is disagreement about how to assign them when we have minimal prior information about the parameters to be estimated, or when we wish to act as if this were so. The basic problem is to assign a prior that, in some well-defined sense, has as small an effect as possible on the final inference. In other words, most physicists want a method that “let’s the data speak for themselves”. At face value, this is the strength of the frequentist approach where no priors appear. However, this strength is illusory because it forces one to answer the wrong question, namely, given a particular model  $M$  one is forced to answer the question: what data-sets are possible? But, the question of direct interest is the inverse: given a particular data-set, namely, the one actually obtained, what models are compatible with it?

A Bayesian analyst is often faced with the following circumstance: that the only prior

information at hand about a parameter  $\theta$  is that it lies within some set, perhaps the set  $\theta \in [0, \infty)$ . What prior probability should we assign to various hypotheses about its value? Laplace argued that if we know nothing about the value of a parameter then we should assign a flat prior density to encapsulate this state of knowledge:  $\pi(\theta) \propto \text{constant}$ . This seems reasonable, until we realize that *any* choice of prior density for a given parameter  $\theta$  specifies, implicitly, the prior density for the infinity of parameters that are functions of  $\theta$ . Clearly, we have specified a lot more than we bargained for!

For example, suppose we transform from  $\theta$  to the parameter  $\alpha = 1/\theta$ . Inferential coherence demands that its prior probability density be  $\pi(\alpha) \propto 1/\alpha^2$ ; a form that looks, at best, non-intuitive. This prior density would be fine were it not for the following question: what reason do we have to suppose that the prior density is flat in the parameter  $\theta$  rather than in the parameter  $\alpha$ , or some other parameter, such as  $\tau = \ln \theta$ ? It seems that the assignment of prior probabilities for a parameter about which we are almost totally ignorant is, indeed, arbitrary. This in a nutshell is the core of the controversy about prior probabilities that has raged for more than 200 years.

The problem of how to assign prior probabilities that, in some sense, have the smallest effect on inferences has a long, difficult, and polemic history [25]. Here, however, is some practical advice. Use the prior density that seems most reasonable to you or, better still, one that has been agreed upon by the community for the given problem. For example, both the CDF and DØ Collaborations have agreed to use a flat prior for a cross-section. Then check the robustness of the inferences (that is, see how much they vary) by trying different reasonable priors. If the answers are unduly sensitive to the choice of prior then the scientifically honest conclusion should be that the data at hand are inadequate and more should be acquired.

## M. Counting Experiments

We have covered the basic elements of the Bayesian theory. In this section, we illustrate some of this theory by applying it to a prototypical example in high energy physics: the analysis of a counting experiment.

Every Bayesian analysis contains at least four ingredients:

- A model

- A data-set
- A likelihood
- A prior probability

For a counting experiment the model is

$$a = s + b, \tag{3.50}$$

where  $a$  is the mean number of events,  $s$  the mean signal count and  $b$  the mean background count. Let  $n$  be the total number of events observed. As discussed in Lecture 2, the probability to observe  $n$  events may be assumed to be

$$P(n|s, b) = \text{Poisson}(n, s + b). \tag{3.51}$$

The prior density for  $s$  and  $b$  can be factorized thus

$$\begin{aligned} \pi(s, b) &= \pi(s|b) \pi(b), \\ &= \pi(s) \pi(b), \end{aligned} \tag{3.53}$$

where we have assumed that the conditional prior density for the signal does not depend on the value of the background. We have two prior densities to assign. We consider first the prior for the background, then that for the signal.

Let us suppose that the background has been estimated from a Monte Carlo simulation of the background process, yielding  $B$  background events, with probability given by  $P(B|\lambda) = \text{Poisson}(B, \lambda)$ . Furthermore, we assume that the relationship between  $b$  and  $\lambda$  is

$$b = k\lambda, \tag{3.54}$$

where  $k$  is a known scale factor, in this example, the ratio of the observed to Monte Carlo integrated luminosities. Given  $B$ , we can compute the posterior density,

$$f(\lambda|B) = \frac{f(B|\lambda) \pi(\lambda)}{\int f(B|\lambda) \pi(\lambda) d\lambda}, \tag{3.55}$$

for  $\lambda$ . But, to do so requires specification of the prior density  $\pi(\lambda)$ . We shall suppose that it is of the form  $\pi(\lambda) = \lambda^p$ , but, for simplicity, we consider  $p = 0$ , that is, a flat prior in  $\lambda$ . The posterior density  $f(\lambda|B)$  contains information about the parameter  $b$ , by virtue of the

relation  $b = k\lambda$ . It can therefore serve as the *prior density* for  $b$ . From Bayes' theorem we obtain the posterior density

$$f(s, k\lambda|n) = \frac{f(n|s, k\lambda) \pi(k\lambda) \pi(s)}{\int \int f(n|s, k\lambda) \pi(k\lambda) \pi(s) d\lambda ds}, \quad (3.56)$$

from which we can eliminate the nuisance parameter  $\lambda$  by marginalization

$$f(s|n) = \int f(s, k\lambda|n) d\lambda. \quad (3.57)$$

The function  $f(s|n)$  suggests that it may be convenient to define the **marginal likelihood**

$$f(n|s) \equiv \int f(n|s, k\lambda) \pi(k\lambda) d\lambda, \quad (3.58)$$

and write Bayes' theorem as

$$f(s|n) = \frac{f(n|s) \pi(s)}{\int f(n|s) \pi(s) ds}. \quad (3.59)$$

For this problem, the marginal likelihood can be calculated. The result is

$$f(n|s) = \frac{1}{(1+k)^{B+1}} \sum_{r=0}^n \left(\frac{k}{1+k}\right)^{n-r} \frac{\Gamma(n-r+B+1)}{(n-r)!B!} \text{Poisson}(r, s). \quad (3.60)$$

We now turn to the signal prior  $\pi(s)$ . Our knowledge of the signal is rather vague: we know it is positive and finite! It is far from clear how to translate this prior knowledge into a prior density. We shall simply adopt as a matter of *convention* the prior  $\pi(s) = 1$ . In practice, one gets intuitively reasonable results with it; but there are better choices [25]. Putting all pieces together we can compute the posterior density  $f(s|n)$ , which is the final, and complete, encoding of our improved knowledge of the possible values of the mean signal count  $s$ .

Exercise: Derive the formulae for  $f(n|s)$  and  $f(s|n)$ .

## IV. LECTURE 4 - STATISTICAL INFERENCE, PART II

### A. Goodness of Fit

Consider the task of fitting a curve to a histogram of counts. The usual way to do this is by the method of maximum likelihood. Let  $f(x, \theta)$  be the curve to be fit by adjusting the parameters  $\theta$ . We minimize the sum

$$\sum_i \ln \text{Poisson}(k_i, f(x_i, \theta)), \quad (4.1)$$

which is equivalent to maximizing the joint likelihood of the counts, with respect to the parameters. Having found the best fit parameters, it is considered sound practice to test the **goodness-of-fit**. The concept of goodness-of-fit was introduced by Fisher. The basic idea is simple: one invents a measure of discrepancy  $D(x)$  between the fitted curve and the data such that large values of  $D$  would tend to cast doubt on the hypothesis that the curve fits the data. One calculates the probability density  $f(D)$  of the discrepancy  $D(x)$ , in principle by the method described in Lecture 2 but in practice by Monte Carlo simulation, and one computes

$$p = \int_{D > D_0} f(D) dD, \quad (4.2)$$

the **p-value** for the observed discrepancy  $D_0$ . Should that number be judged too small, the fit is *rejected* as a *bad* fit because the discrepancy is correspondingly too large. If on the other hand  $p$  is large, the fit may, or may not, be good! Suppose, for example, that the discrepancy is defined by the quadratic form

$$D(x) = \sum_i (k_i - f(x_i, \theta))^2 / \sigma_i^2, \quad (4.3)$$

and we find  $D(x) = 0$ , and therefore  $p = 1$ ! This does not necessarily imply a good fit; goodness-of-fit is a misnomer. These tests should really be called “badness-of-fit” tests!

### B. Confidence Intervals

The purpose of this section is to explain as clearly as possible the important frequentist concept of a confidence interval. Consider the following questions

- What is the mass of the  $\tau$  neutrino?

- What is the mass of the top quark?
- What is the mass of the Higgs boson?

and the following tentative answers

$$\begin{aligned}
 m_\nu &< 18.2 \text{ MeV}, \\
 m_t &= 175.0 \pm 3.1 \text{ GeV}, \\
 m_H &> 114.3 \text{ GeV}.
 \end{aligned}
 \tag{4.4}$$

The statements in Eq. (4.4) are unsatisfactory because they fail to indicate how much *confidence* we should place in them. In the absence of a convention,  $m_t = 175.0 \pm 3.1 \text{ GeV}$  conveys no more information than does  $m_t = 100 \pm 20 \text{ GeV}$ . The statements

$$\begin{aligned}
 m_\nu &< 18.2 \text{ MeV}, \text{ with CL} = 0.950, \\
 m_t &= 175.0 \pm 3.1 \text{ GeV}, \text{ with CL} = 0.683, \\
 m_H &> 114.3 \text{ GeV}, \text{ with CL} = 0.950,
 \end{aligned}
 \tag{4.5}$$

are better because they assign probabilities, called **confidence levels** (CL) that indicate how seriously the statements should be taken. If the statements, Eq. (4.5), were Bayesian there is nothing more to be said. The probabilities would be measures of degrees of belief. However, since we wish to interpret them in a frequentist manner, this involves a bit more work.

But first we ask the following question: do the three statements in Eq. (4.5) convey information that is different in kind? As written, the statements look rather different. However, each can be re-expressed as follows

$$m_\nu \in [0, 18.2] \text{ MeV}, \text{ with CL} = 0.950, \tag{4.6}$$

$$m_t \in [169.2, 179.4] \text{ GeV}, \text{ with CL} = 0.683, \tag{4.7}$$

$$m_H \in [114.3, \infty) \text{ GeV}, \text{ with CL} = 0.950, \tag{4.8}$$

that is, as statements about intervals. Written this way, it is clear that each statement is conveying the same kind of information, which loosely speaking is this: a parameter of interest has a true *fixed* value that has a good chance of being within the specified interval. The second statement in Eq. (4.5) is an example of the conventional way to state the

results of a measurement. The number 3.1, associated with the confidence level of 0.683 (or equivalently, 68.3%), is referred to as a **standard error**. Sometimes (this is especially true in searches for new phenomena) one is interested in only one of the bounds of the interval. For example, in the first statement in Eq. (4.5) the upper bound, that is, the **upper limit**, is of greater interest than the lower one. In the third statement it is the lower bound that is of interest, that is, the **lower limit**.

### 1. Coverage Probability

Imagine a *set of ensembles* of experiments, each element of which is associated with a single *fixed* value  $\theta$  of the parameter to be measured. We might visualize each ensemble, within the set, as a huge box filled with experiments, with each box labeled by (that is to say, associated with) a different value of  $\theta$ . Each experiment  $E$  yields an interval  $[l(E), u(E)]$  for the parameter  $\theta$ . In each ensemble (that is, box) some fraction of the experiments will yield intervals that contain the  $\theta$  value associated with that ensemble. This fraction is called the **coverage probability**, which in general will vary from one ensemble to another. The **confidence level** is the *minimum coverage probability* over the set of ensembles. In terms of our fanciful picture, each box of experiments will have some coverage probability; obviously, at least one box will have the smallest coverage probability, which, by definition, is the confidence level of the set of boxes. Now suppose we choose a box and repeatedly, and randomly, pick an experiment from it. We shall find that the fraction of sampled experiments that yield intervals containing  $\theta$  is greater than or equal to the confidence level for our set of boxes.

The thought experiment we have just described cannot, of course, be carried out in practice. However, coverage (as Neyman stressed) pertains not only to ensembles of identical experiments measuring the same thing, but also to ensembles of *different* experiments measuring *different* things. If one considers the (finite) ensemble of published intervals there is no doubt that they have *some* coverage probability. But it is not clear how useful it is to know this since we are not privy to the true values of all the different quantities to which they pertain. And if we were, the experiments would never have been undertaken! The question remains, in what sense is a confidence level a measure of confidence, as commonly understood? The basic idea is this: an experiment is imagined selected at random from the

ensemble (the box) to which it belongs, presumably the one labeled by a  $\theta$  whose value is equal to that dictated by Nature. The probability that our experiment yields an interval  $[l(E), u(E)]$  containing  $\theta$  is exactly equal to the coverage probability of the ensemble to which it belongs, which by construction is greater than or equal to the confidence level of the set of ensembles. A confidence level is a measure of confidence in the sense that the higher the confidence level the more confident *we* are invited to be that *our* interval actually contains the true value of  $\theta$ .

We now can state the central problem that must be solved in order to make probabilistic statements such as those in Eq. (4.5) within the context of a relative frequency interpretation of probability. The problem is to construct intervals that *a priori* have a coverage probability equal to the desired confidence level, or greater, *whatever the true value of the parameter of interest*. The qualifying clause is necessary because we do not know what the true value is. We do not know from which box our experiment has come! If a set of intervals satisfies the above criterion they are said to **cover**. Intervals so constructed are called **confidence intervals**, a concept introduced by Jerzy Neyman in a seminal paper published in 1937 [26]. Actually, Neyman went further: he required not only that confidence intervals cover for all possible values of the parameter of interest but also for all possible values of *all* the other parameters of the problem, commonly referred to as nuisance parameters. Again, this is necessary because we generally do not know their true values.

## 2. The Neyman Construction

In this section, we give the general algorithm for constructing confidence intervals, which Neyman described in his 1937 paper. For concreteness, we consider the problem of constructing confidence intervals for the Poisson distribution with mean count  $\theta$ .

Happily, the algorithm is conceptually simple. It is illustrated in Fig. 2, which shows a plot of the parameter  $\theta$  versus the observed count  $N$ . Each point of the parameter space of  $\theta$  is associated with an ensemble of experiments, each yielding a count  $N$  and an interval  $[l(N), u(N)]$ , drawn vertically. The algorithm to construct confidence intervals, when the probability density of the observations depends on  $\theta$  only proceeds as follows. For each value of  $\theta$  one finds two counts  $a$  and  $b$ , as indicated in Fig. 2, such that the probability to observe a count within the set  $\{a, \dots, b\}$  is  $\geq \beta$ , where  $\beta$  is the desired confidence level. Figure 2

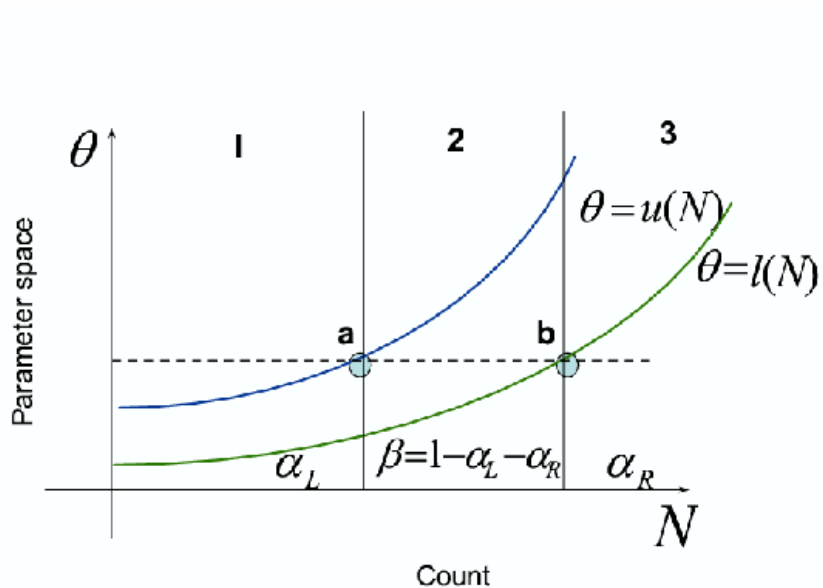


FIG. 2: The plot shows how an observed count  $N$  is mapped into an interval  $[l(N), u(N)]$ , drawn vertically, in the parameter space of  $\theta$ . As the count  $N$  varies, so do the intervals. Counts that land in region 2 lead to intervals that bracket the true value of  $\theta$ , while counts that land in either region 1 or region 3 exclude  $\theta$ . But since the true value of  $\theta$  is unknown we must construct the curves  $\theta = u(N)$  and  $\theta = l(N)$  so that for every value of  $\theta$  that is possible *a priori*, that is, for every box of experiments, the probability to get a count in region 2 is  $\geq \beta$ . The points  $a$  and  $b$ , respectively, define the lower and upper bounds of an interval in  $N$  with probability content  $\geq \beta$ .

shows that, for a given  $\theta$ , the counts  $a$  and  $b$  partition the space of observations into three regions denoted 1, 2 and 3. If an experiment, from the ensemble indexed by  $\theta$ , yields a count  $N$  that lands in region 2 then the interval  $[l(N), u(N)]$  will bracket  $\theta$ . On the other hand, for all observations that fall in either regions 1 or 3 the intervals will fail to include  $\theta$ . By construction, the relative frequency with which a count falls in region 2 is  $\geq \beta$ ; therefore, the coverage probability of the confidence intervals  $[l(N), u(N)]$  will be *exactly* equal to the probability to obtain a count in that region.

### 3. Other Constructions

There are many ways to construct sets of counts  $N$  with probability content greater than or equal to the desired confidence level simply by sliding the points  $a$  and  $b$  along the horizontal line  $\theta = \text{constant}$  (see Fig. 2). One common way is to assign equal probabilities  $\alpha_L$  and  $\alpha_R$  to the regions 1 and 3, respectively. Confidence intervals constructed this way are called **central confidence intervals** and are most efficiently computed by solving the equations

$$\begin{aligned}\alpha_L &= \Pr(r \leq N | \theta = u), \\ &= \sum_{r=0}^N \text{Poisson}(r, u),\end{aligned}\tag{4.9}$$

$$\begin{aligned}\alpha_R &= \Pr(r \geq N | \theta = l), \\ &= \sum_{r=N}^{\infty} \text{Poisson}(r, l), \\ &= 1 - \sum_{r=0}^{N-1} \text{Poisson}(r, l),\end{aligned}\tag{4.10}$$

where  $\beta = 1 - \alpha_L - \alpha_R$ , with  $\alpha_L$  set equal to  $\alpha_R$ . (The subscript  $L$  stands for left and  $R$  for right, corresponding to the regions left and right of region 2 in Fig. 2, that is, regions 1 and 3, respectively.)

Another method that has gained adherents is that of Feldman and Cousins [27]. In this method, as in the general case, one finds for each value of  $\theta$  a set of counts  $\{N\}$  such that the probability to obtain a count within the set is  $\geq \beta$ . The set is populated by first ordering  $N$  according to the likelihood ratio

$$\frac{\text{Poisson}(N, \theta)}{\text{Poisson}(N, N)},\tag{4.11}$$

in descending order, and then adding values of  $N$  to the set until its probability content is equal to or just exceeds the desired confidence level. The counts  $a$  and  $b$  are the minimum and maximum values within the set  $\{N\}$ . A procedure for populating sets of observations, such as  $\{N\}$ , with specified probability content is called an **ordering principle**. The one just described is referred to as Feldman-Cousins ordering.

Figure 3 compares central intervals with those constructed using the Feldman-Cousins

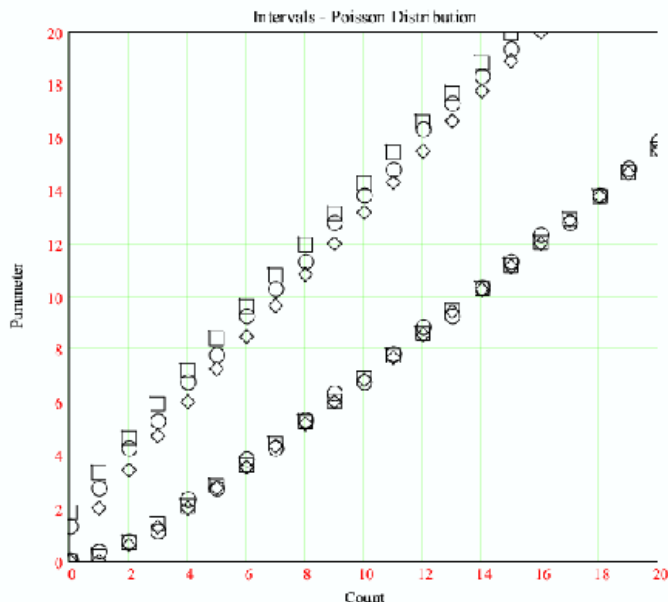


FIG. 3: Confidence intervals for the Poisson distribution. Three sets of intervals are shown: central intervals (boxes), Feldman-Cousins intervals (circles) and “root N” intervals (diamonds).

method. We also show the intervals given by the well-known “root N” rule  $l(N) = N - \sqrt{N}$  and  $u(N) = N + \sqrt{N}$ . We see that all three intervals have approximately the same lower confidence limits, but that the upper limits of central intervals are higher than those of Feldman and Cousins, which in turn are higher than those of the “root N” intervals. However, while both the central and Feldman-Cousins intervals cover, as they necessarily must in view of how they are constructed, the simple “root N” intervals do not, as indicated in Fig. 4. Note, however, that as  $N \rightarrow \infty$  the “root N” intervals become ever more satisfactory approximations to the exact intervals. Incidentally, the use of a confidence level of 0.683 stems from the fact that for  $x \sim \text{Gaussian}(x, \mu, \sigma)$ , with mean  $\mu$  and standard deviation  $\sigma$ , intervals of the form  $[x - \sigma, x + \sigma]$  have a confidence level of 0.683. The “root N” intervals converge to the Gaussian ones as  $N \rightarrow \infty$ .

Clearly there is considerable freedom of choice in constructing confidence intervals. Consequently, with exactly the same data different physicists within a collaboration could compute different confidence intervals all of which cover. So how is one to decide which interval to publish? Unfortunately, there is no consensus, as yet, on the criteria to be used to select a

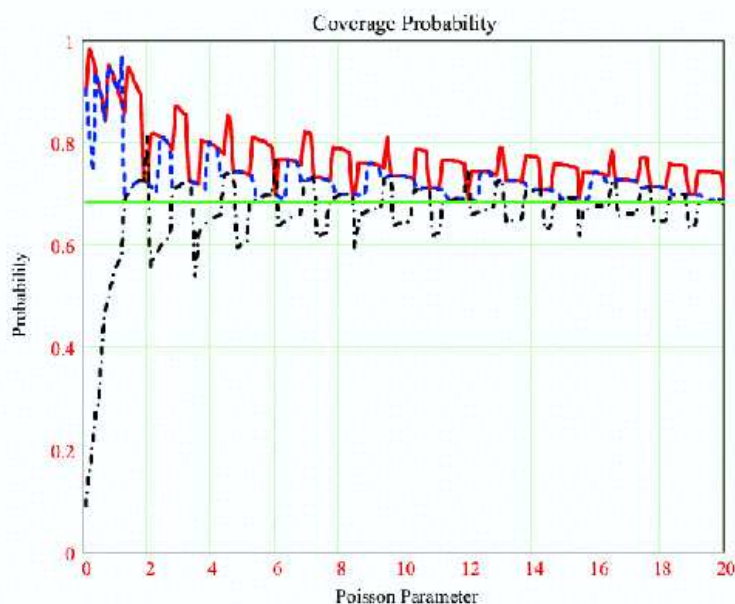


FIG. 4: Coverage probability for three sets of Poisson confidence intervals, central (solid line), Feldman-Cousins (dashed line) and “root N” (dot-dashed line), as a function of the parameter  $\theta$ . By construction the central and Feldman-Cousins intervals cover, whereas the simple “root N” ones do not.

set of confidence intervals from the (infinite) set of possibilities. The only non-controversial advice that can be given is this: in a publication explain precisely what you have done!

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