Exclusion regions and their power.

L. Fleysher,1 R. Fleysher,1 T. J. Haines,2 A. I. Mincer,1 and P. Nemethy1

1Department of Physics, New York University, New York, New York 10003
2Los Alamos National Laboratory, Los Alamos, New Mexico 87545

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The question of exclusion region construction in new phenomenon searches has been causing considerable discussions for many years and yet no clear mathematical definition of the problem has been stated so far. In this paper we formulate the problem in mathematical terms and propose a solution to the problem within the framework of statistical tests. The proposed solution avoids problems of the currently used procedures.

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I. INTRODUCTION

When existence of a new phenomenon is proposed an experiment is designed which exploits the differences between the adopted (old) and the new theories to check if there is evidence to reject the old theory in favor of the new one. It is this difference which provides the signal in the experiment. If such a signal is found, a discovery is claimed and the values of the parameters of the new theory are measured. If, on the other hand, no evidence contradicting the old theory is found, it is desirable to set a constraint on the possible values of the parameters of the new theory. The logic behind this is simple: if the values of the parameters of the new theory were inside a certain region of the parameter space, the experiment would have found evidence against the old theory in favor of the new one. Since no evidence is actually found, such a region is called the exclusion region.

Traditionally, the exclusion regions on the parameters of a theory are constructed based on the upper boundary of a classical one-sided confidence interval. Often, the exclusion regions constructed by one experiment rule out signals reported by the others (see, for instance, CDMS[1] and DAMA[2] or LSND[3] and KARMEN[4]). Therefore, the task of confidence interval construction receives considerable attention and is a subject of many controversies (see, for instance, discussions in[5,6]). There are, however, serious problems associated with the use of confidence intervals for exclusion region construction which are often overlooked. Indeed, one of the pre-requisites of the theory of statistical estimation based on the classical theory of probabilities[10] is the knowledge that the observed data have arisen from the phenomenon being observed. In other words, it is supposed that there is no question whether the observed data x were drawn from the probability distribution p1(x; µ);

it is known for a fact and an attempt is being made to quantify the value of the parameter µ by constructing a one-sided confidence interval.

Hence, it is immediately seen that the classical theory of estimation is not applicable to the situations when it is not known that the phenomenon exists. The application of the theory to such problems may lead to intervals which do not have the desired confidence level. Another problem is that a confidence interval constructed in such a way may exclude values of the parameter µ for which the experiment is insensitive (see, for instance, discussions in[5,6]).

Thus, the dissatisfaction with the classical theory of estimation is not due to imperfections in the theory but is caused by misuse of the theory and by lack of mathematical clarity in problems solutions of which are sought within the framework of the classical estimation theory. Yet, it is desirable to be able to construct exclusion regions objectively without the use of subjective priors.

In this work we formulate the question of what can be stated regarding the parameter µ of the hypothesis H1(µ) of presence of the new phenomenon when the hypothesis H0 of absence of the new phenomenon is not rejected based on the outcome of the experiment. We also propose a solution to this problem formulated within the framework of hypothesis test formalism. In addition, we propose a clear definition of the sensitivity of a detector.

II. STATEMENT OF THE PROBLEM AND ITS SOLUTION

Consider an experiment searching for a new phenomenon where a decision of plausibility of existence of the new phenomenon is made with the help of a statistical test[11]. In such a test, the hypothesis tested (the null hypothesis H0) is the adopted (old) theory with the alternative hypothesis H1 that the observed data is due to the new phenomenon. Each of the hypotheses defines a probability distribution of obtaining every possible outcome x of the experiment p0(x) and p1(x) respectively. The test is set up so that if the observed data lie within some critical region wc, the null hypothesis is rejected and is not rejected otherwise[11].
The error leading to an unjust rejection of the null hypothesis is called the error of the first kind and is denoted by \( \alpha \). It is a common practice to construct the test in such a way as to guarantee that the error does not exceed a preset value \( \alpha_c \) called the level of significance. The power of the test \((1 - \beta)\) is defined as the probability of rejecting the null hypothesis when the alternative is true. In other words:

\[
\alpha_c \geq \int_{w_c} p_0(x)dx \quad (1 - \beta) = \int_{w_c} p_1(x)dx
\]

Example

Suppose that the observable \( X \) is distributed according to the Gaussian distribution with zero mean and known dispersion \( \sigma^2 \) if the new phenomenon does not exist. If, however, the new phenomenon exists, the same observable \( X \) is distributed according to Gaussian with the same dispersion but positive mean \( \mu \). Thus, the hypotheses of the origin of the observed data \( x \) are:

\[
p_0 = \frac{1}{\sqrt{2\pi\sigma^2}} e^{-x^2/2\sigma^2} \quad p_1 = \frac{1}{\sqrt{2\pi\sigma^2}} e^{-(x-\mu)^2/2\sigma^2} \quad \mu > 0
\]

The best critical region is defined as \( x \geq x_c \). That is, if the observed data point \( x \) is greater than \( x_c \), the null hypothesis of absence of the new phenomenon is rejected. Thus, in the proposed test significance and power are:

\[
\alpha_c = \frac{1}{\sqrt{2\pi\sigma^2}} \int_{x_c}^{\infty} e^{-x^2/2\sigma^2} dx
\]

\[
(1 - \beta) = \frac{1}{\sqrt{2\pi\sigma^2}} \int_{x_c}^{\infty} e^{-(x-\mu)^2/2\sigma^2} dx
\]

The level of significance is often selected at \( \alpha_c = 1.35 \cdot 10^{-3} \) which corresponds to \( x_c = 3\sigma \) in this example.

Suppose further that the value of the parameter \( \mu \) of the alternative hypothesis is large (say \( \mu = 5\sigma \)) and the alternative hypothesis is true. Since the existence of the new phenomenon is reported only if \( x > x_c \) is observed, the presence of the new phenomenon will be established with probability \((1 - \beta) = 0.997\). If the alternative hypothesis is true, but the value of the parameter \( \mu \) is small (say \( \mu = 1\sigma \)) the existence of the new phenomenon will be established only in 0.023 cases. Thus, it is hopeless to look for the new phenomenon using the constructed test if the value of \( \mu \) is small.

The general problem which is being addressed in this paper is the following. Given a critical region \( w_c \) constructed for a test of a null hypothesis \( H_0 \) with respect to a composite alternative hypothesis \( H_1(\mu) \) with unknown value of \( \mu \), what kind of restriction can be set on admissible values of \( \mu \) if, based on the outcome of the test, the null hypothesis is not rejected. Intuitively, one would state that the values of the parameter \( \mu \) of the alternative hypothesis for which the null hypothesis can not be rejected reliably should not be excluded based on the non-rejection of the null hypothesis.

To formulate this intuitive notion in mathematical terms it should be realized that the composite hypothesis \( H_1(\mu) \) can be considered as a set of simple hypotheses \( H_1(\mu) \) corresponding to different fixed values of \( \mu \) which can be classified by the power of the test:

\[
(1 - \beta(\mu)) = \int_{w_c} p_1(x; \mu) dx
\]

If the constructed test has low power with respect to the simple alternative hypothesis \( H_1(\mu) \), it is not a surprise that no evidence against the null hypothesis is found. Therefore, if the null hypothesis is not rejected, the admissible values of the parameter \( \mu \) for which the power of the test is small should not be excluded based on the outcome of the experiment.

If however, the constructed test has a high power with respect to the simple alternative hypothesis \( H_1(\mu) \) and no evidence against the null hypothesis is found, it may be concluded that the admissible values of the parameter \( \mu \) for which the power of the test is higher than critical value \((1 - \beta_c)\) can be ruled out as unlikely. The critical value \((1 - \beta_c)\) of the power of the test is motivated by the problem at hand and should be selected at 90% or higher. The value \( \mu^c \) of the parameter \( \mu \) corresponding to the smallest acceptable power of the test \((1 - \beta_c)\) at significance \( \alpha_c \) is the demarcation point (or demarcation hypersurface if \( \mu \) is multi-dimensional) between the allowed and excluded regions of values of the parameter \( \mu \). In the example considered above, the demarcation point corresponding to the power \((1 - \beta_c) = 0.9\) at significance of \( \alpha_c = 1.35 \cdot 10^{-3} \) is \( \mu^c = 4.3\sigma \). The values of \( \mu \) greater than \( \mu^c \) should be considered as unlikely when the null hypothesis is not rejected.

Based on the preceding discussion, it is seen that it is the power of the test which needs to be maximized when constructing experiments. There are several ways to achieve this. One way to increase the power is to set a less stringent level of significance (decrease \( x_c \) in the example considered) which comes at a price of increased probability to falsely claim a discovery. The other, perhaps more desirable way to increase the power is by fundamental modification of the experimental setup. Such modification can be made keeping the significance level intact but may increase the operation cost. Examples of this approach are increased observation time or sample size. In the example considered here, the decrease in the dispersion \( \sigma^2 \) will increase the efficacy of the experiment with respect to weak signals keeping the significance level intact.
III. EXPERIMENT SENSITIVITY

Another question which needs to be addressed is that of sensitivity of an experiment and what it means. Even though sensitivity is usually interpreted as the signal strength which a detector is able to detect, this statement lacks definiteness because the detection is a statistical process. Due to statistical fluctuations a strong signal might be missed and a weak signal might be detected. Thus, the question of sensitivity of the experiment has to be addressed within the framework of statistical tests as well. Therefore, the question is: given a critical region $w_c$ constructed for a test of a null hypothesis $H_0$ what is the efficacy of the test with respect to a set of simple alternative hypotheses $H_1(\mu)$.

The answer, once again, can be found in terms of significance and power. It is reasonable to request that any apparatus to be constructed should have a chance of signal detection of 50% or more with given level of significance. That is why it is proposed to quote the sensitivity of a detector as such signal level that would provide at least 50% power of the test at the specified level of significance and should not be regarded as “absolute” 100% detection level. In the example considered above, the sensitivity of the experiment is $\mu = 3\sigma$ with significance $1.35 \cdot 10^{-3}$.

At this point it is important to note that two identical experiments looking at identical signal at their sensitivity level may provide drastically different outcomes. One of the experiments may get lucky and state a discovery of the other one; there is no contradiction between the two. In order to confirm or refute a signal detected by an experiment at its sensitivity level, it is required to conduct a new test which would have appreciable (90% or more) power with respect to the claimed signal strength with pre-specified significance. Returning to the considered example, to confirm the discovery made on this experiment a new test would have to be built with the new dispersion $\sigma_{new}^2 = 0.48\sigma_{old}^2$ with the same significance of $1.35 \cdot 10^{-3}$.

IV. POISSON PROCESS WITH KNOWN BACKGROUND

The case of tremendous practical importance is when the number $n$ of observed events is distributed according to the Poisson distribution

$$p(n; \mu) = \frac{\mu^n}{n!} e^{-\mu}$$

The experiment searching for a new phenomenon may be a subject to background so that

$$p_0(n; \mu_b) = \frac{\mu_b^n}{n!} e^{-\mu_b}$$

$${p_1(n; \mu_b + \mu_s) = \frac{(\mu_b + \mu_s)^n}{n!} e^{-(\mu_b + \mu_s)}}$$

$${=- p_0(n; \mu_b) + \frac{\mu_s^n}{n!} e^{-\mu_s} + \sum_{n=0}^{\infty} \frac{\mu_s^n}{n!} e^{-\mu_s} \left( \frac{\mu_b^n}{(n-m)!} e^{-\mu_b} \right)$$

FIG. 1: Signal with average strength $\mu_s \geq \mu_c$ can be detected with corresponding probabilities of at least 50% 90% and 99% at significance $1.35 \cdot 10^{-3}$ in the presence of known average background $\mu_b$.

FIG. 2: The upper end $\mu_c^+$ of the 99% confidence level interval for $\mu_s$ from tables VIII, IX [5] can be anywhere between the dashed and dotted lines. If the confidence interval were used to construct the exclusion region, the signals inside the region which are below the solid line could be detected with probability less than 99% at significance $1.35 \cdot 10^{-3}$.

where $\mu_b \geq 0$ is the average background rate and $\mu_s > 0$.

If the average background rate $\mu_b$ is known, the best critical region against the stated alternative is constructed by

$$n \geq n_c \quad \alpha_c \geq \sum_{k=n_c}^{\infty} P_0(k, \mu_b) = P_0(n_c, \mu_b)$$

where $P(x, n)$ is complementary regularized incomplete gamma function.

Thus, if no evidence against the null hypothesis is found, the demarcation point $\mu^c_c$ on the values of $\mu_s$ corresponding to the power $(1 - \beta_c)$ at significance $\alpha_c$ can be constructed by finding the value of $\mu^c_c$ such that:

$$(1 - \beta_c) = \sum_{k=n_c}^{\infty} p_1(k, \mu_b + \mu^c_c) = P(n_c, \mu_b + \mu^c_c)$$

Figure 3 illustrates the situation for the significance of $1.35 \cdot 10^{-3}$ and different requested powers of the test.
It can be seen that even with zero average background events expected, the signal can be reliably detected (with 99% probability) only if its average rate is above \( \mu_s \geq 4.61 \). The surprisingly high value of the signal is due to the discrete nature of the Poisson distribution.

It might be interesting to visualize what would happen if the 99% confidence interval \([0; \mu_s^u]\) proposed in [5] were used for the exclusion region construction. Because the interval depends on the number of observed events, the boundary \( \mu_s^u \) may be anywhere between the dashed and dotted lines on the figure. (The dotted line corresponds to the most confining interval when zero events is observed while the dashed line represents the longest confidence interval obtainable with the left boundary fixed to zero. The figure is produced from the tables VIII and IX from [5].) The values above the boundary \( \mu_s^u \) would be excluded with confidence of 99%. It is seen that signals inside the exclusion region constructed based on the 99% confidence interval which are below the solid line will be detected with probability much smaller than 99% at significance 1.35 \( \cdot \) 10\(^{-3}\).

V. CONCLUSION

In this report we have considered a problem of what can be stated regarding the parameter \( \mu \) of alternative hypothesis \( H_1(\mu) \) of presence of a new phenomenon when no evidence against the null hypothesis \( H_0 \) of absence of the new phenomenon is found. We have proposed a mathematical formulation of this problem and its solution within the framework of hypothesis tests theory [11]. We have also given reasons why the classical theory of estimation [10] is not applicable in situations when the origin of data is questioned.

Nevertheless, we recommend to continue to report the classical confidence intervals assuming that the sought for new phenomenon exists for at least two reasons. First, the confidence intervals constructed now may be validated by a future experiment which will discover the existence of the new phenomenon. Second, the classical confidence interval provides information to future experiments about what the value of the parameter might be.

However, we propose to discontinue the use of the classical confidence intervals for construction of exclusion regions when no evidence against the hypothesis of absence of the new phenomenon is found. Instead, we propose to construct the exclusion regions based on the power of the test, since if the undiscovered process existed with the parameter inside the exclusion region it would have been discovered with probability \((1 - \beta_\alpha)\) or higher at significance \( \alpha \). Other attractive features of the constructed exclusion region are that less powerful experiments will produce less confining exclusion regions, the exclusion regions do not shrink if the number of observed events is less than the average expected background; the procedure for exclusion region construction avoids problems at physical boundaries on the parameter values and does not exclude the values of the parameter for which the experiment is insensitive. Also, the procedure of the exclusion region construction outlined in this paper resolves the illusory contradiction between the opposite results of two independent observations made at the sensitivity level of a detector.

It is proposed to call the detector sensitive if at the specified level of significance at least 50% power of the test can be achieved.

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