DISCOVERING THE SIGNIFICANCE OF $5\sigma$

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ABSTRACT

We discuss the traditional criterion for discovery of requiring a significance corresponding to $5\sigma$; and whether a more nuanced criterion might be better.

1 Introduction

It has become the convention in Particle Physics that in order to claim a discovery of some form of New Physics, the chance of just the background having a statistical fluctuation at least as large as the observed effect is equivalent to the area beyond $5\sigma$ in one tail of a normalised Gaussian distribution, or smaller; i.e. the $p$-value is no larger than $3 \times 10^{-7}$. Indeed, journals are very reluctant to allow the word ‘discovery’ to appear in the title, abstract or conclusions of a paper, unless the $p$-value is that small. In this short note, we list the arguments for and against this attitude.

2 Why $5\sigma$?

Statisticians who hear about the $5\sigma$ criterion are very skeptical about it being sensible. In particular, they claim that it is very uncommon that statistical probability distributions accurately describe reality so far out in the tails. Particle Physics does differ from other fields in that we do believe that in many situations the numbers of observed events do follow a Poisson distribution, and so small tail probabilities may well be meaningful. However, certainly as far as systematic effects are concerned, even in Particle Physics there is often a degree of subjectivity in specifying the exact magnitude of the effect, let alone believing in its assumed distribution far into the tails of the observed effect. Thus the Statisticians’ criticism may well be valid.

The traditional arguments for the $5\sigma$ criterion are:

- History:
  In the past there have been many ‘phenomena’ that corresponded to 3 or $4\sigma$ effects that have gone away when more data were collected. The $5\sigma$
criterion is designed to reduce the number of such false claims. However, it may well be worth checking whether the fraction of false claims at the $5\sigma$ level is indeed smaller than at $4\sigma$.

- **Look Elsewhere Effect (LEE):**

The significance of an interesting peak in a mass spectrum is defined in terms of the probability of a background fluctuation producing an effect at least as large as the one actually seen. If the background fluctuation is required to be at the observed mass, this probability is called the local $p$-value. If, however, the restriction on the location of the background fluctuation is removed, this is instead the global $p$-value, and is larger than the local one because of the LEE.

Ambiguity in the global $p$-value arises because of the choice of requirements that are imposed on the location of the background fluctuation. Possibilities include (a) any reasonable mass; (b) anywhere in the current analysis; (c) anywhere in analyses by members of the experimental Collaboration; etc. In addition to the local $p$-value, it is desirable to quote at least the global one corresponding to option (a). It is clearly important to decide in advance of the analysis what procedure will be used; and to specify in any publication exactly how the global $p$-values are defined.

- **Subconscious Bayes’ Factor:**

When searching for a discovery, the data statistic that is used to discriminate between just background (known as the null hypothesis $H_0$) and ‘background plus signal’ ($H_1$) is often the likelihood ratio $L_1/L_0$ for the two hypotheses; and the $5\sigma$ criterion is applied to the observed value of this ratio, as compared with its expected distribution assuming just background. However, more relevant to the discovery claim is the ratio of probabilities for the two hypotheses. These are related by Bayes Theorem:

$$\frac{P(H_1|data)}{P(H_0|data)} = \frac{p(data|H_1)}{p(data|H_0)} \times \frac{\pi_1}{\pi_0}$$

(1)

where $p(data|H_i)$ and $\pi_i$ are respectively the likelihood and the prior probability for hypothesis $H_i$; and $P(H_i|data)$ is the hypothesis’ posterior probability. So the ratio of probabilities we assign to the hypotheses is their likelihood ratio times their prior probability ratio. Hence, in this approach, even if the likelihood ratio favours $H_1$, we would still prefer $H_0$ if our prior belief in $H_1$ was very low. An example would be that, in order to claim that we had discovered energy non-conservation in proton-proton collisions at the LHC, we would require extremely strong evidence from the data because our prior belief in energy non-conservation is very low. Similarly, if an experiment seemed to show that neutrinos travel faster than light, we might well have a tendency to believe that there was

\footnote{If the width and/or shape of the possible signal are regarded as free parameters, they also contribute to the LEE factor.}
some undiscovered systematic, rather than that neutrinos were a potential source for violating causality.

The above argument is clearly a Bayesian application of Bayes Theorem, while analyses in Particle Physics usually have a more frequentist flavour. Nevertheless, this type of reasoning does and should play a role in requiring a high standard of evidence before we reject well-established theories. There is sense to the oft-quoted maxim ‘Extraordinary claims require extraordinary evidence’.

• Systematics:
  It is in general more difficult to estimate systematic uncertainties than statistical ones. Thus a $n\sigma$ effect in an analysis where the statistical errors are dominant may be more convincing that one where the $n\sigma$ claim is dominated by systematics errors. Thus in the latter case, a $5\sigma$ claim should be reduced to merely $2.5\sigma$ if the systematic uncertainties had been underestimated by a factor of 2; this corresponds to the $p$-value increasing from $3 \times 10^{-7}$ by a dramatic factor of $2 \times 10^4$. The current $5\sigma$ criterion is partially motivated by a cautious approach to somewhat vague estimates of systematic uncertainties.

  Bob Cousins has recommended that for systematic-dominated analyses, it is desirable to assess by how much the systematics must be increased in order to reduce a significance above $5\sigma$ to that level; and then deciding whether this level of systematic effect is plausible or not.

3 Why not $5\sigma$?

There are several reasons why it is not sensible to use a uniform criterion of $5\sigma$ for all searches for new physics. These include most of the features that we included as supporting the use of the $5\sigma$ criterion.

3.1 LEE

This can vary enormously from search to search. Some experiments are specifically designed to measure one parameter, which is sensitive to new physics, while others use general purpose detectors which can produce a whole range of potentially interesting results, and hence have a larger danger of a statistical fluctuation somewhere in the background. An example of an experiment with an enormous LEE is the search for gravitational waves; these can have a variety of different signatures, occur at any time and with a wide range of frequencies, durations, etc.

  It is illogical to penalise a single-measurement analysis simply because others have a significant LEE.
Table 1: Summary of some searches for new phenomena, with suggested numerical values for the number of σ that might be appropriate for claiming a discovery.

| Search                        | Degree of surprise | Impact       | LEE   | Systematics | Number of σ |
|-------------------------------|--------------------|--------------|-------|-------------|-------------|
| Higgs search                  | Medium             | Very high    | Mass  | Medium      | 5           |
| Single top                    | No                 | Low          | No    | No          | 3           |
| SUSY                          | Yes                | Very high    | Very large | Yes        | 7           |
| $B_s$ oscillations            | Medium/low         | Medium       | $\Delta m$ | No        | 4           |
| Neutrino oscillations         | Medium             | High         | $\sin^2(2\theta), \Delta m^2$ | No | 4           |
| $B_s \rightarrow \mu\mu$      | No                 | Low/Medium   | No    | Medium      | 3           |
| Pentaquark                    | Yes                | High/very high | M, decay mode | Medium   | 7           |
| $(g - 2)_{\mu}$ anomaly       | Yes                | High         | No    | Yes         | 4           |
| H spin $\neq 0$               | Yes                | High         | No    | Medium      | 5           |
| $4^{th}$ generation $q, l, \nu$ | Yes               | High         | M, mode | No        | 6           |
| $\nu, \chi > c$              | Enormous           | Enormous     | No    | Yes         | $\geq 8$    |
| Dark matter (direct)          | Medium             | High         | Medium | Yes        | 5           |
| Dark energy                   | Yes                | Very high    | Strength | Yes | 5           |
| Grav waves                    | No                 | High         | Enormous | Yes | 7           |

3.2 Subconscious Bayes’ Factor

Some experiments search for effects which may be very weak but which are predicted to occur in the Standard Model (S.M.), while others may be very speculative (e.g., neutrinos travelling faster than the speed of light; search for mini-Black Holes at the LHC;…..). Clearly, it is unreasonable to require the same level of significance for both types of search.

3.3 Systematics

Some experiments are very sensitive to systematics, while in others it plays a minor role. Thus attempts to discover substructure of quarks by looking at dijet events produced in quark-quark scattering at high energy hadron colliders are dependent on the parton distribution functions (pdf’s) for the initial state beam hadrons. An over-optimistic estimate of the accuracy of pdf’s in the relevant kinematic region can then result in a significant-looking signature of quark substructure, but which would be much less significant when more realistic pdf uncertainties are allowed for.

It is far better to have a procedure which allows in some way for uncertain systematics than to raise the significance level for all experiments as a way of coping with this.
3.4 Summary of some experimental searches

Table 1 provides a summary of some experimental searches for new physics. The topics listed all correspond to searches that have actually been performed; some of these have resulted in actual discoveries, others have made claims which have subsequently been withdrawn, while others have set limits on the sought-for effect. The remarks in the Table, however, are not related to any specific experiment, but are supposed to be more generic. The final column contains a set of suggestions for the significance level required, after making some attempt to correct for the LEE, before a discovery could be claimed. The spirit of these numbers is to provoke discussion of this issue (rather than being a rigid set of rules), by suggesting a graded set of significance levels for different types of experiments.

We briefly contrast the various effects that are important for some of the searches in Table 1:

- \((g - 2)_\mu\):
  This experiment, designed to measure the anomalous magnetic moment of the muon, basically determines just this quantity, and so there is essentially no LEE. Almost by definition, if there is no physics beyond the S.M., the experimental value should agree with the S.M. prediction, so any significant deviation would be an indication of new physics.

- Single top:
  The top quark was discovered in \(t\bar{t}\) pair production in proton-antiproton collisions at the Tevatron. The S.M. also predicts a somewhat smaller production rate for single top-quark production. This was searched for, and also found. Since the mass of the top quark was known from the pair-production discovery mode, there was no LEE due to unknown mass here. Also, the Subconscious Bayes Factor here actually favours single top production, since it is predicted by the S.M., and indeed it would be very surprising if it were not produced or was highly suppressed. Thus this seems to be a good case where \(5\sigma\) should not have been a requirement before confirmation of this production mode was accepted.

- Higgs boson:
  Even before the discovery of a Higgs boson at CERN’s LHC, it was widely expected to exist (although it would not have been completely a surprise if it did not). Thus a discovery claim was not a surprise, but because of its very important role in giving mass to the other elementary particles, its impact was large. The LEE was due to the unpredicted Higgs mass, but there were no further factors from the various possible decay modes, whose branching ratios were predicted by the S.M.

- Supersymmetry (SUSY):
  It would have been very satisfying if SUSY had reduced the number of fundamental particles by pairing each known fermion with a known boson.
This did not happen, and so SUSY has essentially doubled the number of basic particles, by hypothesising SUSY partners for each known particle. Thus there are many different types of SUSY particles to search for and so, combined with a variety of possible masses and decay modes, there is a large SUSY LEE factor. Combined with the high impact of discovering a whole new sector of fundamental particles, the level of significance for a SUSY discovery claim should be high.

- Mini-black holes:

  There have been suggestions that mini-Black Holes could perhaps be produced in the high energy proton-proton collisions at the LHC. These are highly speculative particles, with a large LEE factor arising from their unknown mass and decay modes. A high standard of significance should be required for a claim of their discovery.

3.5 Jeffreys-Lindley Paradox

A criticism of a fixed level of $p$-value for discovery comes from the Jeffreys-Lindley (J-L) paradox[1]. Basically, this draws attention to the way a fixed significance level for discovery does not cope with a situation where the amount of data is increasing. An example involves testing a simple hypothesis $H_0$ (e.g. a Gaussian centred at $\mu = 0$) against a composite one (e.g. $\mu > 0$). It turns out that for a wide variety of priors for $\mu$, the Bayesian posterior probabilities for the hypotheses can favour $H_0$, while the frequentist $p$-value can reject $H_0$.

A simplified version of this effect is illustrated in Table 2; this uses simple hypotheses for both $H_0$ and $H_1$, and does not require priors. This example involves a counting experiment where in the first run 10 events are observed, when the null hypothesis $H_0$ predicts 1.0 and the alternative $H_1$ predicts 10.0; both the $p$-value for the null hypotheses ($p_0$) and the likelihood ratio disfavour $H_0$. Then the running time is increased by a factor of 10, so that the expected numbers according to $H_0$ and $H_1$ both increase by a factor of 10, to 10.0 and 100.0 respectively. With 31 observed events, $p_0$ corresponds to about $5\sigma$ as in the first run; but despite this the likelihood ratio now strongly favours $H_0$. This is simply because the $5\sigma$ $n_{\text{obs}} = 10$ in the first run was exactly the expected value for $H_1$, but with much more data the $5\sigma$ $n_{\text{obs}} = 31$ is way below the $H_1$ expectation. This example thus shows that for a fixed $p$-value such as $3 \times 10^{-7}$ the likelihood-ratio can favour either hypothesis.

The conclusion from the J-L paradox is that the $p_0$ cut used to reject $H_0$ should decrease with increasing amount of data. However, there appears to be no obvious way of implementing this, and Particle Physics tends to use fixed levels of cuts, independent of the data size.

A discussion of the J-L Paradox in its application to Particle Physics will be found in ref. [2].
First data set | Second data set
--- | ---
$H_0$ Poisson, $\mu = 1.0$ | Poisson, $\mu = 10.0$
$H_1$ Poisson, $\mu = 10.0$ | Poisson, $\mu = 100.0$

$\begin{array}{|c|c|}
\hline
n_{obs} & 10 & 31 \\
\hline
p_0 & 1.1 \times 10^{-7} & 0.8 \times 10^{-7} \\
 & 5.2\sigma & 5.3\sigma \\
\hline
L_0/L_1 & 8 \times 10^{-7} & 1.2 \times 10^{-16} \\
 & \text{Strongly favours } H_1 & \text{Strongly favours } H_0 \\
\hline
\end{array}$

Table 2: Comparing $p$-values and likelihood ratios

4 Conclusions

It would be very useful if we could distance ourselves from the attitude of ‘Require 5$\sigma$ for all discovery claims’. This is far too blunt a tool for dealing with issues such as the Look Elsewhere Effect, the plausibility of the searched-for effect, the role of systematics, etc., which vary so much from experiment to experiment. The problem is to produce an agreed alternative. Table 1 is an attempt to stimulate discussion about a graded set of significance levels for different types of experiments.

A possibility would be to replace the significance hurdle, which results in a binary output, by simply quoting the observed local and where relevant global $p$-values. This would make the distinction between 4.9$\sigma$ and 5.0$\sigma$ much less crucial, and it would also show up the difference between 5.0$\sigma$ and 8.0$\sigma$. Unfortunately, however, this may not be acceptable, as the general feeling may well be to maintain emphasis on a fixed criterion to answer the question ‘Is this a discovery or not?’

I wish to thank members of the Statistics Committees of the CMS and CDF Collaborations (especially Bob Cousins and Tom Junk respectively) for enlightening and useful discussions on this and many other statistical issues; and my colleagues on these experiments for asking many thought-provoking questions.

References

[1] H. Jeffreys, ‘Theory of Probability’, Oxford University Press (1939); D. V. Lindley, ‘A Statistical Paradox’, Biometrika 44 (1957) 187.

[2] R. Cousins, ‘Can high energy physicists learn something useful from the Jeffreys-Lindley paradox?’, Banff Workshop (2010), [http://people.stat.sfu.ca/~lockhart/richard/banff2010/cousins.pdf](http://people.stat.sfu.ca/~lockhart/richard/banff2010/cousins.pdf) and preprint in preparation.

Yes we achieved the necessary significance level to claim a discovery or ‘Oh dear, we missed it’.