Statistical Methods in **Particle Physics**

7. Hypothesis Testing

Heidelberg University, WS 2023/24

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Some difficult topics



Errors in independent variables

- What happens if we have errors in x and y?
- Actually quite complex question
- What happens if we repeat the measurement? Do we:
 - A. Draw a new true *x*-value from some distribution?
 - B. Measure the same unknown *x*-value again?
- "A" leads to structural models, while "B" leads to functional models
- When repetition of measurement is fixed, and the x- and y-variances are known, we can calculate a likelihood
- Many models deal with unknown variances, not usual in physics



The measured particle $\beta\gamma$ fluctuates when the experiment is repeated.

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βγ

Errors in independent variables (2)



Example 1: We put the setting on the machine to some x-value (e.g. the voltage), but the true x-value fluctuates around this, giving an uncertainty

Since the fluctuations depend on the formulation of the problem, so must the best fit.



Example 2: There is some true constant x-value, which is unknown. The measurements fluctuate around it.

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Errors in independent variables (3)

Typical case in particle physics

- binned distribution
- Measurement uncertainty leads to entries landing in the wrong bin
- Mostly, when uncertainty is larger than the bin width
- Methods for inverting process via "unfolding"
- Discussed later in the lecture







Asymmetric errors

- Sometimes results are given with asymmetric uncertainties $\chi_{\sigma^{-}}^{\sigma^{+}}$
- This is not consistent with the definition of the error as a standard deviation - which does not have a direction
- There are several ways in which an asymmetric error can come about:
 - From the $\log L_{max} 1/2$ rule of maximum likelihood yielding asymmetric points
 - From using a confidence interval for the edges of the $[x - \sigma^{-}, x + \sigma^{+}]$ interval
 - From some other ad hoc rule, which many or may not be explained
- Usually we need some way to combine (average) measurements and to propagate these uncertainties
- The treatment of the results depends on what the asymmetric uncertainties are supposed to represent



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Asymmetric errors (2)

- Sometimes the question arises: Are the errors Gaussian?
- It is unclear what that means
- Assuming: Is the distribution of the estimator Gaussian?
- Then asymmetry could mean: Sum of two half-Gaussian distributions $[x > 0] \cdot G_1(x, \sigma^+) / \sigma^+ + [x < 0] \cdot G_2(x, \sigma^-) / \sigma^-$
- Mean at 0 but median below
- Taking the mean of several measurements means convolution
- But convolution must lead closer to symmetric distribution
- Therefore: Whatever the reason for asymmetric error bars, it is never justified to add the upper and lower errors in quadrature separately!
- Impossible to calculate χ^2 for goodness-of-fit without specifying what the errors mean
- Similar for weighted mean







Asymmetric errors (3)

- Recommendation for asymmetric uncertainties: Avoid!
- If you have to calculate with other people's errors: Find out precisely what they mean and how they are defined
- R. Barlow looked at two problems:
 - How to combine the $L_{max} 1/2$ estimates from two measurements
 - How to combine uncertainties with asymmetries from a nonlinear function (arXiv:0306138)
- If no clear definition, then you must use some ad-hoc mechanism, e.g. symmetrising the uncertainties, using the larger of the two ... (but don't add them separately)



R. Barlow, PHYSTAT (2005) proceedings arXiv:0406120





The Guide to Uncertainty in Measurement

- There is a document giving an international standard for evaluating and expressing uncertainty
- Published by the International Bureau of Weights and Measures, Joint Committee for Guides in Metrology
- Separates errors into "Type A" and Type B"
 - Type A is estimated via repeated measurements (e.g. from variance of outputs)
 - Type B is everything else
- Essentially adopts a mix of Frequentist and Bayesian methods
 - Type A analysed via unbiased variance estimator
 - "Flat prior" nuisance parameters get $|a b|/\sqrt{12}$ errors - corresponding to marginal
- It is not clear how much it helps in fundamental physics



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Hypothesis testing



Reminder: Bayesian and Frequentist diagnosis example

Bayesian:

- Frequency of disease in population is prior
- Probability for *this* patient to have disease is valid concept
- p(D | +) = 0.032 is the probability for this patient to have the disease, this encodes the uncertainty

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Frequentist:

- Probability for *this* patient to have disease is not a valid concept - there is no random process
- Probability for a patient randomly drawn from the population to have disease is a valid concept
- Two possible statements:
 - "If we randomly select a person from the population, then the people testing positive have a probability of 0.032 of having the disease."
 - "If a patient is healthy, we would get a positive" test with a probability of 0.03"
- Neither are probabilities for this particular person to have the disease

Can we generalise this approach?



Hypotheses and tests

Hypothesis test

- Statement about the validity of a model

Simple hypothesis: a hypothesis with no free parameters

Composite hypothesis: contains unspecified parameter(s)

• Example: data follow Poissonian with mean > 5

Null hypothesis H_0 and alternative hypothesis H_1

- ► H₀ often the background-only hypothesis (e.g. the Standard Model in searches for new physics)
- H₁ often signal or signal + background hypothesis

Question: Can null hypothesis be rejected by the data?

Tells you which of two competing models is more consistent with the data

Examples: the detected particle is a pion; data follow Poissonian with mean 5



Example: Dream speedrunning controversy

- In October 2020, Dream reached 5th place in the "glitchless 1.16" Minecraft speedrunning category
- Two main random processes necessary for completing the game: Ender pearls from trading and blaze rods from blazes
- Number of successes should be distributed by a binomial distribution with $\theta_{\text{pearls}} = 0.05$, $\theta_{\text{rods}} = 0.5$
- Did he cheat? How to assess from frequentist view?
- Asking: How likely is the result? Does not work
 - $p_{\text{binom}}(k = 211 | N = 305, \theta = 0.5) \approx 4.9 \cdot 10^{-12}$ is small
 - But so is the most likely value $p_{\text{binom}}(k = 152 | N = 305, \theta = 0.5) \approx 0.046$
- Need another way to quantify

Bartering Luck



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Example 2: Goodness-of-fit

- Want to know if a model (H_0) is consistent with the data
- χ^2 looks "okay", but how to quantify?
- Probability for any particular χ^2 is always 0 (density)
- If e.g. H_1 were the true model, we would likely have a large χ^2 (wrt. the blue line), but this is a qualitative statement



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Test statistics

- A test statistic t(d) is a function of the data d
- It should be chosen, such that for the hypothesis we are testing, H_0 , the alternatives H_1 (H_2, H_3, \ldots) typically have larger or smaller values (we will assume larger in the following)
- For the "Dream" (binomial) case, we can just use the observer number k - a modification to a higher drop probability yields a higher average k
- For the model comparison, we can use the χ^2 as it will be on average higher if another hypothesis is true
- We thus use k and χ^2 as the test statistics here
- The choice of the test statistic determines how well we can distinguish between hypotheses
- We can now decide to reject or accept a hypothesis based on the test statistic











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Critical region



The probability for H_0 to be rejected while H_0 is true:

Probability to reject H_1 even though it is true:

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Type I and type II errors

Type I error: Null hypothesis is rejected while it is actually true

Type II error: Test fails to reject null hypothesis while it is actually false

Type I and type II errors and their probabilities:

	H_0 is true
H_0 is rejected	Type I error (
<i>H</i> ₀ is not rejected	Correct decision

 H_0 is false (i.e., H_1 is true) Correct decision $(1 - \beta)$ α) on $(1 - \alpha)$ Type II error (β)

What does such a test mean?

- Remember the two statements from diagnosis:
 - If we randomly select a person from the population, then the people testing positive have a probability of 0.032 of having the disease."
 - "If a patient is healthy, we would get a positive test with a probability of 0.03"
- We now define the significance by the second one
- Here, a positive diagnosis would mostly be wrong!
- The Bayesian solution to this would be to use a prior
- The frequentist solution is to require more strict significances, e.g. for particle discoveries $\alpha = 2.9 \cdot 10^{-7}$ also called 5σ .

The p-value - test of significance

- hypothesis without explicit reference to alternative hypotheses
- Define test statistic t that reflects level of agreement with the data
- need to specify them
- Determine distribution $f(t|H_0)$ under hypothesis H_0

p-value = $\int_{-\infty}^{\infty} p(t | H_0) dt$

The *p*-value is the probability of obtaining a test statistic t at least as extreme as the results actually observed, under the assumption that the null hypothesis is correct.

extreme" means.

Often one wants to quantify the level of agreement between the data and a

Larger values should reflect possible alternative hypotheses, but we no not

This means, that the alternative hypothesis is only needed to define what "more

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The p-value - example 1

- For the possible cheating: higher numbers of successes k means "more extreme"
- So we need to sum up all cases at least as extreme as the measured one:

p-value =
$$\sum_{k=211}^{305} p_{\text{binom}}(k | N = 305, \theta = 0.5) = 8.8$$

- Even though this result does not depend on any H_1 , we are implicitly comparing to all hypotheses with $\theta > 0.5$
 - p-value should not be confused with significance level
 - significance level is a pre-specified constant
 - p-value is a function of the data, and is therefore itself a random variable
 - p-value is not the probability for the hypothesis; in frequentist statistics, this is not defined

The p-value: example 2

• For the measured $\chi^2 = 15.6$, the more extreme deviation would be towards higher values

$$p$$
-value = $\int_{15.6}^{\infty} p_{\chi^2}(\chi^2 | N_{dof} = 10) = 0.11$

- Last point gives large contribution to χ^2
- But it actually disfavours H_1 even more
- This shows, that the χ^2 is not the best possible test statistic here
- When someone quotes a significance, always ask: With respect to which test statistic?

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Neyman–Pearson lemma

Neyman-Pearson lemma holds for simple hypotheses and states:

should be chosen such that:

$$t(\vec{x}) := rac{f(\vec{x}|H_1)}{f(\vec{x}|H_0)} > c \quad ext{inside } W$$

c is a constant chosen to give a test of the desired significance level.

Equivalent formulation: optimal scalar test statistic is the likelihood ratio

 $t(\vec{x}) =$

To get the highest power (i.e. smallest possible value of β) of a test of H_0 with respect to the alternative H_1 for a given significance level, the critical region W

and
$$t(\vec{x}) \leq c$$
 outside W

$$\frac{f(\vec{x}|H_1)}{f(\vec{x}|H_0)}$$

The p-value: example 2

- The χ^2 is the log-L of a multidimensional Gaussian
- Thus, the log of the likelihood ratio leads to a difference in χ^2 for the models with $\Delta \chi^2 = -48.5$ p-value = $\int_{-48.5}^{\infty} p(\Delta \chi^2) d\Delta \chi^2 = 0.82$
- Models are much better separated
- However, we need to specify the alternative model

Practical considerations

Problem: often one does not have explicit formulas for $f(x|H_0)$ and $f(x|H_1)$

allow one to generate instances of the data.

events

- Fisher discriminants
- Neural networks
- Support vector machines
- decision trees

• • • •

- One rather has Monte Carlo models for signal and background processes which
- In this case one can use multi-variate classifiers to separate different types of

Simple example: Counting experiment (Poisson statistics) Expected background events: $v_{\rm b} = 1.3$ Expected signal events: $v_s = 2$ Expected signal + bckgr. events: $V_{s+b} = 3.3$

Test statistic t =number of observed events

Critical region $t_c \ge 4$

- significance of the test $\alpha = 0.043$
- power of the test $1 \beta = 0.42$

 H_1 : signal + background

Suppose we observe n = 5 events

• Under H_0 , this correspond to a *p*-value = 0.01

Kolmogorov–Smirnov test (1)

KS test is an unbinned goodness-of-fit test

Q: Do data points come from a given distribution?

Compare cumulative distribution function

$$F(x) = \int_{-\infty}^{x} f(x') \, \mathrm{d}x'$$

with the so-called Empirical Distribution Function (EDF)

$$S(x) = \frac{\text{number of observations with}}{\text{total number of observation}}$$

The test statistic is the maximum difference between the two functions:

$$D = \sup |F(x) - S(x)|$$

One can also test whether two one-dimensional sets of points are compatible with coming from the same parent distribution.

Kolmogorov–Smirnov Test (2)

Expected distribution of D known (Kolmogorov distribution) for given $N \rightarrow p$ -value

 $D^* = \sqrt{N}D$, N = number of data points

Example: Test whether data x_i come from standard normal distribution N(0,1):

from scipy import stats D, $p_value =$ stats.kstest(x, stats.norm.cdf)

Kolmogorov–Smirnov test: only for 1d data

Two-Sample x² Test

Test hypothesis that two binned data sets come from the same underlying distribution.

Two histograms with *k* bins

Number of entries in bin *i*: n_i for measurement 1, m_i for measurement 2

$$\frac{(n_i-m_i)^2}{\sigma_{n_i}^2+\sigma_{m_i}^2}$$

Run test (Wald–Wolfowitz test) Drawback of the χ^2 test: insensitive to the sign of the deviation Consider N bins, $N = N_+ + N_ N_+$: number of positive deviations, N_- : number of negative deviations

++++=--+++++++++=-=- $N = N_+ + N_- = 22$ bins, 6 runs

Mean and variance for the number of runs for the null hypothesis that each assumption about prob. for "+" and "-"):

$$\mu = 1 + rac{2 N_+ N_-}{N}, \qquad \sigma^2 = rac{2 N_+ N_- (2 N_+ N_- - N)}{N^2 (N - 1)} = rac{(\mu - 1)(\mu - 2)}{N - 1}$$

For more than about 20 bins the Gaussian approximation holds and the value in units of the standard deviation is:

Run test is complementary to the χ^2 square test (can be done in addition)

- run = consecutive bins where the data show deviations in the same direction
- element in the sequence is independently drawn from the same distribution (no

significance of the deviation of an observed number *r* of runs from the expected $Z = \frac{r - \mu}{r - \mu}$ σ

p-value for a straight line fit

Constant model ($y = \theta_0$) rejected by small p-value

 χ^2 min = 2.29557, n_{df} = 3:

p-value = 0.51337

from scipy import stats pvalue = 1 - stats.chi2.cdf(chi2, n_dof)

root [1] TMath::Prob(chi2, n_dof)

 χ^2 min = 18.3964, $n_{df} = 4$:

p-value = 0.001032

 $\theta_0 = 2.86 \pm 0.18$

Statistical uncertainty of the fit parameter does not tell us whether model is correct!

p-value for different χ^2_{min} and n_{df}

Wilks' theorem

Let null hypothesis H_0 be a special case of the hypothesis H_1 ("nested hypotheses")

Example: $H_0: f(m) = a_0 + a_1 m$ H_1 : $f(m) = a_0 + a_1m + a_2m^2 + a_3m^3$

Define:

Wilks' theorem: If H_0 is correct then $\Delta \tilde{\chi}^2$ follows χ^2 distribution with $n_{dof} = \#$ added parameters in the large sample limit.

In the above example: $n_{dof} = 2$

Samuel S. Wilks, The Large-Sample Distribution of the Likelihood Ratio for Testing Composite Hypotheses Ann. Math. Statist., Volume 9, Number 1 (1938), 60-62.

$$\ln\left(\frac{L(H_1)}{L(H_0)}\right)$$

Significance of a peak

$$H_0: f(m) = a_0 + a_1 m$$

$$H_1: f(m) = a_0 + a_1 m + a_2 N(m; \mu, \sigma)$$

 $\mu=3.1$, $\sigma=0.03$ fixed in H_1 → one additional parameter

$$\Delta \tilde{\chi}^2 = 2 \log \left(\frac{L(H_1)}{L(H_0)} \right) = 22.5$$

 $\Delta \tilde{\chi}^2$ should follow a χ^2 distribution with $n_{\rm dof} = 1$ if H_0 ist true

p-value = 2.15 \cdot 10⁻⁶

 \rightarrow H₀ can be safely rejected

Why bother with statistical methods?

Presentations by CMS and ATLAS, December 2015: https://indico.cern.ch/event/442432/

Statistics: Draw reliable conclusions from data

In case of doubt: just get more data ...

Yes, but not always easy ...

A heavy Higgs boson?

Peak disappeared with more data ... [<u>link</u>]

A look at other research fields

"Why Most Published Research Findings Are False":

Main thesis: large number, if not the majority, of published medical research papers contain results that cannot be replicated.

Reproducibility crisis:

Affects the social sciences and life sciences most severely (in particular psychology)

Is there a reproducibility crisis? [Nature 533, 2016]

Why Most Published Research Findings Are False John P. A. Ioannidis

blished research findings are metimes refuted by subsequent. evidence, with ensuing confusion and disappointment. Relutation and controversy is seen across the range of esearch designs, from clinical trials and traditional epidemiological studies [1-3] to the most modern molecular research [4,5]. There is increasing oncern that in modern research, false findings may be the majority or even the vast majority of published research ciaims [6-8]. However, this should not be surprising. It can be proven that most claimed research findings are false. Here I will examine the key

The Essay section contains opinion pieces on topics of broad intervet to a general medical audience.

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actors that influence this problem and ome corollaries thereof.

Modeling the Framework for False **Positive Findings**

Several methodologists have sointed out [9-11] that the high rate of nonreplication flack of confirmation) of research discoveris is a consequence of the convenient, ret ill-founded strategy of claiming conclusive research findings solely or the basis of a single study assessed by ormal statistical significance, typically or a p-value less than 0.05. Research is not most appropriately represented and summarized by p-values, but, infortunately, there is a widespread iotion that medical research articles

it can be proven that most claimed research findings are false.

should be interpreted based only on values. Research findings are defined here as any relationship reaching ormal statistical significance, e.g., ffective interventions, informative redictors, risk factors, or association legative" research is also very useful Negative" is actually a misnomer, and the misinterpretation is widespread. However, here we will target relationships that investigators claim exist, rather than null findings.

As has been shown previously, the srobability that a research finding is indeed true depends on the prior probability of it being true (before foing the study), the statistical powe of the study, and the level of statistics significance [10,11]. Consider a 2×2 table in which research findings are compared against the gold standard of true relationships in a scientific field. In a research field both true and false hypotheses can be made about the presence of relationships. Let R be the ratio of the number of "true relationships" to "no relationships ong those tested in the field. R

is characteristic of the field and ca vary a lot depending on whether the field targets highly likely relationship or searches for only one or a few true relationships among thousand and millions of hypotheses that ma he postulated. Let us also conside for computational simplicity reumscribed fields where either then is only one true relationship (among many that can be hypothesized) or the power is similar to find any of the several existing true relationships. Th pre-study probability of a relationship being true is R/(R + 1). The probabil of a study finding a true relationship effects the power 1 - B (one stinu the Type II error rate). The probabili of claiming a relationship when none truly exists reflects the Type I error rate, o. Assuming that crelationship are being probed in the field, the expected values of the 2 × 2 table as ven in Table 1. After a research nding has been claimed based or chieving formal statistical significance he post-study probability that it is true s the positive predictive value, PPV. The PPV is also the complementar obability of what Wacholder et al tave called the false positive repos robability [10]. According to the 2 2 table, one gets $PPV = (1 - \beta)R/(N$ βR + α). A research finding is thus

Citation: learnich JPA (2005) Why most publisher research findings are false PLoS Med 20(: e124.

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Wereviation: NV/ positive predictive val

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01:101171/journal.pmod.000010

August 2005 | Volume 2 | Issue 8 | e124

Yes, a significant crisis

John Ioannidis (Stanford School of Medicine) PLoS Med 2(8): e124., (2005), doi:10.1371/journal.pmed.0020124

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p-value hacking

p-values and Higgs measurement: Expected local *p*-values for a Higgs of a given mass

For each assumed Higgs mass (\rightarrow local *p*-value)

- Calculate expected signal for Standard Model Higgs boson
- Determine *p*-value for H_0 that only SM background processes contribute
- Pure calculation/simulation, no data involved

p-values and Higgs measurement: Observed local *p*-values

"An excess of events is observed above the expected background, with a local significance of 5.0 standard deviations, at a mass near 125 GeV, signaling the production of a new particle. The expected significance for a standard model Higgs boson of that mass is 5.8 standard deviations."

Look-elsewhere effect

CMS Higgs paper

- specified mass range the global *p*-value.
- Local *p*-value corresponds to 5σ
- Global *p*-value for mass range 110–145 GeV corresponds to 4.5σ

In general:

- after *n* tests
- stringent threshold for larger *n*)

A Swedish study in 1992 tried to determine whether or not power lines caused some kind of poor health effects. The researchers surveyed everyone living within 300 meters of high-voltage power lines over a 25-year period and looked for statistically significant increases in rates of over 800 ailments. The study found that the incidence of childhood leukemia was four times higher among those that lived closest to the power lines, and it spurred calls to action by the Swedish government. The problem with the conclusion, however, was that they failed to compensate for the look-elsewhere effect; in any collection of 800 random samples, it is likely that at least one will be at least 3 standard deviations above the expected value, by chance alone. Subsequent studies failed to show any links between power lines and childhood leukemia, neither in causation nor even in correlation.

https://en.wikipedia.org/wiki/Look-elsewhere_effect

The probability for a background fluctuation to be at least as large as the observed maximum excess is termed the local *p*-value, and that for an excess anywhere in a

If one is performing multiple tests then obviously a p-value of 1/n is likely to occur

Solution: "trials penalty" or "trials factors", i.e. make threshold a function of n (more

Digression: *p*-value debate

Null hypothesis ("no effect") rejected and results deemed statistically significant if p-value < 0.05

Relatively weak statistical standard, but often not realized as such

Chance for false positive outcome 1/20

- Might result in too many false positive results in the literature
- Social and biomedical sciences in the focus of the discussion

Problem exacerbated by *p*-value hacking

Data gathered by researches without first creating a hypothesis

Probably contributes to reproducibility crisis in science Proposed solution: lower threshold to p-value < 0.005

<u>www.nature.com/articles/s41562-017-0189-z</u>)

https://www.nature.com/news/big-names-in-statistics-want-to-shake-up-much-maligned-p-value-1.22375

- Search for patterns in the data that can be reported as statistically significant

https://psyarxiv.com/mky9j (published in Nature Human Behavior, https://

Bayesian hypothesis testing

We can write

thus

$$p(H_0 | \vec{d}) = \frac{p}{p(\vec{d} | H_0) p}$$

$$p(H_1 \mid \vec{d}) = \frac{1}{p(\vec{d} \mid E)}$$

The factor $\frac{p(\vec{d} \mid H_1)}{\vec{J}}$ is *independent* of the prior! It tells us how the ratio of the probabilities $p(\vec{d} \mid H_0)$ changes. This is called the Bayes factor.

- It is also the likelihood ratio

 $\frac{p(\vec{d} \mid H_0) p(H_0)}{p(H_0)}$, but also $p(H_0) + p(\vec{d} \mid H_1) p(H_1)$ $\frac{p(\vec{d} \mid H_1) p(H_1)}{H_0 p(H_0) + p(\vec{d} \mid H_1) p(H_1)}$

$$\frac{f_1(p(H_1))}{f_0(p(H_0))} = \frac{p(\vec{d} \mid H_1)}{p(\vec{d} \mid H_0)} \frac{p(H_1)}{p(H_0)}$$

Provides an objective result from Bayesian analysis (when no free parameters are present)

Bayesian hypothesis testing (2)

- We know the $\Delta \chi^2 = 48.5$
- Thus the Bayes factor ratio is \rightarrow

$$\frac{p(d \mid H_1)}{p(\vec{d} \mid H_0)} = \exp\left(-\frac{48.5}{2}\right) \approx 3 \cdot 10^{-11}$$

- So whatever our priors are, the data pushes the posteriors very much towards H_0
- There is no choice of statistic in Bayesian statistics, just Bayes' theorem
- When the models have free parameters, they need to be marginalised out first
 - Then the Bayes factor depends on the prior of the parameters

Why 5σ for discovery in particle physics? $5\sigma \Leftrightarrow p$ -value = 2.87 × 10⁻⁷ (one-tailed test) History: there are many cases of 3σ and 4σ effects that have disappeared with more data

The Look-Elsewhere Effect

Systematics:

- Usually more difficult to estimate than statistical uncertainties
- "Safety margin"

Subconscious Bayes factor:

- $p(H_1|\text{data})$
- H_1 .
- "Extraordinary claims require extraordinary evidence"

Last point \Rightarrow unreasonable to have a single criterion (5 σ) for all experiments

Louis Lyons, Statistical Issues in Searches for New Physics, arXiv:1409.1903

> Physicists subconsciously tend to assess the Bayesian probabilities $p(H_0|$ data) and

If H_1 involves something very unexpected (e.g., neutrinos travel faster than the speed of light) then prior probability for null hypothesis H_0 is much larger than for

