

# Statistical Evaluation of Experimental Determinations of Neutrino Mass Hierarchy

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Statistical methods of presenting experimental results in constraining the neutrino mass hierarchy (MH) are discussed. Two problems are considered and are related to each other: how to report the findings for observed experimental data, and how to evaluate the ability of a future experiment to determine the neutrino mass hierarchy, namely, sensitivity of the experiment. For the first problem where experimental data have already been observed, the classical statistical analysis involves constructing confidence intervals for the parameter  $\Delta m_{32}^2$ . These intervals are deduced from the parent distribution of the estimation of  $\Delta m_{32}^2$  based on experimental data. Due to existing experimental constraints on  $|\Delta m_{32}^2|$ , the estimation of  $\Delta m_{32}^2$  is better approximated by a Bernoulli distribution (a Binomial distribution with 1 trial) rather than a Gaussian distribution. Therefore, the Feldman-Cousins approach needs to be used instead of the Gaussian approximation in constructing confidence intervals. Furthermore, as a result of the definition of confidence intervals, even if it is correctly constructed, its confidence level does not directly reflect how much one hypothesis of the MH is supported by the data rather than the other hypothesis. We thus describe a Bayesian approach that quantifies the evidence provided by the observed experimental data through the (posterior) probability that either one hypothesis of MH is true. This Bayesian presentation of observed experimental results is then used to develop several metrics to assess the sensitivity of future experiments. Illustrations are made using a simple example with a confined parameter space, which approximates the MH determination problem with experimental constraints on the  $|\Delta m_{32}^2|$ .

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## I. INTRODUCTION

Neutrino mass hierarchy (MH), i.e. whether the mass of the third generation neutrino ( $\nu_3$  mass eigenstate) is greater or less than the masses of the first and the second generation neutrinos ( $\nu_1$  and  $\nu_2$ ), is one of the main questions to be answered in the standard model. Besides its fundamental importance to neutrino oscillation physics, the resolution of the neutrino MH plays an important role for the search of neutrinoless double-beta decay, which would determine whether neutrino is a Dirac or Majorana fermion. With the recent discovery of a large value of  $\sin^2 2\theta_{13}$  from Daya Bay [1], T2K [2], MINOS [3], Double Chooz [4], and RENO [5], the stage for addressing the neutrino MH has been set. It became one of the major goals of current and next generation long baseline neutrino experiments (T2K [6], NO $\nu$ A [7] and LBNE [8]) and atmospheric neutrino experiments (Super-K [9], MINOS [10], and INO [11]). Meanwhile, the idea of utilizing a reactor neutrino experiment to determine the MH is also intensively discussed [12–16].

The objective of this paper is to present appropriate ways to do statistical analysis that will help determine

the neutrino mass hierarchy. We start by introducing a few symbols and state the physics problem in terms of a pair of statistical hypotheses. Let  $m_1$ ,  $m_2$  and  $m_3$  denote the masses of the  $\nu_1$ ,  $\nu_2$  and  $\nu_3$  mass eigenstate neutrinos, and let  $\Delta m_{ij}^2 \equiv m_i^2 - m_j^2$  for  $i, j = 1, 2, 3$ . As reviewed in Ref. [17], it is known that  $\Delta m_{21}^2 > 0$  from measurements of solar neutrinos given the definition of mixing angle  $\theta_{12}$ . Whereas the sign of  $\Delta m_{32}^2$  is so far unknown, and it's common to use NH and IH to denote the two hypotheses, the normal hierarchy and the inverted hierarchy, respectively:

$$\begin{cases} \text{NH} : \Delta m_{32}^2 > 0 ; \\ \text{IH} : \Delta m_{32}^2 < 0 . \end{cases} \quad (1)$$

A unique feature to the above hypotheses testing problem is that, there are additional, rather strong information regarding the parameter  $\Delta m_{32}^2$  that need to be taken into account properly. Actually, based on previous experiments, a 68% confidence interval of  $M_{32}^2 \equiv |\Delta m_{32}^2|$  is given by  $(2.43 \pm 0.13) \times 10^{-3} \text{ eV}^2$  [18].

We will mainly address two aspects of the hypotheses testing problem. The first one concerns conducting a test after data has been collected. We discuss a classical testing procedure based on a  $\Delta\chi^2$  statistic (Eq. 3), or equivalently, the procedure of constructing confidence intervals by inverting the test. As a matter of fact, the classical procedure is derived upon the assumption that the best estimator of  $\Delta m_{32}^2$  based on experimental data would fol-

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low a distribution that is approximately Gaussian. But due to existing constraints on  $M_{32}^2$ , this assumption is far from being satisfied. Consequently, actual levels of the resulting confidence intervals may deviate substantially from their nominal levels, as we demonstrate in Sec. II. Instead, a general way to construct confidence intervals that are true to their nominal levels is the Feldman-Cousins approach [19], which we also illustrate in detail in Sec. II.

Still, there is a fundamental limitation to the use of confidence intervals. Note that in the MH determination problem, one of the most crucial questions is, what is the chance that the MH is indeed NH (or IH) given the observed experimental data? Classical confidence intervals are not meant to answer this question directly, whereas credible intervals reported by a Bayesian procedure is. In Sec. III, we present a Bayesian approach, which effortlessly incorporates prior information on  $M_{32}^2$  and output the easy-to-understand (posterior) probability of NH and IH to conclude the test. We will emphasize the importance to differentiate the Bayesian credible interval from the classical confidence interval.

The second aspect of the hypotheses testing problem that we address concerns assessment of experiments in their planning stage. It is critical to evaluate the ‘‘sensitivity’’ of a proposed experiment, i.e., its capability to distinguish NH and IH. Since this evaluation is performed before data collection, it has to be based on potential data from the experiment. An existing evaluation method (such as employed in [8, 20, 21]) assumes that the most typical data set under one hypothesis, say NH, happens to have been observed. Such a data set is referred to as the *Asimov data set* [22]. The method then calculates  $\overline{\Delta\chi^2}$ , which stands for the statistic  $\Delta\chi^2$  in Eq. 3, with the extra bar indicating its dependence on the Asimov data set. It can be seen that  $\overline{\Delta\chi^2}$  reflects how much the Asimov data set under NH disagrees with the alternative model, IH. It is then common practice to quantify the amount of disagreement by finding the p-value corresponding to  $\overline{\Delta\chi^2}$  after comparing it to the quantiles of a chi-square distribution with one degree of freedom (choice of MH). Finally, one minus this p-value is sometimes reported as a quantitative assessment of the experiment. We will show in Sec. II that the comparison of the value of  $\overline{\Delta\chi^2}$  to the quantiles of a chi-square distribution is not justified, when previous knowledge impose constraints on the range of possible values of the parameter  $\Delta m_{32}^2$ .

As an alternative solution, we adopt a Bayesian frame-

work and develop a set of new metrics for sensitivity to evaluate the potential of experiments to identify the correct hypothesis.

The paper is organized as follows. In Sec. II, we review the steps to construct classical confidence intervals for the parameter  $\Delta m_{32}^2$ . In Sec. III, we describe a Bayesian approach that reports the probability of each hypothesis of MH given observed data set. We further extend this Bayesian method to help assess the sensitivity for future experiments. In Sec. IV, we illustrate the Bayesian approach for a simplified version of the MH problem. In particular, analytical formula of the approximations for the probability of the hypotheses, and those for the sensitivity metrics are provided. Also, a numerical comparison is made between the  $\overline{\Delta\chi^2}$  based on the Asimov data set and the sensitivity metrics based on the Bayesian approach. Finally, discussions and a summary are presented in Sec. V and Sec. VI, respectively.

## II. ESTIMATION IN CONSTRAINED VERSUS UNCONSTRAINED PARAMETER SPACES

In this section, we review a classical statistical procedure of forming confidence intervals. For the problem of determining the neutrino mass hierarchy, we demonstrate that the procedure is valid in one scenario, but fails in another where known constraints on  $M_{32}^2$  are taken into consideration. In the latter case, the Feldman-Cousins method [19] based on Monte Carlo (MC) simulation is recommended to obtain valid confidence intervals.

Consider a spectrum that consists of  $n$  energy bins. Assume that the expected number of counts in each bin is a function of  $\Delta m_{32}^2$  and a nuisance parameter  $\eta$ . For simplicity, we denote  $\Delta m_{32}^2$  by  $\theta$ . Then for the  $i$ th bin, let  $\mu_i(\theta, \eta)$  and  $N_i$  represent the expected and the observed counts of neutrino induced reactions, respectively. When  $\mu_i$  is large enough, the distribution of  $N_i$  can be well approximated by a Gaussian distribution with mean  $\mu_i$  and standard deviation  $\sqrt{\mu_i}$ .

Once the data  $x = \{N_i, i = 1, \dots, n\}$  are observed, the deviations from the expected values  $\{\mu_i(\theta, \eta), i = 1, \dots, n\}$  are often calculated to help measure the implausibility of the parameter  $(\theta, \eta)$ . Specifically, when the systematic uncertainties are omitted, and that certain available knowledge concerning the parameters  $\theta$  and  $\eta$  are taken into consideration, one useful definition of the deviation is given by

$$\begin{aligned} \chi^2(\theta, \eta) &= \chi_{stat}^2(\theta, \eta) + \chi_p^2(|\theta|) + \chi_p^2(\eta) \\ &= \sum_i \frac{(N_i - \mu_i(\theta, \eta))^2}{(\delta N_i)^2} + \frac{(|\theta| - |\theta_0|)^2}{(\delta|\theta|)^2} + \frac{(\eta - \eta_0)^2}{(\delta\eta)^2}. \end{aligned} \quad (2)$$

Here, the general notation  $\delta w$  represents the standard

deviation of a variable  $w$ . So  $\delta N_i = \sqrt{\mu_i}$ , and the cor-

responding  $\chi_{stat}^2$  term is called the Pearson's chi-square. Also, note that  $|\theta| = M_{32}^2$ , and it is taken from [18] that  $|\theta_0| = 2.43 \times 10^{-3} \text{ eV}^2$  and  $\delta|\theta| = 0.13 \times 10^{-3} \text{ eV}^2$ .

Based on Eq. 2 and a standard procedure discussed in Ref. [18], confidence intervals can be obtained for the parameter of interest  $\theta$  ( $\Delta m_{32}^2$ ), the sign of which is an indicator of the neutrino MH. First, define  $\theta_{\min}$  to be the best fit to the data in the sense that  $(\theta_{\min}, \eta_{\min}) = \arg \min_{\theta, \eta} \chi^2(\theta, \eta)$  where the minimum is taken over  $\Theta \times H$ , the space of all possible values of  $(\theta, \eta)$ . Here, the general notation  $\arg \min_w h(w)$  denotes the value of  $w$  which corresponds to the minimum of the given function  $h$ . Note that  $\theta_{\min}$  suggested by the observed data set will not be exactly the true value of the parameter  $\theta$ , and a repetition of the experiment would yield a data set that corresponds to a different  $\theta_{\min}$ . So instead of reporting only  $\theta_{\min}$ , it is more rational to report a set of probable values of  $\theta$  that fit the observed data not too much worse than that of the best fit, and state how trust worthy the set is. Indeed, for any given  $\theta$ , let  $\eta_{\min}(\theta) = \arg \min_{\eta} \chi^2(\theta, \eta)$ , and define

$$\Delta\chi_{min}^2(\theta) \equiv \chi^2(\theta, \eta_{min}(\theta)) - \chi^2(\theta_{min}, \eta_{min}), \quad (3)$$

then a *level a confidence interval* based on Eq. 3 is defined to be

$$C_a = \{\theta \in \Theta : \Delta\chi_{min}^2(\theta) \leq t_a\}, \quad (4)$$

where we use the standard set-builder notation  $\{h(w) : \text{restriction } w\}$  to denote a set that is made up of all the points  $h(w)$  such that  $w$  satisfies the restriction to the right of the colon. The key in constructing Eq. 4 is to specify the correct threshold value  $t_a$  for a given confidence level  $a$ . (See the final paragraph of this section for a more detailed description of what confidence level means.) Most commonly examined confidence levels use  $a = 68.27\%(1\sigma)$ ,  $95.45\%(2\sigma)$ ,  $99.73\%(3\sigma)$ , which are often linked to threshold values  $t_a = 1, 4, 9$  respectively [18]. Note that these three values are the 68.27%, 95.45% and 99.73% quantiles of the chi-square distribution with one degree of freedom, respectively. They are used as threshold values because the parameter space  $\Theta$  is of dimension one and that, under certain regularity conditions,  $\Delta\chi_{min}^2(\theta)$  would follow approximately a chi-square distribution with one degree of freedom when  $\theta$  is the true parameter value. This procedure and its extensions to cases where  $\theta$  is of higher dimension have been successfully applied in many studies [8, 20, 21, 23–29] in order to constrain various parameters in the neutrino physics.

Although this procedure has been widely used in analyzing experimental data, note that it is not universally applicable. Its limitations has been addressed by Feldman and Cousins [19]. Below, we illustrate this point through a simple MC simulation study. It will be shown that, in a situation that is similar in nature to the MH determination problem in Eq. 1 where there exist special constraints on the possible values of  $\theta$ , the aforemen-

tioned threshold values based on chi-square approximation could result in bad confidence intervals. That is, the actual coverage probabilities of the intervals strongly disagree with their nominal levels.

In the simulation, we set  $n = 10$ ,  $\mu_i(\theta) = 1000 + 15 \cdot \theta$  for  $i = 1, \dots, n$ . (Here, no nuisance parameter  $\eta$  is introduced, and all the expected bin counts are assumed equal for simplicity. Nevertheless, these assumptions are not essential to the purpose of our simulation.) The following two cases are investigated:

- Case I:  $\Theta = (-\infty, \infty)$ ,
- Case II:  $\Theta = \{-1, 1\}$ .

Case I is a typical situation where nothing was known about  $\theta$  before the current experiment, whereas case II is designed to imitate the situation where existing measurements of  $|\theta| = M_{32}^2$  are very accurate at around  $2.43 \times 10^{-3} \text{ eV}^2$ , and we simply denoted this value to 1 for clarity of presentation. Further, the definition of deviation analogue to Eq. 2 is taken to be  $\chi^2(\theta) = \sum_i \frac{(N_i - \mu_i(\theta))^2}{\mu_i(\theta)}$  for case I. For case II, the chi-square definition is  $\chi^2(\theta) = \sum_i \frac{(N_i - \mu_i(\theta))^2}{\mu_i(\theta)} + \frac{(|\theta| - |\theta_0|)^2}{(\delta|\theta|)^2}$  with experimental constrains on  $|\theta|$ . It is then reduced to  $\chi^2(\theta) = \sum_i \frac{(N_i - \mu_i(\theta))^2}{\mu_i(\theta)}$  with  $\theta$  being only 1 or -1.

Under each case, we set the true value of  $\theta$  to be  $\theta_0 = 1$ , based on which 100,000 MC samples are simulated, denoted by  $\{N_1^{(j)}, \dots, N_{10}^{(j)}\}$  for  $j = 1, \dots, 100000$ . Then for the  $j$ th sample, confidence intervals of levels  $a = 68.27\%$ ,  $95.45\%$ ,  $99.73\%$  are constructed according to Eq. 4 using threshold values 1, 4, 9, respectively. Finally, at each of the three levels, we record the proportion of confidence intervals out of the 100,000 that include the truth  $\theta_0 = 1$ . The results are reported in the last three columns of Table I. It can be seen that, in case I, the actual coverage probabilities closely match the nominal levels. However, in case II, the actual coverage probabilities are always higher!

Without too much technical detail, we try to explain the reason why the chi-square procedure produced valid confidence intervals for case I, but not for case II. In general, having observed data  $x$  from a parametric model  $P(x|\theta)$ , a sensible test for a pair of hypotheses,  $H_0 : \theta \in \Theta_0$  and  $H_1 : \theta \in \Theta - \Theta_0$  (the counterpart of  $H_0$ ), is the likelihood ratio test that is based on the test statistic

$$\Delta\chi_{min}^2 \equiv -2\log\left(\frac{P(x|\theta_{0,\min})}{P(x|\theta_{\min})}\right), \quad (5)$$

where  $\theta_{0,\min} = \arg \min_{\{\theta \in \Theta_0\}} P(x|\theta)$ , and  $\theta_{\min} = \arg \min_{\{\theta \in \Theta\}} P(x|\theta)$  are the best fit over the null parameter set  $\Theta_0$  and the full parameter set  $\Theta$ , respectively. If the observed data  $x$  yields a large  $\Delta\chi_{min}^2$ , it means that  $\Theta_0$  is implausible, which further leads to the rejection of  $H_0$ . Note that, the statistic  $\Delta\chi_{min}^2(\theta)$  in Eq. 3 is a special case of Eq. 5 with  $\Theta_0$  consisting of a single point,  $\theta$ .

Case	$\Delta\chi_{min}^2(\theta_{true})$ distribution	$\theta_{min}$ distribution	distribution parameter within this example	$\Delta\chi_{min}^2 \leq 1$ confidence level	$\Delta\chi_{min}^2 \leq 4$ confidence level	$\Delta\chi_{min}^2 \leq 9$ confidence level
I	Chi-square	Gaussian	mean = 1 and $\sigma = 0.67$	68.27%	95.48%	99.73%
II	-	Bernoulli	$p = 0.0679$	95.12%	98.48%	99.86%

TABLE I: Confidence levels for various of  $\Delta\chi_{min}^2$  region for the Gaussian and the Bernoulli distribution from MC. In Case I, the mean and the standard deviation of the Gaussian distribution is found to be about 1 and  $\sigma = 0.67$  respectively. In Case II, the parameter  $p$  of the Bernoulli distribution (e.g. percentage of  $\theta_{min} < 0$ ) is found to be about 6.8%.

In order to determine the correct threshold values in rejecting, or equivalently, in constructing confidence intervals defined by Eq. 4, the distribution/quantiles of  $\Delta\chi_{min}^2(\theta_0)$  considering all possible data set needs to be known, when the true parameter value is some  $\theta_0 \in \Theta_0$ . An important result in statistics, Wilks Theorem [30, 31] states that, under certain regularity conditions,  $\Delta\chi_{min}^2(\theta_0)$  follows approximately a chi-square distribution with degree of freedom equal to the difference between the dimension of  $\Theta$  and that of  $\Theta_0$ , when the data size is large. (In our problem, the data size is simply  $\sum_i N_i$ .) The main regularity conditions are, as we quote [31], “the model is differentiable in  $\theta$  and that  $\Theta_0$  and  $\Theta$  are (locally) equal to linear spaces”. Essentially, such conditions imply that  $\theta_{min}$  follows an approximately Gaussian distribution centered at the true  $\theta$  value, which eventually implies an approximate chi-square distribution for  $\Delta\chi_{min}^2(\theta_0)$ .

In case I of our simulation, the best estimation of  $\theta$  can be calculated directly from the number of events in each bin:  $\theta_{min} = \frac{(\sum_{i=1}^{10} N_i)/10 - 1000}{15}$ . The aforementioned regularity conditions are satisfied in this case, and the distribution of  $\theta_{min}$  and that of  $\Delta\chi_{min}^2(\theta_0)$  follow the Gaussian and the chi-square distribution respectively as what Wilks theorem predicts. In the top two panels of Fig. 1, we reconfirm this fact by comparing their histograms based on the 100,000 MC samples (black shaded area) to the probability density function of the Gaussian and the chi-square distribution (blue long dash-dotted line). On the other hand, the full parameter space in case II consists of two isolated points and clearly violates the conditions required by Wilks theorem. Indeed, in case II, the best estimation of  $\theta$  is given by

$$\theta_{min} = \begin{cases} 1 & \text{if } \chi^2(\theta = 1) < \chi^2(\theta = -1) \\ -1 & \text{otherwise} \end{cases}$$

follows a Bernoulli distribution, and  $\Delta\chi_{min}^2(\theta_0)$  follows a distribution quite different from a canonical chi-square distribution. Approximations to the actual distributions of  $\Delta\chi_{min}^2(\theta_0)$  and  $\theta_{min}$  can be obtained from the 100,000 MC samples, and are shown (black shaded area) in the bottom two panels of Fig. 1. Further, an analytical approximation (red dash-dot-dotted line) to the distribution is derived in Appendix A. The analytical calculation implies that, independent of whether the truth  $\theta_0$  is 1 or

$-1$ , the p-value<sup>1</sup> corresponding to an observed value of  $\Delta\chi_{min}^2(\theta_0)$ , say  $t$ , is approximately given by

$$\text{p-value}(t) = P(\Delta\chi_{min}^2(\theta_0) \geq t) \approx \frac{1}{2} - \frac{1}{2} \text{erf} \left( \frac{t + \overline{\Delta\chi^2}}{\sqrt{8\overline{\Delta\chi^2}}} \right) \quad (6)$$

for any  $t > 0$ ; and the p-value is 1 for any  $t \leq 0$ . Here erf is the Gaussian error function:  $\text{erf}(x) = \frac{2}{\sqrt{\pi}} \int_0^x e^{-t^2} dt$ . (We use the general notation  $P(A)$  to denote the probability of an event  $A$ .)

The discussions above suggest that, when constructing confidence intervals in special cases where conditions of Wilks theorem do not hold (or that the user can not be sure if the conditions hold), the regular threshold values (such as  $t_\alpha = 1, 4, 9$  mentioned earlier) should not be taken for granted. Instead, alternative thresholds based on MC or case-specific analytical approximations are needed. We recommend using the MC method with a large MC sample size whenever possible, because unlike other methods, it is guaranteed to produce a valid confidence interval for  $\theta$ . We hereby review how to produce a valid  $1-\sigma$  (68.27%) confidence interval for  $\theta$  using the MC method [19]. This method can easily be generalized to build confidence intervals of any level.

- Having observed data  $x = \{N_1, \dots, N_n\}$ , apply the following procedure to every  $\theta$  in the parameter space  $\Theta$  (fix one  $\theta$  at a time):

1. Calculate  $\Delta\chi_{min}^2(\theta)^x$  with Eq. 3 based on the observed data.
2. Simulate a large number of MC samples, say  $\{x^{(j)}\}_{j=1}^T$ , where  $x^{(j)} = \{N_1^{(j)}, \dots, N_n^{(j)}\}$  is generated from the model with true parameter value  $\theta$ . For  $j = 1, \dots, T$ , calculate  $\Delta\chi_{min}^2(\theta)^{(j)}$ , that is Eq. 3 based on the  $j$ th MC sample  $x^{(j)}$ . This produces an empirical distribution of the statistic  $\Delta\chi_{min}^2(\theta)$ .

<sup>1</sup> The p-value at  $t$  is defined to be the percentage of potential measurements that result in the same or a more extreme value of the test statistic, say  $\Delta\chi_{min}^2$ , than  $t$ .

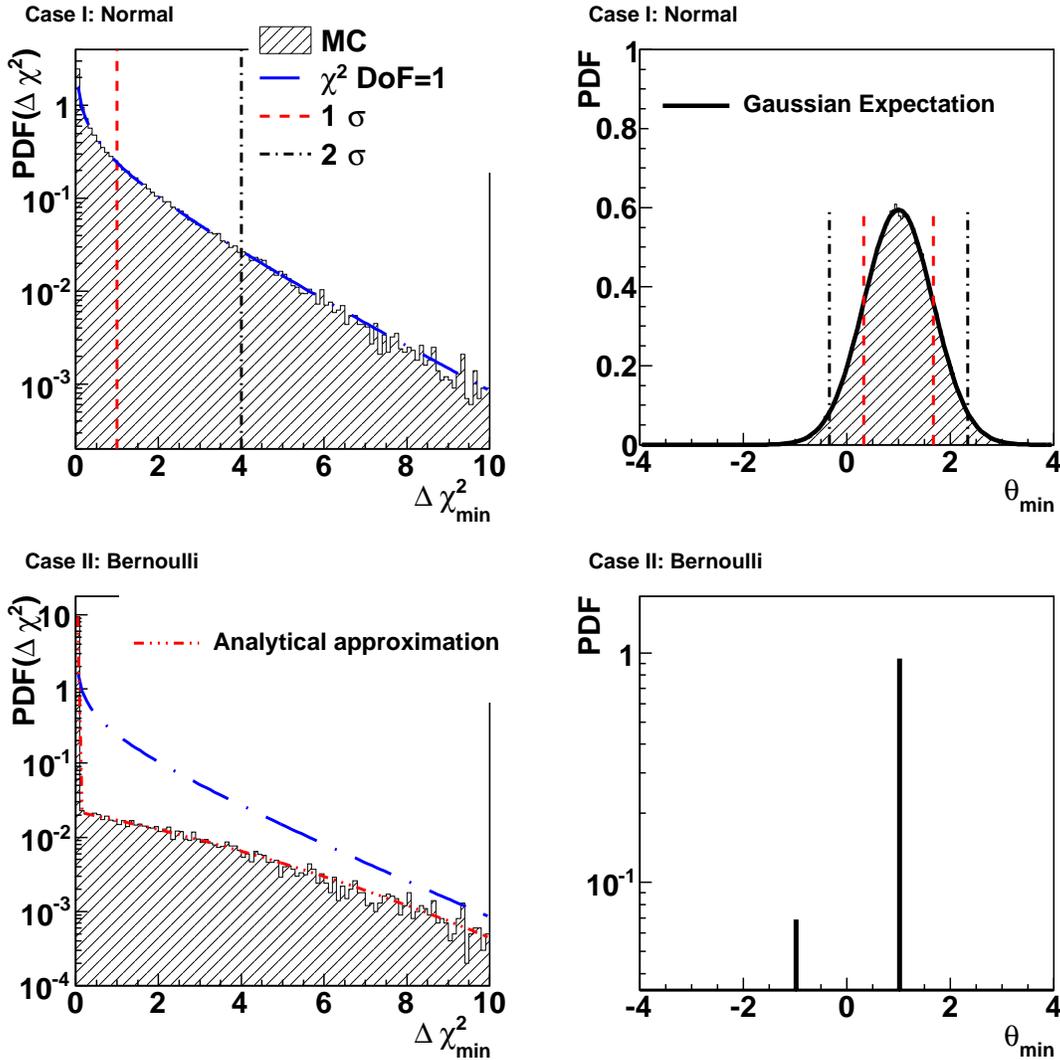


FIG. 1: (color online) Distributions of  $\Delta\chi_{min}^2(\theta)$  and  $\theta_{min}$  for case I and case II with 100,000 MC samples. The  $\theta_{min}$  distribution of case I (top right) and case II (bottom right) are a Gaussian and a Bernoulli distribution, respectively. The  $\Delta\chi_{min}^2(\theta)$  distribution of case I (top left) is consistent with the chi-square distribution with degree of freedom one. The commonly used  $1\sigma$ , (68.27% confidence level) and  $2\sigma$ , (95.45% confidence level) regions are labelled with red dashed and black dash-dotted lines for case I. The  $\Delta\chi_{min}^2(\theta)$  distribution of case II (bottom left) strongly deviates from the chi-square distribution. In case II, we also show the analytical approximation (derived in Appendix. A) of the distribution of  $\Delta\chi_{min}^2$ . We should emphasize while chi-square distribution does not depend on any additional parameter (other than  $\Delta\chi_{min}^2$ ), the analytical approximation depends on  $\overline{\Delta\chi^2}$ .

3. Calculate the percentage of MC samples such that  $\Delta\chi_{min}^2(\theta)^{(j)} < \Delta\chi_{min}^2(\theta)^x$ . Then  $\theta$  is included in the  $1\text{-}\sigma$  confidence interval if and only if the percentage is smaller than 68.27%.

One can easily check that p-values analytically obtained from Eq. 6 for case II (basically the MC method) are consistent with the simulation results listed in Table I.

On a separate issue that was also emphasized in Ref. [19], classical confidence intervals should not be confused with Bayesian credible intervals. On one hand, the **confidence-level** of a confidence interval, say  $a$ , is

an evaluation of this interval estimation procedure based on many **potential** repetitions of the experiment. More specifically, had the experiment been independently repeated 100 times, applying the estimation procedure to each would result in 100 intervals, and  $a$  represents the proportion of these intervals that we expect to contain the true value of the unknown parameter  $\theta$ . The level- $a$  confidence interval reported in practice is the result of applying such a procedure to the data observed in the current experiment. On the other hand, a Bayesian credible interval, say of **credible-level**  $b$ , is a region in the parameter space such that, given the **observed** data, it

contains the true value of the unknown parameter with probability  $b$ . In general, an  $a$ -level confidence interval does not coincide with an  $a$ -level Bayesian credible interval. In other words, if  $C_a$  is an  $a$ -level confidence interval built from the observed data  $x$ , then it is generally inappropriate to give the interpretation that  $P(\theta \in C_a|x)$  (the probability of true  $\theta$  inside  $C_a$  given data  $x$ ) is  $\alpha$ . Nevertheless, in Appendix B, we discuss when confidence intervals approximately match Bayesian credible intervals. In the next section, we present a Bayesian approach to the problem of determining neutrino mass hierarchy.

### III. A BAYESIAN APPROACH TO DETERMINE NEUTRINO MASS HIERARCHY

#### A. Bayesian inference based on observed data

The MH determination problem is concerned with comparing two competing models, NH and IH, having observed data  $x$ . The Bayesian approach to the problem is based on the probabilities that each model is true given  $x$ , namely,  $P(NH|x)$  and  $P(IH|x) = 1 - P(NH|x)$ . (In general, we adopt the notation  $P(A|B_1, \dots, B_n)$  to represent the probability of event  $A$  given events  $B_1, \dots, B_n$ . Also, we use capital letters such as  $S_1, \dots, S_n$  and  $T$  to denote random variables, and use small letters such as  $s_1, \dots, s_n$  and  $t$  to denote numbers inside the range of possible values of the random variables. Then  $P_{T|S_1, \dots, S_n}(t|s_1, \dots, s_n)$  denotes for the conditional probability density function (pdf) or the conditional probability mass function (pmf) given events  $S_1, \dots, S_n = s_1, \dots, s_n$ . The subscript to  $P$  is often omitted when it is clear what random variable is being considered.) Model NH will be preferred over IH if the odds  $r(x) = P(IH|x)/P(NH|x) < 1$ . Moreover, the size of  $r$  serves as an easy-to-understand measure for the amount of certainty of this preference. Alternatively, some people may feel more comfortable in interpreting  $P(NH|x) = 1/(1 + r(x))$  directly.

One can determine  $P(NH|x)$  and  $P(IH|x)$  within a Bayesian framework as follows. Let the true value of MH be either NH or IH, and let the counts  $N_i$  follow a Gaussian distribution with mean  $\mu_i^{\text{MH}}(\theta, \eta_{\text{MH}})$  and standard deviation  $\sqrt{\mu_i^{\text{MH}}(\theta, \eta_{\text{MH}})}$  for  $i = 1, \dots, n$ . Here,  $\theta$  is the parameter of interest, and  $\eta_{\text{MH}}$  denotes other unknown nuisance parameter(s). Here, a subscript accompanies  $\eta$  to emphasize that the nuisance parameter is allowed to have different interpretations and behavior under the two hypotheses. (We will omit this subscript whenever there is no possibility of confusion.) If prior knowledge is available for  $\theta$  and  $\eta$ , then they should be elicited to form prior distributions,  $P(\theta, \eta|MH)$  for MH=IH, NH. Sometimes, it is reasonable to assume that the parameters  $\theta$  and  $\eta$  are independent conditional on MH, hence  $P(\theta, \eta|MH) = P(\eta|MH)P(\theta|\eta, MH) = P(\eta|MH)P(\theta|MH)$ .

Specific to the MH problem at hand, under NH (IH), previous knowledge (e.g., from [18]) suggests that a sen-

sible prior for  $\theta$  would be a Gaussian with mean  $2.43 \times 10^{-3} \text{ eV}^2$  ( $-2.43 \times 10^{-3} \text{ eV}^2$ ) and standard deviation  $0.13 \times 10^{-3} \text{ eV}^2$ . Since the hypotheses being tested are NH :  $\theta \in \Theta_{\text{NH}} = (0, \infty)$  versus IH :  $\theta \in \Theta_{\text{IH}} = (-\infty, 0)$ ,  $P(\theta|NH)$  and  $P(\theta|IH)$  are specified to be the truncated version of the above Gaussian distributions supported within  $\Theta_{\text{NH}}$  and  $\Theta_{\text{IH}}$ , respectively. Nevertheless, in our Bayesian model,  $P(\theta \in \Theta_{\text{IH}}|NH)$  and  $P(\theta \in \Theta_{\text{NH}}|IH)$  based on the Gaussian prior are so tiny that they will yield the same numerical results as the truncated version. Similar choice can be made for  $P(\eta|MH)$ .

According to Bayes' theorem, we have

$$\begin{aligned} P(NH|x) &= \frac{P(x|NH) \cdot P(NH)}{P(x)} \\ &= \frac{P(x|NH) \cdot P(NH)}{P(x|NH) \cdot P(NH) + P(x|IH) \cdot P(IH)}. \end{aligned} \quad (7)$$

Here,  $P(NH)$  and  $P(IH) = 1 - P(NH)$  should reflect one's knowledge in NH and IH prior to the experiment. In the MH problem, it is reasonable to assume that NH and IH are equally likely, that is  $P(NH) = P(IH) = 50\%$ . We will make this assumption throughout the paper. Consequently, Eq. 7 reduces to

$$P(NH|x) = \frac{P(x|NH)}{P(x|NH) + P(x|IH)}. \quad (8)$$

Based on probability theory,  $P(x|MH)$ , i.e. the likelihood of model MH, is a "weighted average" of  $P(x|\theta, \eta, MH)$  over all possible values of  $(\theta, \eta)$ :

$$\begin{aligned} P(x|MH) &= \int_{H_{\text{MH}}} \int_{\Theta_{\text{MH}}} P(\eta|MH)P(\theta|\eta, MH)P(x|\theta, \eta, MH)d\theta d\eta, \end{aligned} \quad (9)$$

in which  $H_{\text{MH}}$  represents the phase space of nuisance parameter  $\eta$  given the choice of MH. Further, under the assumption that  $\theta$  and  $\eta$  are independent, Eq. 9 is reduced to:

$$\begin{aligned} P(x|MH) &= \int_{H_{\text{MH}}} \int_{\Theta_{\text{MH}}} P(\eta|MH)P(\theta|MH)P(x|\theta, \eta, MH)d\theta d\eta. \end{aligned} \quad (10)$$

In practice, the integral in Eq. 9 is often analytically intractable, but can be approximated using MC methods. Using a basic MC scheme, first, a large number of samples  $\{(\theta^{(j)}, \eta^{(j)}), j = 1, \dots, T\}$  are randomly generated from the prior distribution  $P(\theta, \eta|MH)$ . Then for the observed data  $x$ , obtain  $\hat{P}_T(x|MH) := T^{-1} \sum_{j=1}^T P(x|\theta^{(j)}, \eta^{(j)}, MH)$ . As the MC size  $T$  increases, the estimator  $\hat{P}_T(x|MH)$  will have probability approaching 1 of being arbitrarily close to the true  $P(x|MH)$ . Note that there exist much more efficient MC algorithms, such as importance sampling algorithms,

$\alpha$	0.475	1	1.281	1.645	2	3	4	5
one-sided p-value: $p_\alpha$	31.74%	15.87%	10%	5%	2.28%	0.13%	3.2e-5	3.0e-7
$\Delta\chi_{\alpha\sigma}^2$	1.53	3.33	4.39	5.89	7.52	13.29	20.70	30.04

TABLE II: Tabulated results of  $\Delta\chi_{\alpha\sigma}^2$ . For a given  $\alpha$ , the one-sided p-value is  $p_\alpha = P(Z \geq \alpha)$  (probability of  $Z \geq$  than  $\alpha$ ) where  $Z$  stands for a standard Gaussian random variable. The corresponding  $\Delta\chi^2$  value is given by  $\Delta\chi_{\alpha\sigma}^2 = -2 \log(p_\alpha/(1 - p_\alpha))$ .

that require smaller, more affordable  $n$  for the resulting estimators to achieve the same amount of accuracy as that of the basic MC scheme. Interesting readers are pointed to [32] for further details and references.

There also exist (relatively crude) approximations to  $P(x|MH)$  in Eq. 9 that avoid the intense computation in the MC approach. A most commonly used one is the one on which a popular model selection criteria, the Bayesian information criterion (BIC) is based. This approximation is often presented in terms of an approximation to a one-to-one transformation of  $P(x|NH)$ , namely

$$\Delta\chi^2(x) \equiv -2 \log r(x) = -2 \log (P(IH|x)/P(NH|x)). \quad (11)$$

Denote

$$\mathcal{T}_{MH}(x) \equiv -2 \log \left\{ \max_{\theta, \eta} P(x|\theta, \eta, MH) P(\eta|MH) P(\theta|MH) \right\},$$

where the maximum is taken over  $(\theta, \eta) \in \Theta_{MH} \times H_{MH}$  and

$$\Delta\mathcal{T}(x) \equiv \mathcal{T}_{IH}(x) - \mathcal{T}_{NH}(x). \quad (12)$$

Then if the sample size  $\sum_i N_i$  is large, and  $\eta_{NH}$  and  $\eta_{IH}$  are of the same dimension, then

$$\Delta\chi^2(x) = 2 \log P(x|NH) - 2 \log P(x|IH) \approx \Delta\mathcal{T}(x). \quad (13)$$

Here, the equality follows from Eq. 8 and the approximation is supported by a crude Taylor expansion around the maximum likelihood estimator for the parameters. There are other approximations that follow the same line, that are more accurate but also computationally more demanding. See [32] for details.

One remark should be made regarding  $\Delta\mathcal{T}$ , as it is closely related to a commonly used test statistic in the classical testing procedure. Indeed, if the truncated Gaussian priors mentioned earlier are assigned for  $\theta$  and a Gaussian prior with mean  $\eta_0$  and standard deviation  $\delta\eta$  is assigned for  $\eta$  under both NH and IH, then according to the definition of  $\chi^2$  in Eq. 2, we have

$$\delta\chi^2 \equiv \chi^2(\hat{\theta}', \hat{\eta}') - \chi^2(\hat{\theta}, \hat{\eta}) = \Delta\mathcal{T} - \sum_{i=1}^n \log \frac{\mu_i(\hat{\theta}', \hat{\eta}')}{\mu_i(\hat{\theta}, \hat{\eta})}, \quad (14)$$

where  $(\hat{\theta}, \hat{\eta})$  and  $(\hat{\theta}', \hat{\eta}')$  denote maximizers of

$$P(x|\theta, \eta, MH)P(\eta|MH)P(\theta|MH), \quad \text{MH}=\text{NH, IH.}$$

within their respective range. (Note that  $\delta\chi^2$  is essentially an alternative version of  $\Delta\chi_{\min}^2$  in Eq. 3, bearing some technical difference only.) Here, the term  $\sum_{i=1}^n \log \frac{\mu_i(\hat{\theta}', \hat{\eta}')}{\mu_i(\hat{\theta}, \hat{\eta})}$  is the result of the normalization factor (e.g.  $(2\pi\sigma^2)^{-\frac{1}{2}}$ ) of the Gaussian pdf, and is in general small compared to  $\Delta\mathcal{T}$ . In the classical testing procedure, the observed value of  $\delta\chi^2$  will be compared to its parent distribution to get a p-value. Whereas the Bayesian approach described in this section directly interprets the value of  $\Delta\mathcal{T}$ , by transforming it to either the odds ratio between NH and IH,  $r(x) = e^{-\Delta\chi^2(x)/2} \approx e^{-\Delta\mathcal{T}(x)/2}$ , or the probability of NH,

$$\begin{aligned} P(NH|x) &= \frac{1}{1 + r(x)} \\ &= \frac{1}{1 + e^{-\Delta\chi^2(x)/2}} \approx \frac{1}{1 + e^{-\Delta\mathcal{T}(x)/2}}, \end{aligned} \quad (15)$$

and similarly, the probability of IH,

$$\begin{aligned} P(IH|x) &= \frac{r(x)}{1 + r(x)} \\ &= \frac{e^{-\Delta\chi^2(x)/2}}{1 + e^{-\Delta\chi^2(x)/2}} \approx \frac{e^{-\Delta\mathcal{T}(x)/2}}{1 + e^{-\Delta\mathcal{T}(x)/2}}. \end{aligned} \quad (16)$$

## B. Sensitivity of experiments

So far, we described the Bayesian procedure for testing the two hypotheses, NH and IH, given observed data  $x = \{N_1, \dots, N_n\}$ . Reasoning backwards, foreseeing what analysis will be done after data collection allows us to address the question that, before data is collected from a proposed experiment, how confidently do we expect it to be able to distinguish the two hypotheses NH and IH. We loosely refer to such an ability as ‘‘sensitivity’’ of the experiment. There could be many ways to define sensitivity, and we list a few below. In practice, evaluating a proposed experiment using one or several of these sensitivity criteria provides views from different angles of the potential return from the experiment.

Note that sensitivity depends on the underlying true model as well as future experimental results generated from this model. For example, if NH is true, then we have a population of potential experimental results  $x \sim P(x|NH) = \int \int P(x|\theta, \eta, NH)P(\theta, \eta|NH)d\theta d\eta$ . And each potential  $x$  is associated with a posterior probability  $P(NH|x)$ . Then one could evaluate the ability of

an experiment to confirm NH when it is truly the underlying model by looking at the distribution of  $P(NH|x)$ . The most typical numerical summaries of this distribution include its mean, quantiles and tail probabilities, all of which can be used to address sensitivity. It is important to repeat such an evaluation procedure under the assumption that IH is the true model, because the sensitivity of an experiment for NH is not directly related that for IH.

Below we develop measures for sensitivity under the assumption that NH is true, knowing that they can be similarly defined when IH is true.

1. The average posterior probability of NH is given by

$$\begin{aligned} \bar{P}_{T=NH}^{NH} &= \int P(NH|x) P(x|NH) dx \\ &= \int_{-\infty}^{\infty} \frac{1}{1 + e^{-\Delta\chi^2/2}} P(x|NH) dx \\ &= \int_{-\infty}^{\infty} \frac{1}{1 + e^{-\Delta\chi^2/2}} P(\Delta\chi^2|NH) d\Delta\chi^2. \end{aligned} \quad (17)$$

Note that the first integral above involves calculating an  $N$ -dim integral, and the last one is of 1-dim only. The latter is much easier to obtain, an example of which will be presented in the next section.

Besides  $\bar{P}_{T=NH}^{NH}$ , one also needs to obtain  $\bar{P}_{T=IH}^{IH}$ , the average probability of IH if nature is indeed IH. Note that  $\bar{P}_{T=IH}^{IH}$  is the same as  $1 - \bar{P}_{T=NH}^{NH}$ , but is not directly related to  $\bar{P}_{T=NH}^{NH}$ , and hence must be obtained independently.

2. The fraction of measurements  $x$  that favor NH, i.e., the fraction of  $x$  such that  $P(NH|x) > .5$ , is given by

$$\begin{aligned} F_{T=NH} &= \int_{\{x:P(NH|x)>.5\}} P(x|NH) dx \\ &= \int_0^{\infty} P(\Delta\chi^2|NH) d\Delta\chi^2. \end{aligned} \quad (18)$$

Here, ‘‘F’’ and the subscript ‘‘ $T = NH$ ’’ stand for fraction and the NH assumption, respectively.

If NH is the correct hypothesis, then a good experiment should have a high probability of producing data that not only favors NH but indeed provides substantial evidence for NH. Hence, it is useful to generalize the term in Eq. 18 to gauge the chance of  $P(NH|x) > 1 - p$  for any threshold value  $1 - p$  of interest. In particular, physicists are familiar with thresholds associated with the so-called  $\alpha\sigma$  level, with one-sided  $\alpha\sigma$  corresponding to  $1 - p_\alpha = 1 - P(Z \geq \alpha)$  for a standard Gaussian

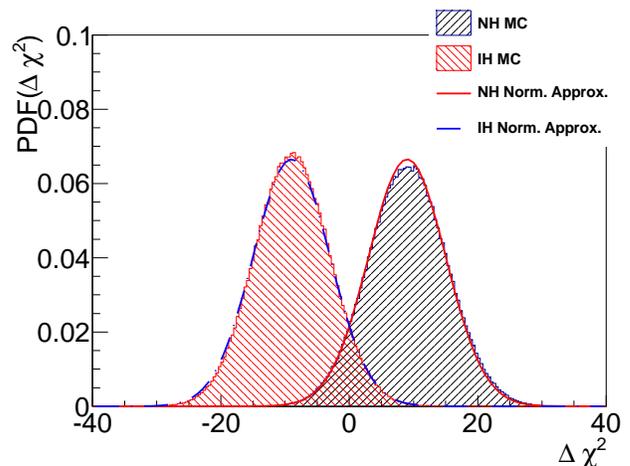


FIG. 2: (color online) The probability density functions  $P(\Delta\chi^2|NH)$  and  $P(\Delta\chi^2|IH)$  in the Bernoulli model are shown as the solid and dotted lines, respectively. The  $|\overline{\Delta\chi^2}|$  is assumed to be 9.

random variable  $Z$ <sup>2</sup>. Accordingly, define

$$\begin{aligned} F_{T=NH}^{\alpha\sigma} &= \int_{\{x:P(NH|x)>1-p_\alpha\}} P(x|NH) dx \\ &= \int_{\Delta\chi_{\alpha\sigma}^2}^{\infty} P(\Delta\chi^2|NH) d\Delta\chi^2. \end{aligned} \quad (19)$$

A list of common  $\alpha\sigma$  values, the corresponding  $p_\alpha$ , as well as  $\Delta\chi_{\alpha\sigma}^2 = -2 \log(p_\alpha/(1 - p_\alpha))$  are listed in Table. II.

3. In addition, probability intervals (PI) for  $P(NH|x)$  also provide useful information. For example, one can define  $P_{T=NH}^{90\%}$ , such that, had NH been the truth, 90% of the potential data would yield  $P(NH|\Delta\chi^2)$  larger than  $P_{T=NH}^{90\%}$ . And the interval  $(P_{T=NH}^{90\%}, 1)$  is referred to as a 90% probability interval.

In summary, all the above criteria reflect the capability of the experiment distinguish the two competing hypotheses, and they convey different messages.

In the next section, we use an example to show how one can easily calculate the posterior probability and the sensitivity measurements introduced above. We also contrast the resulting sensitivity measurements to a commonly used quantity that is known as ‘‘ $\Delta\chi^2$  of Asimov data set’’.

<sup>2</sup> Another commonly used term is two-sided  $\alpha\sigma$  which corresponds to  $1 - P(|Z| \geq \alpha)$ .

#### IV. ILLUSTRATION OF THE BAYESIAN APPROACH IN A CONSTRAINED PARAMETER SPACE

In this section, we consider a situation where  $\theta$  can only take on two possible values, 1 and  $-1$ , which correspond to the hypotheses NH and IH respectively. This simplified setting is motivated by the fact that existing measurements of  $|\theta| = M_{32}^2$  are very accurate at around  $2.43 \times 10^{-3} \text{ eV}^2$ , and we simply denote this value to 1 for clarity of presentation. It is a special case of the Bayesian treatment in the previous section, where  $P(\theta|NH)$  and  $P(\theta|IH)$  are assigned degenerate distributions at 1 and  $-1$  respectively. That is,  $P(\theta = 1|NH) = P(\theta = -1|IH) = 1$ . Further, there is no nuisance parameter  $\eta$ . As a result, the expected bin counts will be denoted by  $\mu_i^{NH} = \mu(1)$  and  $\mu_i^{IH} = \mu(-1)$  respectively.

Below, we showcase numerical calculations of various sensitivity criteria for this example. In particular, we introduce approximations that are simple functions of a term commonly known as “ $\overline{\Delta\chi^2}$  of Asimov data set” in the physics literature. According to the definition in Ref. [22], “the Asimov data set” under hypothesis MH is given by  $x^{MH} = (\mu_1^{MH}, \dots, \mu_N^{MH})$ , where  $\mu_i^{MH} = \mu_i(\theta_0^{MH}, \eta_0^{MH})$  and  $(\theta_0^{MH}, \eta_0^{MH}) = \arg \max_{(\theta, \eta)} P(\theta, \eta|MH)$  is the prior mode under MH. In words, the Asimov data set is the most typical data set under the most likely parameter values based on prior knowledge subject to the given model.

Interestingly,  $\overline{\Delta\chi^2}$  is itself often used as a measure of sensitivity. Here, we’ll contrast the typical usage of  $\overline{\Delta\chi^2}$  to that of the sensitivity criteria developed in the previous section. More accurate evaluations of these sensitivity criteria are also attainable via MC methods.

Suppose that the proposed experiment will collect enough data such that the expected counts under NH and IH are much larger than the difference between them:  $\mu_i^{NH} \sim \mu_i^{IH} \gg |\mu_i^{NH} - \mu_i^{IH}|$ . Using the notations introduced in Sec. II, if the nature is NH, then the observed counts  $N_i$  can be represented as

$$N_i = \mu_i^{NH} + \sqrt{\mu_i^{NH}} \cdot g_i, \quad (20)$$

where  $g_1, \dots, g_n$  are mutually independent standard Gaussian random variables. Then, the statistic  $\Delta\chi^2$  of Eq. 11 becomes

$$\begin{aligned} \Delta\chi_{T=NH}^2 &= \sum_{i=1}^n \frac{(\mu_i^{NH} - \mu_i^{IH})^2}{\mu_i^{IH}} \\ &+ \sum_{i=1}^n 2 \frac{(\mu_i^{NH} - \mu_i^{IH})}{\mu_i^{IH}} \sqrt{\mu_i^{NH}} g_i \\ &+ \sum_{i=1}^n \frac{\mu_i^{NH} - \mu_i^{IH}}{\mu_i^{IH}} g_i^2 \\ &- \sum_{i=1}^n \log\left(1 + \frac{\mu_i^{NH} - \mu_i^{IH}}{\mu_i^{IH}}\right). \end{aligned} \quad (21)$$

Here, the subscript  $T = NH$  indicates that nature is NH. Since  $\mu_i^{iH} \gg |\mu_i^{NH} - \mu_i^{IH}|$ , the summation of the last two terms in Eq. 21 is negligible as it is approximately  $\sum_{i=1}^n \frac{\mu_i^{NH} - \mu_i^{IH}}{\mu_i^{IH}} \cdot (g_i^2 - 1)$  by a Taylor expansion of the last term. Therefore,  $\Delta\chi_{T=NH}^2$  follows a Gaussian distribution, with mean and standard deviation:

$$\begin{cases} \overline{\Delta\chi^2} &\equiv \sum_{i=1}^n \frac{(\mu_i^{NH} - \mu_i^{IH})^2}{\mu_i^{IH}} \\ \sigma_{\Delta\chi^2} &\equiv 2\sqrt{\sum_{i=1}^n \frac{(\mu_i^{NH} - \mu_i^{IH})^2 \cdot \mu_i^{NH}}{(\mu_i^{IH})^2}} \\ &= 2\sqrt{\sum_{i=1}^n \left( \frac{(\mu_i^{NH} - \mu_i^{IH})^2}{\mu_i^{IH}} + \frac{(\mu_i^{NH} - \mu_i^{IH})^3}{(\mu_i^{IH})^2} \right)} \\ &\approx 2\sqrt{\overline{\Delta\chi_{NH}^2}} \end{cases} \quad (22)$$

In the last step, since  $\mu_i^{NH} - \mu_i^{IH} \ll \mu_i^{NH} \sim \mu_i^{IH}$ , we further neglect the term  $\frac{(\mu_i^{NH} - \mu_i^{IH})^3}{(\mu_i^{IH})^2}$ . Similarly, it is straightforward to show that when nature is IH,  $\Delta\chi_{T=IH}^2$  would follow an approximate Gaussian distribution with mean  $= -\overline{\Delta\chi^2}$  and standard deviation  $\sigma_{\Delta\chi^2}$ .

To see how the above approximation works, we look at the example in Sec. II, where  $\overline{\Delta\chi^2} \approx 9$ . Fig. 2 shows histograms (shaded area) based on large MC samples of  $\Delta\chi^2$  under NH and IH respectively. They agree very well with the analytical approximation (dashed lines) in Eq. 22.

Now, we are ready to calculate (1) the probability of a hypothesis post data collection, and (2) various measurements of sensitivity for an experiment concerning potential data generated from it.

First, given observed data  $x = (N_1, \dots, N_n)$ , the probability  $P(NH|x)$  can be directly calculated from Eq. 7.

Let  $G(t; m, \sigma) = \frac{1}{\sqrt{2\pi}\sigma} e^{-\frac{(t-m)^2}{2\sigma^2}}$  denote the pdf of a Gaussian random variable with mean  $m$  and standard deviation  $\sigma$ , evaluated at  $t$ , then

$$\begin{aligned} P(NH|x) &= \frac{P(x|NH) \cdot P(NH)}{P(x|NH) \cdot P(NH) + P(x|IH) \cdot P(IH)} \\ &= \frac{\prod_i G(N_i; \mu_i^{NH}, \sqrt{\mu_i^{NH}})}{\prod_i G(N_i; \mu_i^{NH}, \sqrt{\mu_i^{NH}}) + \prod_i G(N_i; \mu_i^{IH}, \sqrt{\mu_i^{IH}})} \\ &= \frac{1}{1 + e^{-\Delta\chi^2(x)/2}} \end{aligned}$$

where

$$\Delta\chi^2(x) = \sum_{i=1}^n \left[ \log \frac{\mu_i^{IH}}{\mu_i^{NH}} + \frac{(N_i - \mu_i^{IH})^2}{\mu_i^{IH}} - \frac{(N_i - \mu_i^{NH})^2}{\mu_i^{NH}} \right].$$

We mention that, if one reduces the full data  $x$  to its function  $\Delta\chi^2(x)$ , then calculating  $P(NH|\Delta\chi^2)$  based on our approximation in Eq. 22 will recover  $P(NH|x)$ :

$$\begin{aligned}
P(NH|\Delta\chi^2) &= \frac{P(\Delta\chi^2|NH) \cdot P(NH)}{P(\Delta\chi^2)} = \frac{P(\Delta\chi^2|NH)}{P(\Delta\chi^2|NH) + P(\Delta\chi^2|IH)} \\
&= \frac{G\left(\Delta\chi^2; \overline{\Delta\chi^2}, 2\sqrt{\overline{\Delta\chi^2}}\right)}{G\left(\Delta\chi^2; \overline{\Delta\chi^2}, 2\sqrt{\overline{\Delta\chi^2}}\right) + G\left(\Delta\chi^2; -\overline{\Delta\chi^2}, 2\sqrt{\overline{\Delta\chi^2}}\right)} = \frac{1}{1 + e^{-\Delta\chi^2/2}}. \tag{23}
\end{aligned}$$

Next, we evaluate various sensitivity metrics of a future experiment, using again the Gaussian distribution

for  $\Delta\chi^2$  in Eq. 22:

$$\overline{P}_{T=NH}^{NH} \approx \int_{-\infty}^{\infty} \frac{1}{1 + e^{-t/2}} G\left(t, \overline{\Delta\chi^2}, 2\sqrt{\overline{\Delta\chi^2}}\right) dt \equiv \overline{P}(\overline{\Delta\chi^2}), \tag{24}$$

$$F_{T=NH} \approx \int_0^{\infty} G\left(t; \overline{\Delta\chi^2}, 2\sqrt{\overline{\Delta\chi^2}}\right) dt = \frac{1}{2} \left( 1 + \operatorname{erf}\left(\sqrt{\frac{\overline{\Delta\chi^2}}{8}}\right) \right), \tag{25}$$

$$F_{T=NH}^{\alpha\sigma} \approx \int_{\Delta\chi_{\alpha\sigma}^2}^{\infty} G\left(t; \overline{\Delta\chi^2}, 2\sqrt{\overline{\Delta\chi^2}}\right) dt = \frac{1}{2} \left( 1 + \operatorname{erf}\left(\frac{\overline{\Delta\chi^2} - \Delta\chi_{\alpha\sigma}^2}{\sqrt{8\overline{\Delta\chi^2}}}\right) \right), \tag{26}$$

$$P_{T=NH}^A \approx 1 / \left( 1 + e^{-\frac{1}{2}(\overline{\Delta\chi^2} - 2z_A^* \sqrt{\overline{\Delta\chi^2}})} \right). \tag{27}$$

In the above,  $\overline{P}_{T=NH}^{NH}$  was approximated by  $\overline{P}(\overline{\Delta\chi^2})$ , which is a function of  $\overline{\Delta\chi^2}$  only. Also,  $z_A^*$  represents the  $A$  percentile of a standard Gaussian distribution. For example, In order to calculate the probability intervals (PI), one needs to find out the corresponding  $\Delta\chi_{PI}^2$  values as inputs of Eq. 15. In Table. III, we list the  $\Delta\chi_{PI}^2$  values for a few typical choices of probability intervals, assuming that nature is NH.

For the example experiment used in the simulation of section II, its  $\overline{\Delta\chi^2} = 9$ . Had one followed common practice that directly compares  $\sqrt{\overline{\Delta\chi^2}}$  to the quantiles of a Gaussian distribution, one would report the ‘‘specificity’’ of the experiment to be 99.87% (1 - ‘‘one-sided p-value’’). In contrast, we obtained various sensitivity metrics for the experiment according to Eq. 24-27, and listed them in Table IV. First, assuming the ‘‘Asimov data set’’ is observed, we have  $P(NH|x^{NH}) \approx P(IH|x^{IH}) \approx P(NH|\Delta\chi^2 = 9) = 98.90\%$ . Secondly, we calculated  $\overline{P}_{NH}^{NH} \approx \overline{P}_{IH}^{IH} \approx \overline{P}(\overline{\Delta\chi^2} = 9) = 90.14\%$ . That is, the average posterior probability for NH (or IH) when it is indeed the correct hypothesis is only about 90%, which is much lower than its Asimov counterpart of  $P(NH|\Delta\chi^2 = 9) = 98.90\%$ . Thirdly, the fraction  $F_{T=NH} = 93.32\%$  of potential data sets would yield a  $\Delta\chi^2$  that favors NH. And to contrast with the Gaussian

interpretation, we calculated that only  $F_{T=NH}^{3\sigma} = 23.73\%$  of potential data sets would yield a  $\Delta\chi^2$  above 9, or say, yield an evidence as strong as  $P(NH|x) \geq 99.87\%$ . Further, the left panel of Fig. 3 displays the distribution (vertical axis in log scale) of  $P(NH|x) = P(NH|\Delta\chi^2)$ . The two vertical dashed lines show that 68% of potential data sets will result in  $P(NH|x) > 95.67\%$ , whereas 90% of potential data sets will result in  $P(NH|x) > 65.79\%$ .

Moving forward from a fixed  $\overline{\Delta\chi^2}$  value, we next study how the various sensitivity metrics compare to each other for experiments with different  $\overline{\Delta\chi^2}$  values. The right panel of Fig. 3 displays the lower bound of the 90% probability interval  $P_{T=NH}^{90\%}$ , the average probability  $\overline{P}_{NH}^{NH}$ , and the Gaussian interpretation based on one-sided p-value as functions of  $\overline{\Delta\chi^2}$ . Note that we plotted 1 minus the aforementioned metrics in order to zoom in the high probability regions. Interestingly, the line of average probability  $\overline{P}$  yields a higher value than the lower bound of 90% P.I. for  $\overline{\Delta\chi^2} < \sim 18$ , and yields a lower value than the lower bound of 90% P.I. for  $\overline{\Delta\chi^2} > \sim 18$ . Such behavior is natural given the definition of each curve. Nevertheless, both curves are much higher than the Gaussian interpretation, suggesting that the Gaussian interpretation is over-optimistic in describing the ability of an experiment to differentiate NH and IH.

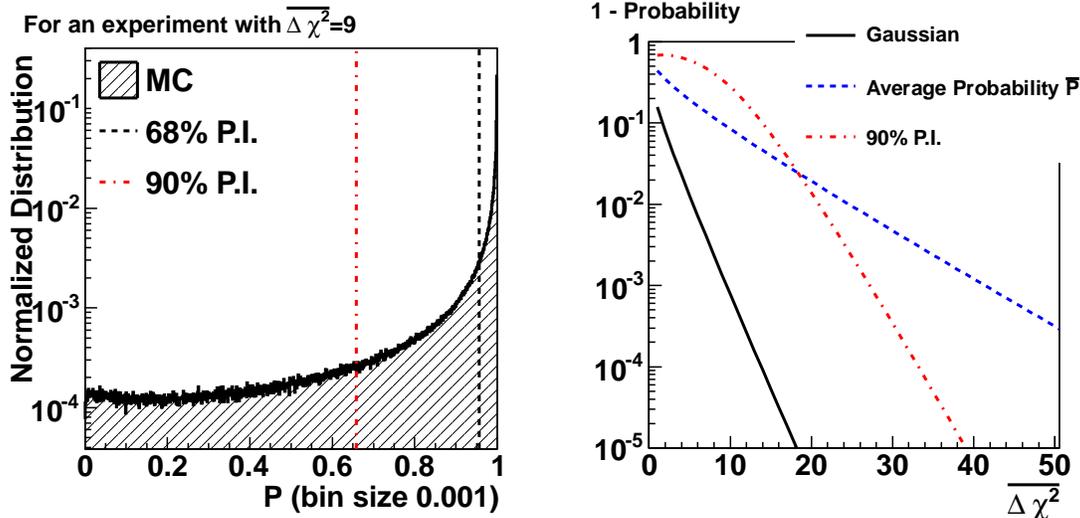


FIG. 3: (color online) The left panel shows the distribution of  $P(NH|x) = P(NH|\Delta\chi^2)$  over the population of potential data  $x$  that arises from an experiment with  $\overline{\Delta\chi^2} = 9$  where the truth is NH. The mean of this distribution is 90.14%. Lower bound of the 68% and 90% probability intervals are plotted. That is, 68% (90%) of the data  $x$  would yield a  $P(NH|x)$  that falls to the right of the dash-dotted (dashed) line. These two lines are also commonly referred as the 32 and the 10 percentile. The right panel plots several sensitivity metrics (subtracted from 1 for clarity), against  $\overline{\Delta\chi^2}$  that ranges from 1 to 50. Note that all the lines are decreasing because higher values of  $\overline{\Delta\chi^2}$  corresponds to more sensitive experiments. This is done for three different criteria: the Gaussian interpretation (derived from the one-sided p-value with one degree of freedom),  $\overline{P}$  and  $P_{T=NH}^{90\%}$ . The Gaussian interpretation is seen to be over-optimistic in describing the ability of the experiment to differentiate the two hypotheses.

Probability Intervals (PI)	68%	90%	95%	99%
$\Delta\chi_{PI}^2$	$\overline{\Delta\chi^2} - 0.936\sqrt{\overline{\Delta\chi^2}}$	$\overline{\Delta\chi^2} - 2.564\sqrt{\overline{\Delta\chi^2}}$	$\overline{\Delta\chi^2} - 3.29\sqrt{\overline{\Delta\chi^2}}$	$\overline{\Delta\chi^2} - 4.656\sqrt{\overline{\Delta\chi^2}}$

TABLE III: Tabulated  $\Delta\chi_{PI}^2$  values for a few typical choice of probability intervals, assuming that nature is NH.

## V. DISCUSSIONS

A couple of comments should be made regarding the  $\sqrt{\Delta\chi^2}$  representation for sensitivity in determining the MH.

1. We have seen that the distribution of the best estimator of  $\theta = \Delta m_{32}^2$  is closer to a Bernoulli distribution than to a Gaussian distribution. Therefore, Wilks' theorem is not applicable, and direct interpretation of  $\sqrt{\Delta\chi_{min}^2}$  as the number of  $\sigma$  in the Gaussian approximation leads to incorrect confidence intervals. We provided an analytical formula (Eq. 6) for confidence interval in an ideal Bernoulli case, which can be used to generate approximate confidence intervals for similar cases. For more general cases, a full MC simulation is needed to construct confidence intervals, as advocated in Ref. [19].
2. Even if a confidence interval for  $\Delta m_{32}^2$  is constructed correctly, its confidence level can not be

directly interpreted as how much the current measurement would favor the NH (IH) against the other. Despite possible agreement between confidence intervals and Bayesian credible intervals under certain circumstances as discussed in Appendix. B, such agreement does not apply to the current MH problem where there are strong constraints imposed on  $M_{32}^2$ .

Additional comments should be made regarding the Bayesian approach.

1. In principle, results from different experiments can be combined within the Bayesian framework. One example can be found in Ref. [33], in which a Bayesian method was applied to constrain  $\theta_{13}$  and CP phase  $\delta$  with existing experimental data. Regarding to the MH, results from different experiments can be combined through the integral in Eq. 9. Specifically, one can integrate over the nuisance parameters regarding experimental systematic uncertainties, while leaving nuisance parameters regarding the relevant neutrino masses and mixing parameters unintegrated. For example,

Symbol Description	$\overline{P}$ Average	Gaussian Interpretation	$P(NH x)$ Asimov data set	$F_{T=NH}$ $\Delta\chi^2 > 0$	$F_{T=NH}^{3\sigma}$ $P > 99.87\%$	$P_{T=NH}^{68\%}$ 68% P.I.	$P_{T=NH}^{90\%}$ 90% P.I.
Sensitivity Metric	90.14%	99.87%	98.90%	93.32%	23.73%	95.67%	65.79%

TABLE IV: Sensitivity metrics for an experiment with  $\overline{\Delta\chi^2} = 9$ .

suppose there are two independently conducted experiments, labeled by  $j = 1, 2$ , and that their respective observed data  $x_j$  corresponds to the model  $P(x_j|\theta, \eta^*, \eta_j, MH)$  under MH=NH or IH. Here the vector of nuisance parameter  $\eta$  in experiment  $j$  is separated into two pieces  $\eta^*$  and  $\eta_j$ , where  $\eta_j$  is unique to the experiment and  $\eta^*$  is common to both experiments. Of course,  $\theta$  is the parameter of interest and hence always common to both. Then, it would be useful for the different experiments to not only present  $\Delta\chi^2$  (Eq. 11), but to also present

$$P(x_j|\theta, \eta^*, MH) = \int P(x_j|\theta, \eta^*, \eta_j, MH)P(\eta_j|\theta, \eta^*, MH)d\eta_j,$$

in order that one can calculate the overall likelihood  $P(x_1, x_2|\theta, \eta^*, NH) = \prod_{j=1}^2 P(x_j|\theta, \eta^*, NH)$  for further inferences.

- We have listed a few variables to represent sensitivity of future experiments in Sec. III. Each of them convey different information. In the case that one has to choose a single variable to represent the sensitivities, one natural choice would be  $\overline{P}_{T=NH}^{NH}$  and  $\overline{P}_{T=IH}^{IH}$ , the average probability of NH given that the nature is NH, as well as the average probability of IH given that the nature is IH. Note that  $\overline{P}_{T=NH}^{NH}$  is generally not guaranteed to be equal to  $\overline{P}_{T=IH}^{IH}$ , so they need to be calculated separately.
- For general models where nuisance parameters are present, it is possible to measure the specificity of an experiment conditional on different possible values of the nuisance parameters. For instance, suppose NH, and that a particular value of the nuisance parameter, say  $\eta = \eta_0$ , is true. Then the relevant population of potential experimental results consists of  $x$  generated from  $P(x|NH, \eta_0) = \int P(x|\theta, \eta_0, NH)P(\theta, \eta_0|NH)d\theta$ . Accordingly,  $P(NH|x)$  can be obtained for each  $x$  in this population with Eq. 8<sup>3</sup>, and for e.g., their mean  $\overline{P}_{T=NH}^{NH}(\eta_0)$  and quantiles  $P_{T=NH}^A(\eta_0)$  serve as more refined sensitivity metrics for the experiment, and can be plotted against a range of possible

$\eta_0$  values. Such application is particularly useful when the separation of MH strongly depends on the value of  $\eta$ . One such example is long baseline  $\nu_e$  or  $\bar{\nu}_e$  appearance measurements (from  $\nu_\mu$  or  $\bar{\nu}_\mu$  beam), in which the sensitivity of MH strongly depends on the value of CP phase of lepton section  $\delta_{CP}$  and neutrino mixing angle  $\theta_{23}$ .

- The Gaussian approximation in Eq. 22 allows analytical calculation of various sensitivity metrics. Be aware that such calculations are valid under the assumption that the possible range of  $\theta$  under either hypothesis is narrow enough that it can be reasonably represented by a single point, and that  $\mu_i^{NH} - \mu_i^{IH} \ll \mu_i^{NH} \sim \mu_i^{IH}$ . For more general cases, numerical such as MC methods are needed.
- Finally, we emphasize that sensitivity metrics are designed to evaluate an experiment in its planning stage. It can be used to see if an experiment with a proposed sample size, i.e., the expected bin counts  $\{\mu_i, i = 1, \dots, n\}$ , will be large enough to have a high probability of generating desired strength of evidence to support the true hypothesis. But once the data are observed, the calculation of sensitivity metrics is no longer relevant. One should clearly differentiate results deduced from data from that from the sensitivity calculations.

## VI. SUMMARY

In this paper, we perform a statistical analysis for the problem of determining the neutrino mass hierarchy. A classical method of presenting experimental results is examined. Such method produces confidence intervals through the parameter estimation of  $\Delta m_{32}^2$  based on approximating the distribution of  $\sqrt{\Delta\chi^2}$  as the standard Gaussian distribution. However, due to strong existing experimental constraints of  $M_{32}^2 \equiv |\Delta m_{32}^2|$ , the parent distribution of the best estimation of  $\Delta m_{32}^2$  is better approximated as a Bernoulli distribution rather than a Gaussian distribution, which leads to a very different estimation of the confidence level. The importance of using the Feldman-Cousins approach to determine the confidence interval is emphasized.

In addition, the classical method is shown to be inadequate to convey the message of how much results from an experiment favor one hypothesis than the other, as the agreement between the confidence interval and the

<sup>3</sup> One should not take into account the information of  $\eta = \eta_0$  in calculating the probability, since one does not know the true value of  $\eta$  when analyzing experimental data.

Bayesian credible interval also breaks down due to the constraints on  $M_{32}^2$ .

We therefore introduce the Bayesian approach to quantify the probability of MH. We further extend the discussion to quantify experimental sensitivities of future measurements.

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### Appendix A: Derivation of $P(\Delta\chi_{min}^2)$ for case II: $\Theta = \{-1, 1\}$

Let  $\theta_0$  denote the true parameter value from which the data are generated. Under case II, when  $\theta_0 = 1$ , the statistic  $\Delta\chi_{min}^2(\theta_0)$  in Eq. 3 is directly related to  $\Delta\chi^2$  in Eq. 21 (recall that the notation  $\theta = 1, -1$  refers to NH and IH, respectively) as  $\Delta\chi_{min}^2(1) = \max\{0, -\Delta\chi^2\}$ . The result in section IV implies that, under  $\theta_0 = 1$ ,  $-\Delta\chi^2$  follows an approximately Gaussian distribution with mean  $-\overline{\Delta\chi^2}$  and standard deviation  $2\sqrt{\overline{\Delta\chi^2}}$ . Similarly, when  $\theta_0 = -1$ , the statistic  $\Delta\chi_{min}^2(\theta_0) = \max\{0, \Delta\chi^2\}$ , where  $\Delta\chi^2$  follows approximately Gaussian distribution

with mean  $\overline{\Delta\chi^2}$  and standard deviation  $2\sqrt{\overline{\Delta\chi^2}}$ . Therefore, whether the truth is  $\theta_0$  is 1 or  $-1$ , the distribution of  $\Delta\chi_{min}^2(\theta_0)$  is such that  $P(\Delta\chi_{min}^2(\theta_0) \geq t) = 1$  for  $t \leq 0$ , and that  $P(\Delta\chi_{min}^2(\theta_0) \geq t) \approx \frac{1}{2} - \frac{1}{2}\text{erf}\left(\frac{t + \overline{\Delta\chi^2}}{\sqrt{8\overline{\Delta\chi^2}}}\right)$  for  $t > 0$ .

### Appendix B: Confidence Interval vs. Bayesian Credible Interval

As emphasized in Ref. [19], the classical confidence interval should not be confused with the Bayesian credible interval. However, it is rather common that physicists approximate the confidence interval as the Bayesian credible interval, especially in MC simulations, where previous measurements of some physics quantities are used as inputs. Such approximations turn out to be acceptable under the following condition.

Consider the condition that the pdf (or pmf) of the best estimation of the unknown parameter  $\theta_{min}$  only depends on its relative location with respect to the true parameter value, that is,

$$P_{\Theta_{min}|\Theta_{true}}(\theta_{min}|\theta_{true}) = h(\theta_{min} - \theta_{true}), \quad (\text{B1})$$

for some non-negative function  $h$  such that  $\int_{-\infty}^{\infty} h(t)dt = 1$ . Models that satisfy Eq. B1 are said to belong to a location family, where  $\theta_{true}$  is called the location parameter. When there is a lack of strong prior information for  $\theta_{true}$ , it is usually reasonable to assign a uniform prior for it, that is, to assign  $P_{\Theta_{true}}(\theta_{true}) \propto 1$ . If so, we have

$$\begin{aligned} P_{\Theta_{true}|\Theta_{min}}(\theta_{true}|\theta_{min}) &= P_{\Theta_{min}|\Theta_{true}}(\theta_{min}|\theta_{true})P_{\Theta_{true}}(\theta_{true})/P_{\Theta_{min}}(\theta_{min}) \\ &\propto P_{\Theta_{min}|\Theta_{true}}(\theta_{min}|\theta_{true})P_{\Theta_{true}}(\theta_{true}) \quad (\text{as a function of } \theta) \\ &\propto P_{\Theta_{min}|\Theta_{true}}(\theta_{min}|\theta_{true}) = h(\theta_{min} - \theta_{true}). \end{aligned}$$

In the above, the first step follows from the Bayes' theorem, and the third step incorporates the uniform prior on  $\theta_{true}$ . Since for any fixed  $\theta_{true}$ ,  $\int_{-\infty}^{\infty} h(\theta_{min} - \theta_{true})d\theta_{min} = 1$ , the above indeed implies that

$$P_{\Theta_{true}|\Theta_{min}}(\theta_{min}|\theta_{true}) = h(\theta_{min} - \theta_{true}). \quad (\text{B2})$$

For any threshold level  $c$  and the observed value of  $\theta_{min}$ , define a plausible region for  $\theta_{true}$  by  $A(\theta_{min}, c) = \{\theta : P_{\Theta_{min}|\Theta_{true}}(\theta_{min}|\theta) > c\}$ , then

$$\begin{aligned} A(\theta_{min}, c) &= \{\theta : h(\theta_{min} - \theta) > c\} \\ &= \{\theta_{min} + t : h(0 - t) > c\} = \theta_{min} + A(0, c), \end{aligned} \quad (\text{B3})$$

where the transformation  $t = \theta - \theta_{min}$  is used in step 2, and in general, the notation  $\alpha + A$  for a point  $\alpha$  and a set  $A$  represents the set that consists of points  $\alpha + a$  for all  $a \in A$ . In words, Eq. B3 says that the plausible regions based on different  $\theta_{min}$  with a fixed threshold  $c$  are simply shifts in location of each other. First, under the Bayes framework,  $A(\theta_{min}, c)$  can be considered as a credible region (most often an interval). The probability that  $\theta$  falls in  $A(\theta_{min}, c)$  is called the level of the credible region, and is given by

$$\begin{aligned}
P_{\Theta_{\text{true}}|\Theta_{\text{min}}}(\theta \in A(\theta_{\text{min}}, c)|\theta_{\text{min}}) &= \int_{A(\theta_{\text{min}}, c)} P_{\Theta_{\text{true}}|\Theta_{\text{min}}}(\theta|\theta_{\text{min}})d\theta \\
\text{(by Eq. B2 and Eq. B3)} &= \int_{\theta_{\text{min}}+A(0, c)} h(\theta - \theta_{\text{min}})d\theta \\
\text{(letting } t = \theta - \theta_{\text{min}}) &= \int_{A(0, c)} h(t)dt.
\end{aligned}$$

On the other hand, under the classical framework,  $A(\theta_{\text{min}}, c)$  serves as a confidence interval, the level of

which is given by

$$\begin{aligned}
&P_{\Theta_{\text{min}}|\Theta_{\text{true}}}(\theta \in A(\theta_{\text{min}}, c)|\theta) \\
\text{(by Eq. B3)} &= P_{\Theta_{\text{min}}|\Theta_{\text{true}}}(\theta \in \theta_{\text{min}} + A(0, c)|\theta) \\
&= P_{\Theta_{\text{min}}|\Theta_{\text{true}}}(\theta_{\text{min}} \in \theta - A(0, c)|\theta) \\
\text{(by Eq. B1)} &= \int_{\theta - A(0, c)} h(\theta_{\text{min}} - \theta)d\theta_{\text{min}} \\
\text{(letting } t = \theta_{\text{min}} - \theta) &= \int_{A(0, c)} h(t)dt.
\end{aligned}$$

In summary, the region  $A(\theta_{\text{min}}, c)$  can be interpreted both as a confidence interval and a credible region of the same level.

A most useful special case where Eq. B1 is satisfied is the case where  $\theta_{\text{min}}$  strictly follows a Gaussian distribution with mean  $\theta_{\text{true}}$  (such as Case I of section II) and that the standard deviation of the Gaussian distribution did not depend on  $\theta_{\text{true}}$ . As we mentioned in section II, it is shown by Wilks [30] that, based on a large data sample size, the statistic  $\theta_{\text{min}}$  does approximately follow a Gaussian distribution with mean at  $\theta_{\text{true}}$  under certain regular conditions. Hence, it is not unacceptable to construct an  $\alpha$  level confidence interval and interpret it as an  $\alpha$  level credible interval, as long as the standard deviation of the Gaussian distribution has weak or no dependence on  $\theta_{\text{true}}$ .

However, in the MH determination problem, the regularity conditions are violated due to the existing experimental constraints on  $|\theta| = M_{32}^2$ . As a result, condition Eq. B1 is far from being satisfied, and there is no

longer a correspondence between confidence intervals and Bayesian credible intervals. Indeed, strong inconsistency between implications of the two types of intervals can be seen from the following specific example belonging to case II of section II. It is easy to come up with an observed data  $x$  that results in  $\Delta\chi^2 = 1$  and  $\overline{\Delta\chi^2} = 9$  (defined in Eq. 11 and 22 respectively). Then, according to the Bayesian approach, the probability is about 62.2% that NH is the correct hypothesis, or an odds of 5 : 3 of NH against IH. Most people would consider this a fairly weak preference for NH. On the other hand, the classical estimation procedure turns out to exclude the point IH from the 95% confidence interval according to (the correct table) Table. I. Had one attempted to interpret this 95% confidence interval as a Bayesian credible interval, one would conclude that the odds of NH against IH is at least 19 : 1. This conclusion is over confident in the MH determination compared to the odds of 5 : 3 suggested by the well-founded Bayesian approach.

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