The Gaussian CL_s Method for Searches of New Physics

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We describe a method based on the CL_s approach to present results in searches of new physics, under the condition that the relevant parameter space is continuous. Our method relies on a class of test statistics developed for non-nested hypotheses testing problems, denoted by ΔT , which has a Gaussian approximation to its parent distribution when the sample size is large. This leads to a simple procedure of forming exclusion sets for the parameters of interest, which we call the Gaussian CL_s method. Our work provides a self-contained mathematical proof for the Gaussian CL_s method, that explicitly outlines the required conditions. These conditions are milder than that required by the Wilks' theorem to set confidence intervals (CIs). We illustrate the Gaussian CL_s method in an example of searching for a sterile neutrino, where the CL_s approach was rarely used before. We also compare data analysis results produced by the Gaussian CL_s method and various CI methods to showcase their differences.

I. INTRODUCTION

The Standard Model of particle physics has been extremely successful since its establishment in the mid-1970s. In particular, the Higgs particle discovered at LHC in 2012 [1, 2] completed the list of fundamental particles predicted by the minimal Standard Model. On the other hand, there has been experimental evidence that point to new physics beyond the Standard Model: neutrino oscillations indicate non-zero neutrino mass; various gravitational effects indicate the existence of non-baryonic dark matter; the accelerating expansion of our universe indicates the existence of dark energy; the large observed matter-anti-matter asymmetry in the universe indicates the existence of additional CP violation source beyond that in the quark mixing matrix, etc. Searches for new physics beyond the Standard Model have been and still are at the frontier of high energy particle physics.

Given experiment data, a problem of searching for new physics often turns into a parameter estimation problem, and the findings are presented in the form of constraints on some continuous parameter(s). One example is the search for sterile neutrino suggested by LSND [3], MiniBooNE [4], and reactor antineutrino anomalies [5].¹ In this case, data collected from an experiment consists of neutrino interaction counts in multiple energy bins, $x = (N_1, \dots, N_n)$. Data analysis results are generally shown as constraints in the two-dimensional parameter space of $(\sin^2 2\theta, |\Delta m^2|)$, where θ is the mixing angle involving the sterile neutrino, and $|\Delta m^2|$ is the mass-

squared difference of neutrino mass eigenstate beyond three generations.

One way to set constraints is to form confidence intervals² (CI), which contains parameter values that are compatible with the data. Let β denote the parameter(s), such as $\beta = (\sin^2 2\theta, |\Delta m^2|)$ in the neutrino oscillation problem. A CI can be obtained by inverting a testing procedure. Specifically, the set of all β_1 such that the hypothesis $H_0 : \beta = \beta_1$ is not rejected at level $1 - c$, forms a level- c CI. A testing procedure is often performed by thresholding a test statistic, which is a user-chosen function that, for any given β_1 , defines a criterion to order all possible values of x . To test $H_0 : \beta = \beta_1$, a commonly used type of test statistic takes the form

$$\Delta\chi^2(\beta_1; x) := \chi^2(\beta_1; x) - \chi_{\min}^2(x), \quad (1)$$

where χ^2 is a function that measures the compatibility between β_1 and x . One important example of χ^2 is the negative-two-log-likelihood function, and the corresponding $\Delta\chi^2$ is called the likelihood ratio (LR) test statistic. In the field of high energy physics, the unified approach to construct CIs advocated by Feldman and Cousins [6] is indeed based on the likelihood ratio test statistic.

A parameter value β_1 is included in a level- c CI if $\Delta\chi^2(\beta_1; x)$ is below a threshold t_c , such that $\text{Prob}_{\beta_1}(\Delta\chi^2(\beta_1; X) \leq t_c) \geq c$. Here, the subscript β_1 means that X is a random outcome from a model with true parameter value β_1 . In general, Monte Carlo (MC) simulation can be used³ to approximate the parent dis-

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¹ Other examples include dark matter searches (the interaction cross section vs. the mass of the dark matter particle) and SUSY (super symmetry) particle searches at LHC (the interaction coupling vs. the mass scale).

² Rigorously speaking, the word “confidence set” should be used instead of “confidence interval” when the dimension of the parameter space is higher than one. But as long as there is no ambiguity, we will refer to all confidence sets as confidence intervals for simplicity.

³ When the model contains nuisance parameters, extra care are needed in performing Monte Carlo simulation. See Ref. [7] for example.

tribution of $\Delta\chi^2$. We refer to the corresponding method of constructing CIs as *the MC CI method*. An example of the MC CI method, tailored for the LR test statistic, can be found in section V.B of Feldman and Cousins [6]. The MC CI method is often computationally intensive. Alternatively, t_c can be approximated using a Chi-square distribution, a summary of its usage in particle physics is provided by the Particle Data Group [8]. This method is simple to carry out, but the approximation is only valid under relatively stringent conditions. Specifically, the Chi-square thresholds are justified by the Wilks' theorem [9] for the LR test statistic under regularity conditions C1—C3 in Sec. II, and they are justified for the variations of $\Delta\chi^2$ listed in Sec. IV A under similar conditions [10, 11]. We conveniently refer to any method that constructs approximate CIs based on Chi-square thresholds as a *Wilks' CI method*.

In theory, forming CIs using test statistics of the form $\Delta\chi^2(\beta; X)$ is desirable, because it leads to a unified approach in setting limits in the absence of new physics signals and in estimating parameters after the discovery of new physics [6]. However, in the problem of searching for sterile neutrinos, the computationally expensive MC CI method is usually necessary to obtain valid thresholds t_c for the $\Delta\chi^2$ statistic, making the application difficult.

Compared to $\Delta\chi^2$, the following test statistic, ΔT , has a parent distribution that is easy to approximate under mild conditions. By fixing a reference value of β , say β_{ref} , one can test a pair of non-nested hypotheses $H_0 : \beta = \beta_{\text{ref}}$ versus $H_1 : \beta = \beta_1$ using a test statistic of the form

$$\Delta T(\beta_{\text{ref}}, \beta_1; x) := \chi^2(\beta_1; x) - \chi^2(\beta_{\text{ref}}; x). \quad (2)$$

An example of ΔT is the negative-two-log-likelihood ratio statistic for H_0 and H_1 . Given observed data x and a fixed β_{ref} , all β_1 values that result in $\text{Prob}_{\beta_1}(\Delta T(\beta_{\text{ref}}, \beta_1; X) \leq t'_c) \geq c$ constitute a level- c CI. It is proven in Sec. III B that under fairly mild conditions, one can approximate t'_c using quantiles of a Gaussian distribution. Specifically, we show that when the data size is large, the distribution of $\Delta T(X)$, where X represents potential data from a model that satisfies either one of the two hypotheses, say H , can be approximated by the Gaussian distribution with mean $\overline{\Delta T_H}$ and standard deviation $2\sqrt{|\overline{\Delta T_H}|}$. Here, $\overline{\Delta T_H}$ is defined to be $\Delta T(x_H^{\text{Asimov}})$ as in Eq. (19), where x_H^{Asimov} is the *Asimov data set* [12] as introduced in Sec. III.

However, CIs constructed from ΔT can exclude β_1 values that are not much less compatible with the data than β_{ref} is, which we demonstrate in Sec. V D. To avoid counter-intuitive results based on ΔT , we take the CL_s approach of setting *exclusion sets* [13–15] as an alternative to the CI approach. We refer to the simple procedure of setting exclusion sets based on the ΔT statistic using a Gaussian approximation as *the Gaussian CL_s method*.

Note that an exclusion set imposes a different kind of constraint than that of (the complement of) a CI. An exclusion set aims at identifying parameter values that

fit the data much worse than the reference model. Consequently, the CL_s approach is more reluctant than the CI approach to exclude models where the experiment has little sensitivity. An example comparing the two can be found in Sec. V D.

The main contribution of this paper is to provide a mathematical proof for a Gaussian approximation to the distribution of ΔT . This result justifies the Gaussian CL_s method, which requires a computational load similar to that of the Wilks' CI method, and the former is valid in situations where the latter is not. Results similar to ours can be found in Ref. [12] in the context of searching new particles, and in Ref. [16, 17] in the context of neutrino mass hierarchy determinations. The self-contained proof provided in this paper makes it easier to fully articulate the required conditions, which were missing in the previous work. Also, we make a more general and realistic assumption in accordance with the physics problem of interest than that of Ref. [12] and the paper by Wald [10] cited therein. For details, see assumptions [A0] and [A1] in Sec. III B 2.

Another contribution of this paper is that we compare various methods that take the CI approach or the CL_s approach in a problem of searching for neutrino oscillations, where the CL_s approach was rarely used before. Based on the comparisons, we advocate the Gaussian CL_s as an attractive alternative method to the CI approach in the application of searching for new physics through precision measurements. First, the Gaussian CL_s method is inexpensive to carry out and is valid in very general setups. Secondly, researchers often need to combine results from different experiments. When conditions in the Wilks' theorem are not satisfied, it is simple to combine the test statistics from different experiments and form an overall CI using the Wilks' method. Otherwise, expensive MC methods have to be used to form CIs for each experiment, and there is no rigorous way to combine these results together other than to rerun a more expensive MC for the combined data. In contrast, we explain in Sec. VI that experimental results can be easily combined using the Gaussian CL_s method, and is valid under mild conditions.

This paper is organized as follows. In Sec. II, we briefly review the CI approach that utilizes a class of statistics, $\Delta\chi^2$. We look at both the Wilks' CI method and the MC CI method, and discuss their advantages and limitations. In Sec. III, we describe an alternative class of statistics, ΔT . In Sec. IV, we describe the CL_s approach based on the ΔT statistic, and outline a simple procedure to carry it out using the Gaussian approximation. In Sec. V, using an example of the search for a sterile neutrino, we check the validity of the approximation in the Gaussian CL_s method, and compare different methods of forming constraints in the parameter space. Finally, we present discussions and summaries in Sec. VI and Sec. VII, respectively.

II. THE CONFIDENCE INTERVAL APPROACH BASED ON THE $\Delta\chi^2$ STATISTIC

In this section, we briefly review the traditional method of setting CIs in the context of neutrino oscillations. We consider a neutrino energy spectrum that consists of n energy bins, and assume that the mean number of counts in each bin is a function of the vector of parameters of main interest, $\beta = (\sin^2 2\theta, |\Delta m^2|)$, and a vector of nuisance parameters (such as the overall normalization), η . Let Θ , M , and $\mathcal{H}$ denote the parameter space of $\sin^2 2\theta$, $|\Delta m^2|$, and η , respectively. There are two further physical constraints: $\sin^2 2\theta \geq 0$ and $|\Delta m^2| \geq 0$. Then for the i -th bin, $\lambda_i(\sin^2 2\theta, |\Delta m^2|, \eta)$ and N_i represent the mean and the observed counts of neutrino induced interactions, respectively. When λ_i is large enough, the distribution of N_i can be well approximated by a Gaussian distribution with mean λ_i and standard deviation $\sqrt{\lambda_i}$.

Given any specific guess of the value of the parameters $(\sin^2 2\theta, |\Delta m^2|, \eta)$, once the data $x = \{N_i, i = 1, \dots, n\}$ are observed, one can calculate the deviation of the data from the mean values λ_i to measure the compatibility of the hypothesized parameter values to x . Commonly used deviations include negative-two-log-likelihood ratio, Pearson chi-square and Neyman chi-square. Further, when certain knowledge concerning the nuisance parameter η (e.g. knowledge of detecting efficiency and neutrino flux) is available, it can be reflected in the definition of the deviation. For example, to modify the Pearson Chi-square, denoted by χ_P^2 , when previous experiments suggest an estimate of η to be η_0 with standard deviation σ_η , one can define the following deviation function:

$$\begin{aligned} & \chi^2(\sin^2 2\theta, |\Delta m^2|, \eta; x) \\ &= \chi_P^2(\sin^2 2\theta, |\Delta m^2|, \eta; x) + \chi_\eta^2(\eta) \\ &= \sum_i \frac{(N_i - \lambda_i(\sin^2 2\theta, |\Delta m^2|, \eta))^2}{\lambda_i(\sin^2 2\theta, |\Delta m^2|, \eta)} + \frac{(\eta - \eta_0)^2}{(\sigma_\eta)^2}. \end{aligned} \quad (3)$$

The term t_c represents the threshold value such that, $\min_\eta \text{Prob}_{\sin^2 2\theta, |\Delta m^2|, \eta}(\Delta\chi^2 \leq t_c) \geq c$. The key in constructing a CI is to specify t_c correctly for a given confidence level c .

Most commonly examined confidence levels use $c = 68.3\%$ (1σ), 95.5% (2σ), 99.7% (3σ), which are often linked to threshold values $t_c = 2.31, 5.99, 11.8$, respectively [8]. Note that these three values are the 68.3%, 95.5% and 99.7% quantiles of the Chi-square distribution with two degrees of freedom, respectively. The reason why these threshold values are used is that, CI_c is indeed constructed upon screening the entire param-

Below, we use the notation $\arg \min_w h(w)$ to denote the value of w that minimizes any given function h , and 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. Let

$$(\sin^2 2\theta_{\min}, |\Delta m_{\min}^2|, \eta_{\min}) = \arg \min \chi^2(\sin^2 2\theta, |\Delta m^2|, \eta; x), \quad (4)$$

that is, the value of $(\sin^2 2\theta, |\Delta m^2|, \eta) \in \Theta \times M \times \mathcal{H}$ that best fits the data according to the deviation χ^2 . Also, let

$$\chi_{\min}^2(x) = \chi^2(\sin^2 2\theta_{\min}, |\Delta m_{\min}^2|, \eta_{\min}; x). \quad (5)$$

And for any given $(\sin^2 2\theta, |\Delta m^2|)$, let

$$\eta_{\min}(\sin^2 2\theta, |\Delta m^2|) = \arg \min_\eta \chi^2(\sin^2 2\theta, |\Delta m^2|, \eta; x). \quad (6)$$

Then we can define a test statistic that reflects how much worse $(\sin^2 2\theta, |\Delta m^2|)$ is than that of the best fit, namely,

$$\begin{aligned} & \Delta\chi^2(\sin^2 2\theta, |\Delta m^2|; x) \equiv \\ & \chi^2(\sin^2 2\theta, |\Delta m^2|, \eta_{\min}(\sin^2 2\theta, |\Delta m^2|); x) - \chi_{\min}^2(x) \end{aligned} \quad (7)$$

The corresponding CI with confidence level c is defined to be

$$CI_c = \{(\sin^2 2\theta, |\Delta m^2|) \in \Theta \times M : \Delta\chi^2(\sin^2 2\theta, |\Delta m^2|; x) \leq t_c\}. \quad (8)$$

eter space by inspecting one point at a time, denoted by $(\sin^2 2\theta_1, |\Delta m_1^2|)$, and testing the pair of hypotheses, $H_0 : (\sin^2 2\theta, |\Delta m^2|) = (\sin^2 2\theta_1, |\Delta m_1^2|)$ versus H_1 : otherwise. To test the above hypotheses using the Chi-square statistic $\Delta\chi^2$ in Eq. (7), the full parameter space for $(\sin^2 2\theta, |\Delta m^2|, \eta)$ is $\Theta \times M \times \mathcal{H}$, and the null hypothesis space is $\{(\sin^2 2\theta_1, |\Delta m_1^2|)\} \times \mathcal{H}$. According to the Wilks' theorem [9], if certain regularity conditions hold, mainly

- C1. the full parameter space $\Theta \times M \times \mathcal{H}$ is a continuous space, and the the model likelihood function is a smooth function (for example three times differen-

tiable) in the parameters,

C2. the full parameter space contains an open neighborhood around the true value $(\sin^2 2\theta_1, |\Delta m_1^2|, \eta_1)$, and

C3. the data size N_i is large for each $i = 1, \dots, n$,

then the statistic $\Delta\chi^2(\sin^2 2\theta_1, |\Delta m_1^2|; X)$ follows approximately a Chi-square distribution when X is data generated from H_0 . Further, the degree of freedom of this Chi-square distribution equals the difference between the dimension of the full parameter space and that of the null hypothesis space, namely 2, in the current case. This procedure of constructing CIs and its extensions have been successfully applied in many studies in order to constrain various parameters in the field of neutrino physics (e.g. Ref. [18]).

Although the above Wilks' CI method has been widely used in analyzing experimental data, it does not always produce CIs that have correct coverage. Its limitations have been addressed by, for example, Feldman and Cousins [6]. One example is the searches for neutrino oscillations in the disappearance mode. The oscillation probability with $(\sin^2 2\theta, |\Delta m^2|)$ in a 2-flavor framework is written as:

$$P_i = 1 - \sin^2 2\theta \cdot \sin^2(1.27 \cdot |\Delta m^2| \cdot L/E_i^\nu), \quad (9)$$

where L and E_i^ν are the distance neutrino travels and the neutrino energy at the i -th bin, respectively. Then the mean bin counts $\lambda_i = E(N_i)$ are such that $\lambda_i = m \cdot (a_i \cdot P_i + b_i)$, where a_i and b_i are coefficients that depend on the vector of nuisance parameters η , and m represents the amount of accumulated data (e.g. the elapsed time for data collection).

The reason why the Wilks' CI method fails for the above neutrino oscillations example is the following. A key middle step in the proof of the Wilks' theorem is that conditions C1–3 together ensure that the estimator of $(\sin^2 2\theta, |\Delta m^2|)$ based on minimizing χ^2 , has a distribution close to a Gaussian distribution. This suggests two cases. (1) When testing a hypothesis H of the form: $\sin^2 2\theta = 0$ for any value of $|\Delta m^2|$, C2 is violated, hence the Wilks' theorem does not apply no matter how large the data size is. (2) When testing hypotheses of all other forms, C1 and C2 are both satisfied, hence as the sample size grows to infinity, the distribution of $\Delta\chi^2$ will eventually converge to a Chi-square distribution. However, for instance if the true $\sin^2 2\theta$ is close to 0, then there could be a non-ignorable probability that we observe a data set that results in $\sin^2 2\theta_{\min} = 0$. This clearly prevents the distribution of $(\sin^2 2\theta_{\min}, |\Delta m_{\min}^2|)$ from being closely approximated by a Gaussian distribution. Indeed, the closer $\sin^2 2\theta_0$ is to 0, the larger the data size is needed to overcome the above phenomena.

The latter point can also be understood intuitively. The parameter space of $\sin^2 2\theta$ vs. $|\Delta m^2|$, as is usually displayed in Fig. 1a, is uniform. But the effective parameter space of $(\sin^2 2\theta, |\Delta m^2|)$, in which the distance

between any two points is measured by χ^2 defined in Eq. (3), is no longer uniform (Fig. 1b). Due to the functional form of the oscillation formula, the effective parameter space becomes more compact at smaller $\sin^2 2\theta$, as the differences between spectra with different values of $|\Delta m^2|$ become smaller. Therefore, more data is needed to reach the large data limit required by the Wilks' theorem in order to maintain the open neighborhood around the true parameter values (regularity condition C2). For example, the true $\sin^2 2\theta = 0$ hypothesis does not have an open neighborhood, as $\sin^2 2\theta < 0$ is not allowed. It is therefore impossible to reach the large data limit. Even for non-zero but small true value of $\sin^2 2\theta$, the required data size could be well beyond the experimental reach.

When these regularity conditions are not satisfied, there are instances when the parent distribution of $\Delta\chi^2$ can have simple approximations that are not necessarily Chi-square. See, for e.g. Ref. [12, Sec. 3], where the parameter β has dimension 1. For more general cases, one needs the MC method to set CIs. Below, we review how to produce a valid 1- σ (68%) CI of $(\sin^2 2\theta, |\Delta m^2|)$ using MC, which can be easily generalized to build CIs of any level.

Having observed data $x = \{N_1, \dots, N_n\}$, apply the following procedure to every $(\sin^2 2\theta, |\Delta m^2|)$ in the parameter space $\Theta \times M$:

1. Calculate $\Delta\chi^2(\sin^2 2\theta, |\Delta m^2|; x)$ with Eq. (7) 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 $(\sin^2 2\theta, |\Delta m^2|)$. Here, the nuisance parameters can be either randomly generated according to the common hybrid Bayesian/Frequentist approach [19] or fixed at the best-fit values from data according to the full Frequentist approach [7, 20]. For $j = 1, \dots, T$, calculate $\Delta\chi^2(\sin^2 2\theta, |\Delta m^2|; x^{(j)})$. This produces an empirical distribution of the statistic $\Delta\chi^2$.
3. Calculate the percentage of MC samples such that $\Delta\chi^2(\sin^2 2\theta, |\Delta m^2|; x^{(j)}) < \Delta\chi^2(\sin^2 2\theta, |\Delta m^2|; x)$. Then $(\sin^2 2\theta, |\Delta m^2|)$ is included in the 1- σ CI if and only if the percentage is smaller than 68%.

The key of the above procedure is to generate an empirical distribution of $\Delta\chi^2$, which is not necessarily close to a Chi-square distribution.

Unlike the Wilks' CI method, the MC CI method guarantees the validity of the resulting CIs when the MC sample size is large. However, the procedure can be very time-consuming when the dimension of the vector of unknown parameters is high and/or when a fine grid of the parameter space needs to be examined. In addition, the number of MC samples needed to produce an empirical distribution that leads to an accurate enough CI increases quickly as the required confidence level increases. The procedure can become prohibitively expensive if the

FIG. 1. (color online) Left panel (a): The parameter space of $\sin^2 2\theta$ vs. $|\Delta m^2|$ in the Cartesian coordinate. Physical constraints are $\sin^2 2\theta \geq 0$ and $|\Delta m^2| \geq 0$. Right panel (b): Schematic illustration of the effective parameter space of $\sin^2 \theta$ vs. $|\Delta m^2|$ taking into account the spectral difference measured by χ^2 defined in Eq. (3). When $\sin^2 2\theta = 0$, points with different values of $|\Delta m^2|$ will converge into a single point. This can be easily seen from Eq. (9). At $\sin^2 2\theta = 0$, $|\Delta m^2|$ has no impact on the neutrino spectrum. Therefore, when $\sin^2 2\theta = 0$, there is no open neighborhood around the true value, leading to a failure of regularity conditions required by the Wilks' theorem.

minimization process used to find $(\sin^2 2\theta_{\min}, |\Delta m_{\min}^2|)$ is slow due to the existence of many nuisance parameters or other technical difficulties.

Furthermore, there is no simple recipe to strictly combine the CIs generated with the MC CI method from different experiments to form an overall CI. To see this, consider an example where several experiments are carried out to probe the parameter space of $(\sin^2 2\theta, |\Delta m^2|)$. For any space point $(\sin^2 2\theta, |\Delta m^2|)$, the $\Delta\chi^2$ statistic of the j th experiment is given by $\chi^2(\sin^2 2\theta, |\Delta m^2|; x^{(j)}) - \chi^2(\sin^2 2\theta_{\min}^{(j)}, |\Delta m_{\min}^2|^{(j)})$. Note that the minimum-value parameter space point, $(\sin^2 2\theta_{\min}, |\Delta m_{\min}^2|)$, based on different experiments are typically different. Once the experiments are combined, a strict implementation of the MC CI method requires to know the global minimum-value parameter space point, which is in general unattainable. Indeed, one has to redo MC simulations for the combined data, which is expensive in computation since minimization has to be done for each MC sample.

In the next section, we introduce a different test statistic from $\Delta\chi^2$, which allows for a simple approximation to its distribution under mild conditions. Using this new test statistic helps circumvent the computational problems mentioned above.

III. THE ΔT STATISTIC

A. Non-nested hypotheses testing

Recall that we used β and η to denote the parameter of interest and the nuisance parameter respec-

tively. The corresponding model has mean bin counts $(\lambda_1(\beta, \eta), \dots, \lambda_n(\beta, \eta))$. Let B denote the parameter space for β . In this section, we consider pairs of non-nested hypotheses $H_0 : \beta = \beta_0$ and $H_1 : \beta = \beta_1$, one pair at a time, for any $\beta_0 \neq \beta_1 \in B$. For convenience and clarity, we update some of our notations and refer to the nuisance parameter under H_0 and H_1 as η and ζ respectively, and they can be of different dimensions. Also, we refer to the mean bin counts associated with β_0 and β_1 as μ and ν respectively, that is, the mean count of the i th bin is $\mu_i(\eta) = \lambda_i(\beta_0, \eta)$ under H_0 and $\nu_i(\zeta) = \lambda_i(\beta_1, \zeta)$ under H_1 .

We now introduce a test statistic, denoted by $\Delta T(\beta_0, \beta_1; x)$, or simply $\Delta T(x)$, for testing H_0 versus H_1 . More than one version of the definition of ΔT will be listed below.

We start with either the Poisson or the Normal distribution to model the data x , and use the general notation $L(x, \lambda)$ to denote the corresponding likelihood, where λ equals to $\mu(\eta)$ under H_0 , and $\nu(\zeta)$ under H_1 , respectively. Following the practice of Ref. [21, sec. 2], we convert⁴ the likelihood functions under H_0 and H_1 into $T_{H_0}(\eta; x)$ and $T_{H_1}(\eta; x)$ respectively. Let

$$a(x) = 2 \log L(x, \lambda = x), \quad (10)$$

⁴ This is usually done in order that $T_{H_0}(\eta; x)$ and $T_{H_1}(\eta; x)$ are asymptotically equivalent under certain conditions to their counterparts in the classical Chi-square forms, namely, the Neyman and the Pearson Chi-square statistics.

and define

$$T_{H_0}(\eta; x) = -2 \log(L(x, \mu(\eta))) + a(x), \text{ and } (11)$$

$$T_{H_1}(\zeta; x) = -2 \log(L(x, \nu(\zeta))) + a(x), \quad (12)$$

both of which can be interpreted as likelihood ratios. Take the Poisson model for example, we have

$$\begin{aligned} 2 \log L(x, \lambda) &= \sum_{i=1}^n -2N_i \log \lambda_i + 2\lambda_i + 2 \log(N_i!) \\ &\approx \sum_{i=1}^n [2(\lambda_i - N_i + N_i \log(N_i/\lambda_i)) \\ &\quad + \log N_i] + n \log(2\pi), \end{aligned} \quad (13)$$

and $a(x) = \sum_{i=1}^n \log N_i + n \log(2\pi)$. Then, looking at

the definition of T_{H_0} for instance, we have

$$T_{H_0}(\eta; x) = \sum_{i=1}^n 2(\mu_i(\eta) - N_i + N_i \log(N_i/\mu_i(\eta))). \quad (14)$$

In practice, when there are prior experiments carried out to study the nuisance parameters, an additional term that reflects deviation from this prior knowledge is added to the definition of $T_{H_0}(\eta; x)$. We denote this term by $\chi_{\text{penalty}}^2(\eta)$, an example of which is the term $\frac{(\eta - \eta_0)^2}{(\sigma_\eta)^2}$ in Eq. (3). And when the data size is large, terms of smaller order are sometimes omitted from the definition of $T_{H_0}(\eta; x)$. There are at least four common variations for $T_{H_0}(\eta; x)$ used in practice:

$$T_{H_0}(\eta; x) = \sum_{i=1}^n 2 \left(\mu_i - N_i + N_i \log \frac{N_i}{\mu_i} \right) + \chi_{\text{penalty}}^2(\eta), \quad (15)$$

$$T_{H_0}(\eta; x) = \sum_{i=1}^n \log \frac{\mu_i}{N_i} + \sum_{i=1}^n \frac{(N_i - \mu_i)^2}{\mu_i} + \chi_{\text{penalty}}^2(\eta), \quad (16)$$

$$T_{H_0}(\eta; x) = \sum_{i=1}^n \frac{(N_i - \mu_i)^2}{\mu_i} + \chi_{\text{penalty}}^2(\eta), \quad (17)$$

$$T_{H_0}(\eta; x) = \sum_{i=1}^n \frac{(N_i - \mu_i)^2}{N_i} + \chi_{\text{penalty}}^2(\eta). \quad (18)$$

Here, Eq. (15) and Eq. (16) origin from the likelihood function of the Poisson and the Gaussian distribution, respectively. Eq. (17) and Eq. (18) are variations of Eq. (16), and are commonly referred to as the Pearson and the Neyman Chi-square, respectively.⁵ Note that Eq. (3) is a specific example of Eq. (17). We can define four versions of $T_{H_1}(\zeta; x)$ similarly.

En route to form the test statistic ΔT , $T_{H_0}(\eta; x)$ and $T_{H_1}(\zeta; x)$ are further minimized over all nuisance parameters, to obtain $T_{H_0}^{\min}(x) = \min_{\eta} T_{H_0}(\eta; x)$ and $T_{H_1}^{\min}(x) = \min_{\zeta} T_{H_1}(\zeta; x)$, respectively. Finally, we define the test statistic

$$\Delta T(x) = T_{H_1}^{\min}(x) - T_{H_0}^{\min}(x). \quad (19)$$

Note that $\Delta T(x)$ has the interpretation of being a log-likelihood ratio test statistic (or certain variations of it, depending on which version of the definition of T_{H_0} and

T_{H_1} are used) between the two hypotheses. It is easy to see that a positive $\Delta T(x)$ would favor H_0 , and a negative $\Delta T(x)$ would favor H_1 . In addition, the absolute size of $\Delta T(x)$ reflects how much one hypothesis is favored over the other.⁶

Remark. We emphasize that $\Delta T(x)$ is a different type of test statistic than $\Delta\chi^2(x)$ in Eq. (7). Specifically, $\Delta T(x)$ involves the best fit under the restrictions H_0 and H_1 , respectively, while $\Delta\chi^2(x)$ involves the best fit under the restrictions H_0 and over the full parameter space, respectively. The way ΔT is defined is key to why there is a Gaussian approximation that works under very general setups, even in the cases where simple approximations for the conventional $\Delta\chi^2$ statistic fails. Nevertheless, we should note that, when the computing is affordable, forming CIs using $\Delta\chi^2$ is more desirable

⁵ As summarized in Ref. [21], all the above estimators had a set of properties which the authors considered optimal. They called them "best asymptotically normal" (BAN) estimators. The versions of test statistics based directly on likelihood functions are considered superior due to their faster convergence to the limiting chi-square distributions.

⁶ An alternative way to define $\Delta T(x)$ is to replace $T_{H_0}^{\min}(x)$ and $T_{H_1}^{\min}(x)$ by $T_{H_0}^{\text{mag}}(x)$ and $T_{H_1}^{\text{mag}}(x)$, respectively, which are the marginalized, or say integrated version of $T_{H_0}(\eta; x)$ and $T_{H_1}(\zeta; x)$ over all nuisance parameters. These two methods generally give very similar results in practice. From the statistics point of view, while the minimization method adopts the Frequentist's philosophy, the marginalization method adopts the Bayesian philosophy.

because it leads to a unified approach for setting limits in absence of new physics signals and in estimating parameters after the discovery of new physics [6].

Next, we introduce the concept of *the Asimov data set* [12]. Let $x_{H_0}^{\text{Asimov}}$ denote the Asimov data set under H_0 , which is, loosely speaking, the mean counts corresponding to the true model in H_0 without any statistical fluctuation nor variations of systematics (change in nuisance parameters from their true value). In mathematical symbols, $x_{H_0}^{\text{Asimov}} = \mu(\eta^0)$, where η^0 stands for the true value of the nuisance parameter. In practice, we do not know η^0 , so it is commonly approximated by an existing nominal value of the nuisance parameter (such as the term η_0 in Eq. (3)).

Finally, we define a term that will help describe the distribution of the test statistic ΔT under H_0 . Assuming that H_0 is the correct hypothesis, define

$$\begin{aligned}\overline{\Delta T_{H_0}} &= \Delta T(x_{H_0}^{\text{Asimov}}) \\ &= T_{H_1}^{\min}(x_{H_0}^{\text{Asimov}}) - T_{H_0}^{\min}(x_{H_0}^{\text{Asimov}}) \\ &= T_{H_1}^{\min}(x_{H_0}^{\text{Asimov}}),\end{aligned}\quad (20)$$

where the last step holds because $T_{H_0}^{\min}(x_{H_0}^{\text{Asimov}}) = 0$ by the definition of $T_{H_0}^{\min}$ and $x_{H_0}^{\text{Asimov}} := \mu(\eta^0)$.

Analogously, let $x_{H_1}^{\text{Asimov}} = \nu(\zeta^0)$ denote the Asimov data set under H_1 , where we can approximate ζ^0 by an existing nominal value. Then the following term will help describe the distribution of the test statistic ΔT , had H_1 been the correct hypothesis:

$$\begin{aligned}\overline{\Delta T_{H_1}} &= \Delta T(x_{H_1}^{\text{Asimov}}) \\ &= T_{H_1}^{\min}(x_{H_1}^{\text{Asimov}}) - T_{H_0}^{\min}(x_{H_1}^{\text{Asimov}}) \\ &= -T_{H_0}^{\min}(x_{H_1}^{\text{Asimov}}).\end{aligned}\quad (21)$$

B. A Gaussian Approximation to the Distribution of $\Delta T(X)$ with Large Data Size

In this section, we show that by omitting terms of relatively small orders, the distribution of $\Delta T(X)$ under hypothesis H follows approximately a Gaussian distribution with mean $\overline{\Delta T_H}$ and standard deviation $2\sqrt{|\overline{\Delta T_H}|}$, where H could be either H_0 or H_1 .

1. Description of the mathematical problem and notations

Recall that we defined four versions of $(T_{H_0}(\eta; x), T_{H_1}(\zeta; x))$ that yield four different definitions of the test statistic $\Delta T(X)$. In this section, we focus on studying $\Delta T(X)$ based on Eq. (17), namely the Pearson Chi-square statistic. For clarity, we call it $D(X)$ from here on. The main part of Sec. IIIB2 will be devoted to develop a Gaussian approximation for the distribution of $D(X)$ under H_0 . And in the remarks in the end of Sec. IIIB2, we show that under

H_0 , the differences between the other three versions of $\Delta T(X)$ to $D(X)$ are insignificant under fairly general conditions, so the approximate distribution derived for $D(X)$ can also be used for all the different versions of $\Delta T(X)$. Note that due to the symmetry between H_0 and H_1 , the aforementioned result also applies to $D(X)$ and its variations under H_1 .

The mathematical problem concerning $D(X)$ is the following. Let

$$\begin{aligned}\chi_{H_0}^2(\eta; X) &:= \sum_{i=1}^n \frac{(N_i - \mu_i(\eta))^2}{\mu_i(\eta)} \quad \text{and} \\ \chi_{H_1}^2(\zeta; X) &:= \sum_{i=1}^n \frac{(N_i - \nu_i(\zeta))^2}{\nu_i(\zeta)}\end{aligned}\quad (22)$$

and let

$$\begin{aligned}\hat{\eta} &= \arg \min_{\eta} \chi_{H_0}^2(\eta; X) \\ \hat{\zeta} &= \arg \min_{\zeta} \chi_{H_1}^2(\zeta; X).\end{aligned}\quad (23)$$

Then the definition of $D(X)$ is

$$D(X) = \chi_{H_1}^2(X, \hat{\zeta}) - \chi_{H_0}^2(X, \hat{\eta}).\quad (24)$$

Note that $(\chi_{H_0}^2(X, \hat{\eta}), \chi_{H_1}^2(X, \hat{\zeta}))$ stands for the version of $(T_{H_0}^{\min}(X), T_{H_1}^{\min}(X))$ that is based on Eq. (17).

Our goal is to obtain an approximation of the distribution of $D(X)$ under H_0 , when the data size is large. Hence a specific quantity, say m , is needed to reflect the magnitude of the data, in order that we can describe how other quantities in the model change along with it. For example, m could be the duration of the experiment or the total number of events. For the ease of description, let m represent the duration of the experiment in this section. Then $p = \frac{X}{m}$ stands for the per unit time observed counts in a potential experiment, and it would remain stable (instead of tending to infinity or zero) as m grows. So we say p is of order $O_p(1)$ (with respect to m)⁷.

In order to describe the modeling of counts rigorously, we introduce a set of notations, a summary of which is provided in Table I. Recall that when H_0 is the correct hypothesis, we employed $\mu(\eta)$ to denote the mean bin counts for models under this hypothesis, where η is the

⁷ The Big O , the small o , the Big O_p , and the small o_p notation are standard mathematical symbols, such that for two sequences of random variables $\{X_m\}$ and $\{Y_m\}$, we write

- $Y_m = o_p(X_m)$ if and only if $Y_m/X_m \rightarrow 0$ in probability as $m \rightarrow \infty$, and
- $Y_m = O_p(X_m)$ if and only if Y_m/X_m is bounded in probability as $m \rightarrow \infty$.

In the special case where $\{X_m\}$ and $\{Y_m\}$ are deterministic sequences, the stochastic o_p and O_p symbols reduce to the o and O symbols. See Ref. [22, sec 2.2] for details on the rules of calculus with these symbols.

vector of unknown nuisance parameters of dimension q . Denote the true value of η by η^0 , that is, $\mu^0 = \mu(\eta^0)$ is the true mean counts of the observation such that

$$N_i \stackrel{\text{indep}}{\sim} \text{Poisson}(\mu_i^0) \quad \text{for } i = 1, \dots, n.$$

When the data size is large, a very good approximation to the model above is given by

$$N_i \stackrel{\text{indep}}{\sim} \text{N}(\mu_i^0, \mu_i^0) \quad \text{for } i = 1, \dots, n.$$

Further, let $\pi := \mu/m$ denote the per unit time mean counts. To help explain these notations, take the example from Sec. IV B for instance, if $H_0 : (\sin^2 2\theta, |\Delta m^2|) = (\sin^2 2\theta_0, |\Delta m_0^2|)$ is the correct hypothesis, then $\pi_i = \mu_i(\eta)/m = a_i(\eta) \cdot P_i + b_i(\eta)$. The terms a_i and b_i are functions of order $O(1)$, and are determined by the con-

figuration of the experiment. For example, a_i can represent the detector efficiency, neutrino flux from reactor, target mass, etc., b_i can represent the backgrounds. Also, $P_i = 1 - \sin^2 2\theta_0 \cdot \sin^2(1.27 \cdot |\Delta m_0^2| \cdot L/E_i^\nu)$ represents the survival probability in a disappearance model.

Meanwhile, a competing framework, namely the collection of models that satisfy H_1 , specifies the mean counts incorrectly as $\nu(\zeta)$, where ζ is the unknown nuisance parameter of dimension q^* . Also, define the per unit time mean counts under H_1 by $\tau = \nu/m$. When H_0 is the correct hypothesis and that the true model is μ^0 , there exists a unique ζ^0 , such that $\hat{\zeta}$ approaches ζ^0 as $m \rightarrow \infty$. We will show in Appendix A that ζ^0 has the interpretation that it corresponds to the model $\nu(\zeta)$ among all that belong to the alternative framework that is the closest to the true model μ^0 in terms of the deviation $\sum_{i=1}^n \frac{(\mu_i^0 - \nu_i(\zeta))^2}{\nu_i(\zeta)}$. Denote $\nu^0 = \nu(\zeta^0)$.

2. Approximating the distribution of the test statistic $D(X)$

In this section, we always assume that H_0 is the correct hypothesis, under which we study the distribution of $D(X)$ defined in Eq. (24). For convenience, we will suppress the dependence on X in the notation, and write $D = \chi_{H_1}^2(\hat{\zeta}) - \chi_{H_0}^2(\hat{\eta})$. On one hand, it's well known that the distribution of $\chi_{H_0}^2(\hat{\eta})$ approaches the Chi-square distribution with degree of freedom $(n - q)$ as m increases. On the other hand, the limiting distribution of $\chi_{H_1}^2(\hat{\zeta})$ as m increases does not always exist. Indeed, the behavior of $\chi_{H_1}^2(\hat{\zeta})$ for large m is dependent on how far apart the mean counts of the best model under the alternative theoretical frameworks are from that of the true model. Denote the difference of per unit mean counts between the two models by $\delta = \pi^0 - \tau^0$. First, we state a classical assumption made in many statistical literatures (such as Ref. [10] and Ref. [12]) in order to obtain the limiting distribution of test statistics analogous to $\chi_{H_1}^2(\hat{\zeta})$, that is, the different versions of $T_{H_1}^{\min}(X)$:

$$[\text{A1}] \quad \delta = \pi^0 - \tau^0 = O(m^{-\frac{1}{2}}), \text{ that is, } \mu^0 - \nu^0 = O(m^{\frac{1}{2}}).$$

Assumption [A1] means that the best model under the wrong hypothesis is just barely incorrect. For example, under [A1], Ref. [10] showed that the likelihood ratio test statistic for testing H_1 against the full parameter space (that is, the statistic $T_{H_1}^{\min}(X)$ based on Eq. (15) and Eq. (16)) has a limiting non-central Chi-square distribution. The non-centrality parameter has the same form as the test statistic, but with $\hat{\mu}$ and $\hat{\nu}$ replaced by μ^0 and ν^0 . For a simplified presentation of this result, see, for example, Ref. [12, Sec. 3.1]. Under [A1], the non-centrality parameter is finite and the non-central Chi-square approximations are accurate to the extent that the $O_p(m^{-\frac{1}{2}})$ terms are neglected.

In contrast to [A1], we consider the following assumption, which is more general and realistic for the physics problem at hand:

$$[\text{A0}] \quad \delta = \pi^0 - \tau^0 = O(1), \text{ that is, } \mu^0 - \nu^0 = O(m).$$

In words, [A0] assumes that the difference in mean bin counts between the best model under the wrong hypothesis and the true model increases at the same rate as the data size m , or slower. Clearly, [A0] is a more relaxed condition than [A1], in the sense that [A1] implies [A0], but not vice versa. An example where [A0] holds and [A1] does not, is the case that the nuisance parameter is absent: each hypothesis allows exactly one model, such that the per unit mean bin counts of the model under H_0 is π^0 , and that under H_1 is τ^0 , where π^0 and τ^0 are vectors of constants that do not change with the data size m . As for general cases where there are nontrivial nuisance parameters, it is possible that the best model under H_1 can lead to τ^0 values that move closer to the truth π^0 as more data become available. Hence [A1] may become satisfied, while [A0] is always satisfied. In situations where one is unwilling to assert a convergence rate as fast as $O(m^{-\frac{1}{2}})$ for $(\tau^0 - \pi^0)$, if the convergence occur at all, [A0] is more appropriate than [A1].

To see the impact of using [A0] instead of [A1], it turns out that when $\lim_{m \rightarrow \infty} m^{\frac{1}{2}}\delta = \infty$, various test statistics similar to $\chi_{H_1}^2(\hat{\zeta})$ (these are the different versions of $T_{H_1}^{\min}$ that we mentioned in Sec. III A) would be unbounded in

	Under the correct hypothesis	Under the alternative hypothesis
General notation		
Mean bin counts	$\mu(\eta) = (\mu_1(\eta), \dots, \mu_N(\eta))$	$\nu(\zeta) = (\mu_1(\zeta), \dots, \mu_N(\zeta))$
Per-unit mean counts	$\pi(\eta) = \mu(\eta)/m$	$\tau(\zeta) = \nu(\zeta)/m$
True values or their closest approximations under the give model		
nuisance parameter	η_0 (a q -dim vector)	ζ_0 (a q^* -dim vector)
Mean bin counts	$\mu^0 = \mu(\eta_0)$	$\nu^0 = \nu(\zeta_0)$
Per-unit mean counts	$\pi^0 = \mu^0/m$	$\tau^0 = \nu^0/m$
Estimation based on observed data		
nuisance parameter	$\hat{\eta} = \arg \min \chi_{H_0}^2(\eta; X)$	$\hat{\zeta} = \arg \min \chi_{H_1}^2(\zeta; X)$
Mean bin counts	$\hat{\mu} = \mu(\hat{\eta})$	$\hat{\nu} = \nu(\hat{\zeta})$
Per-unit mean counts	$\hat{\pi} = \hat{\mu}/m$	$\hat{\tau} = \hat{\nu}/m$

TABLE I. Legend of symbols used in describing the correct model and the alternative model, respectively.

probability. Take the likelihood ratio test statistic mentioned above for example, the non-centrality parameter in the previous approximation grows to infinity as m increases. Further, the differences between the different versions of $\chi_{H_1}^2(\hat{\zeta})$ usually do not converge to 0 as m increases.

Although the limiting distribution does not necessarily exist under assumption [A0], it is still possible to approximate the distribution of $\chi_{H_1}^2(\hat{\zeta})$ at a finite, but large enough m . We make such an attempt, but this certainly requires a different derivation than the existing proofs that assume [A1]. In our derivation, we keep track of the terms that have higher order than constants when the data size m grows. Our proof follows the lines of that of Ref. [23, Chap. 16], but with significant modifications.

Write

$$\chi_{H_1}^2(\hat{\zeta}) = \sum_{i=1}^n \frac{(N_i - \hat{\nu}_i)^2}{\hat{\nu}_i} =: \sum_i f_i^2 \quad \text{and} \quad \chi_{H_0}^2(\hat{\eta}) = \sum_{i=1}^n \frac{(N_i - \hat{\mu}_i)^2}{\hat{\mu}_i} =: \sum_i e_i^2.$$

Here

$$f_i = f_i(\mathbf{a}, \mathbf{b}, \mathbf{c}) = \frac{N_i - \hat{\nu}_i}{\hat{\nu}_i^{\frac{1}{2}}} = \sqrt{m} \frac{p_i - \hat{\tau}_i}{\hat{\tau}_i^{\frac{1}{2}}} = \sqrt{m} \frac{(p_i - \pi_i^0) - (\hat{\tau}_i - \tau_i^0) + (\pi_i^0 - \tau_i^0)}{((\hat{\tau}_i - \tau_i^0) + \tau_i^0)^{\frac{1}{2}}} =: \sqrt{m} \frac{a_i - c_i + \delta_i}{(c_i + \tau_i^0)^{\frac{1}{2}}},$$

and

$$e_i = e_i(\mathbf{a}, \mathbf{b}, \mathbf{c}) = \frac{N_i - \hat{\mu}_i}{\hat{\mu}_i^{\frac{1}{2}}} = \sqrt{m} \frac{p_i - \hat{\pi}_i}{\hat{\pi}_i^{\frac{1}{2}}} = \sqrt{m} \frac{(p_i - \pi_i^0) - (\hat{\pi}_i - \pi_i^0)}{((\hat{\pi}_i - \pi_i^0) + \pi_i^0)^{\frac{1}{2}}} =: \sqrt{m} \frac{a_i - b_i}{(b_i + \pi_i^0)^{\frac{1}{2}}},$$

where $a_i = p_i - \pi_i^0 = O_p(m^{-\frac{1}{2}})$, $b_i = \hat{\pi}_i - \pi_i^0$, and $c_i = \hat{\tau}_i - \tau_i^0 = O_p(m^{-\frac{1}{2}})$, for $i = 1, \dots, n$. Then by the Taylor expansion of $\mathbf{f} = (f_1, \dots, f_n)^T$ and $\mathbf{e} = (e_1, \dots, e_n)^T$ around $(\mathbf{a}, \mathbf{b}, \mathbf{c}) = (0, 0, 0)$, we have

$$\mathbf{f} = \sqrt{m} \text{diag}\{\tau^0\}^{-\frac{1}{2}} \delta + \text{diag}\{\tau^0\}^{-\frac{3}{2}} \left[\text{diag}\{\tau^0\} - \frac{1}{2} \text{diag}\{\pi^0 + \tau^0\} E^* \right] \sqrt{m} (p - \pi^0) + O_p(m^{-\frac{1}{2}}),$$

where the three terms in the above expression are of order $O_p(m^{\frac{1}{2}})$, $O_p(1)$ and $O(m^{-\frac{1}{2}})$ respectively. Further,

$$\mathbf{e} = \text{diag}\{\pi^0\}^{-\frac{1}{2}} (I - D) \sqrt{m} (p - \pi^0) + O_p(m^{-\frac{1}{2}}),$$

where $D = B(B^T \text{diag}\{\pi^0\}^{-1} B)^{-1} B^T \text{diag}\{\pi^0\}^{-1}$, and the two terms in the above expression are of order $O_p(1)$ and $O_p(m^{-\frac{1}{2}})$ respectively. Therefore

$$\begin{aligned} D &= \chi_{H_1}^2(\hat{\eta}) - \chi_{H_0}^2(\hat{\zeta}) = \mathbf{f}^T \mathbf{f} - \mathbf{e}^T \mathbf{e} \\ &= m \delta^T \text{diag}\{\tau^0\}^{-1} \delta + 2\sqrt{m} \delta^T \text{diag}\{\tau^0\}^{-2} \left[\text{diag}\{\tau^0\} - \frac{1}{2} \text{diag}\{\pi^0 + \tau^0\} E^* \right] \sqrt{m}(p - \pi^0) + O_p(1) \\ &= m \delta^T \text{diag}\{\tau^0\}^{-1} \delta + 2\sqrt{m} \delta^T \text{diag}\{\tau^0\}^{-1} \sqrt{m}(p - \pi^0) \\ &\quad - \frac{1}{2} \sqrt{m} \left[\delta^T \text{diag} \left\{ \frac{\pi^0 + \tau^0}{(\tau^0)^2} \right\} B^* \right] \left(B^{*T} \text{diag} \left\{ \frac{(\pi^0)^2}{(\tau^0)^3} \right\} B^* \right)^{-1} B^{*T} \text{diag} \left\{ \frac{\pi^0}{(\tau^0)^2} \right\} \sqrt{m}(p - \pi^0) + O_p(1) \end{aligned}$$

According to Eq. (40) of Lemma 1, the term in the closed bracket above reduces to 0. Hence

$$D = m \delta^T \text{diag}\{\tau^0\}^{-1} \delta + 2\sqrt{m} \delta^T \text{diag}\{\tau^0\}^{-1} \sqrt{m}(p - \pi^0) + O_p(1).$$

Denote the first term of D by

$$D_1 = m (\pi^0 - \tau^0)^T \text{diag}\{\tau^0\}^{-1} (\pi^0 - \tau^0) = \sum_{i=1}^n \frac{(\mu_i^0 - \nu_i^0)^2}{\nu_i^0} = \min_{\nu} \sum_{i=1}^n \frac{(\mu_i^0 - \nu_i)^2}{\nu_i} =: \bar{D}, \quad (25)$$

where the second to last equality follows from Appendix A. Note that under assumption [A0], $D_1 = \bar{D}$ is of order $O(m)$. Next denote the second term of D by D_2 . The central limit theorem implies that as m increases to infinity, $\sqrt{m}(p - \pi^0)$ converges in distribution to the $N(0, \text{diag}\{\pi^0\})$ distribution. Hence $D_2/(2\sqrt{m})$ converges in distribution to the $N(M_2, V_2)$ where

$$M_2 = \delta^T \text{diag}\{\tau^0\}^{-1} 0 = 0,$$

and

$$\begin{aligned} V_2 &= \delta^T \text{diag}\{\tau^0\}^{-1} \text{diag}\{\pi^0\} \text{diag}\{\tau^0\}^{-1} \delta \\ &= \delta^T \text{diag}\{(\tau^0)^{-1}\} \delta + \delta^T \text{diag}\left\{ \frac{\pi^0 - \tau^0}{(\tau^0)^2} \right\} \delta \\ &= \frac{\bar{D}}{m} + \sum_{i=1}^n \frac{(\pi_i^0 - \tau_i^0)^3}{(\tau_i^0)^2} =: \frac{\bar{D}}{m} + s. \end{aligned}$$

Note that both $\frac{\bar{D}}{m}$ and s are of order $O(1)$ under assumption [A0], hence $D_2 = O_p(m^{\frac{1}{2}})$. In summary, under assumption [A0], we have $D = D_1 + D_2 + O_p(1)$, where

$$D_1 + D_2 \stackrel{\text{approx.}}{\sim} N(\bar{D}, 4\bar{D} + 4ms). \quad (26)$$

Remarks and Implications of Eq. (26)

or in other words,

1. For the common physics problem that we are interested in, additional simplification can be made to the approximating distribution, $N(\bar{D}, 4\bar{D} + 4ms)$. Specifically, in searching for new physics through precision measurements, the mean bin counts of the true model and that of the best model under the alternative hypothesis are relatively close to each other, that is,

$$|\mu_i^0 - \nu_i^0| \ll \mu_i^0 \sim \nu_i^0,$$

$$\begin{aligned} \frac{(\mu_i^0 - \nu_i^0)}{\mu_i^0} &= \frac{\delta_i^0}{\pi_i^0} \ll 1 \quad \text{and} \\ \frac{(\mu_i^0 - \nu_i^0)}{\nu_i^0} &= \frac{\delta_i^0}{\tau_i^0} \ll 1. \end{aligned} \quad (27)$$

In such situations, one can ignore the ms term in Eq. (26), because $ms = \sum_i \frac{(\mu_i^0 - \nu_i^0)^2}{\nu_i^0} \cdot \frac{\mu_i^0 - \nu_i^0}{\nu_i^0} \ll \sum_i \frac{(\mu_i^0 - \nu_i^0)^2}{\nu_i^0} = \bar{D}$. Then our main result becomes

$$D(X) \stackrel{\text{approx.}}{\sim} N(\bar{D}, 4\bar{D}). \quad (28)$$

2. We claimed in Sec. IV A that, at large data limit, the three versions of $\Delta T(X) = T_{H_1}^{\min}(X) - T_{H_0}^{\min}(X)$ based on the definition of T_{H_0} (and the corresponding T_{H_1}) in Eq. (15), (16), and Eq. (18), each have negligible difference from the $D(X)$. We validate this claim as follows.

For the moment, we drop the penalty term $\chi_{\text{penalty}}^2(\eta)$ from Eq. (15)–(18) for simplicity. And we will address the issue of the penalty term in the next remark.

First, for Eq. (15), we have,

$$\begin{aligned} T_{H_0}(X) &= \sum_i 2 \left(\mu_i - N_i + N_i \log \left(1 - \frac{\mu_i - N_i}{\mu_i} \right) \right) \\ &= \sum_i \frac{(\mu_i - N_i)^2}{\mu_i} + O_p(m^{-\frac{1}{2}}). \end{aligned}$$

The last step was obtained through expanding $\log \left(1 - \frac{\mu_i - N_i}{\mu_i} \right)$ at large data limit, ($|N_i - \mu_i| =$

$O_p(\mu_i^{\frac{1}{2}}) = O_p(m^{\frac{1}{2}})$). Next, for Eq. (16), we have,

$$\begin{aligned} T_{H_0}(X) &= \sum_i \left(\frac{(\mu_i - N_i)^2}{\mu_i} + \log \left(1 + \frac{\mu_i - N_i}{N_i} \right) \right) \\ &= \sum_i \frac{(\mu_i - N_i)^2}{\mu_i} + O_p(m^{-\frac{1}{2}}). \end{aligned}$$

Finally, for Eq. (18), we have,

$$\begin{aligned} T_{H_0}(X) &= \sum_i \frac{(\mu_i - N_i)^2}{N_i} \\ &= \sum_i \frac{(\mu_i - N_i)^2}{\mu_i} + O_p(m^{-\frac{1}{2}}). \end{aligned}$$

The differences between each version of $T_{H_0}(X)$ and $\sum_i \frac{(\mu_i - N_i)^2}{\mu_i}$ are negligible. Next we examine the differences between each version of $T_{H_1}(X)$ and $\sum_i \frac{(\nu_i - N_i)^2}{\nu_i}$. We will only consider situations where condition Eq. (27) hold. If so, the term $\frac{\nu_i - N_i}{N_i} = \frac{\delta_i}{\pi_i} + O_p(m^{-\frac{1}{2}}) \ll 1$, which will help validate the following three approximations. First, for Eq. (15), we have,

$$\begin{aligned} T_{H_1}(X) &= \sum_i 2 \left(\nu_i - N_i + N_i \log \frac{N_i}{\nu_i} \right) = \sum_i 2 \left(\nu_i - N_i + N_i \log \left(1 - \frac{\nu_i - N_i}{\nu_i} \right) \right) \\ &= \sum_i \frac{(\nu_i - N_i)^2}{\nu_i} \cdot \left(1 + O \left(\frac{(\nu_i - N_i)}{\nu_i} \right) \right). \end{aligned}$$

Next, for Eq. (16), we have,

$$T_{H_1}(X) = \sum_i \frac{(\nu_i - N_i)^2}{\nu_i} - \sum_i \log \left(1 - \frac{\nu_i - N_i}{\nu_i} \right) = \sum_i \frac{(\nu_i - N_i)^2}{\nu_i} \cdot \left(1 + O \left(\frac{1}{\nu_i - N_i} \right) \right).$$

Finally, for Eq. (18), we have,

$$T_{H_1}(X) = \sum_i \frac{(\nu_i - N_i)^2}{N_i} = \sum_i \frac{(\nu_i - N_i)^2}{\nu_i} \cdot \left(1 + O \left(\frac{\nu_i - N_i}{N_i} \right) \right).$$

In situations where Eq. (27) is satisfied, the differences between each version of $T_{H_1}(X)$ and $\sum_i \frac{(\nu_i - N_i)^2}{\nu_i}$ are very small compared to the latter and are hence negligible.

It follows that the different versions of the test statistic $\Delta T(X)$ will behave similarly as $D(X)$. Finally, it is easy to see that our definition for $\bar{D}$ in Eq. (25) is equivalent to $\bar{\Delta T}$ (defined in Eq. (20)) based on Eq. (17). Our main result in Eq. (28) can

be stated as

$$\Delta T \stackrel{\text{approx.}}{\sim} N(\bar{\Delta T}, 4|\bar{\Delta T}|). \quad (29)$$

3. We emphasize that Eq. (24) is a specific form of T in Eq. (15), (16), (17), and Eq. (18). The penalty term in T represents the constraint of systematic uncertainties, and is commonly obtained by dedicated measurements. When one includes the dedicated measurements as part

of Chi-square definition, one naturally recovers Eq. (24). Therefore, our proof in Sec. IIIB is also valid for test statistics with the format of T in Eq. (15), (16), (17), and Eq. (18).

4. We comment on the large data limit, which is required to reach the final conclusion (Eq. (28)) and to show the equivalence of Eq. (15), (16), (17), and Eq. (18). For a single bin, $\frac{N_i - \mu_i}{\mu_i}$ is negligible if N_i is greater than about 100. For multiple bins, the contributions from each bin will likely cancel and the condition can be relaxed in practice to that the total number of events, $\sum_i N_i$, is greater than about 100.

In summary of this section, we showed the following result. Assume the following set of conditions hold:

1. CD1: the parameter space ($\mathcal{H}$) of the nuisance parameters η and ζ are both continuous and the model likelihood function is a smooth function (for example three times differentiable) in the parameters,
2. CD2: the data size N_i is large for each $i = 1, \dots, n$,
3. CD3: the best model under the null hypothesis H_0 and the alternative hypothesis H_1 are relatively close, in the sense that $|\mu_i^0 - \nu_i^0| \ll \mu_i^0 \sim \nu_i^0$, for $i = 1, \dots, n$.

Then a simple approximation for the distribution of $\Delta T(X)$ under H_j , for either $j = 0$ or 1 , is the Gaussian distribution with mean $\overline{\Delta T_{H_j}}$ and standard deviations $2\sqrt{|\overline{\Delta T_{H_j}}|}$. Based on the Gaussian approximation, the CL_s value is easily calculated with $\Delta T(x)$, $\overline{\Delta T_{H_0}}$, and $\overline{\Delta T_{H_1}}$. In case any of the above conditions (CD1-CD3) breaks down, the distribution of $\Delta T(X)$ is not necessarily well approximated by the Gaussian distribution, and should instead be estimated through Monte Carlo simulations.

IV. THE CL_s APPROACH BASED ON THE ΔT STATISTIC

The $\Delta T(x)$ statistic described in the previous section can be used to form both CIs and CL_s , and they differ in how the associated p-values are utilized. Note that both procedures are easy to carry out because of the simple Gaussian approximation for the distribution of $\Delta T(x)$. We will introduce the CL_s approach with the $\Delta T(x)$ statistic below. The principle of forming CIs with $\Delta T(x)$ is the same as that with $\Delta\chi^2$.

FIG. 2. (color online) Illustration of the CL_s approach with log-likelihood ratio ΔT . In order to be consistent with the convention in Ref. [24], we plot the densities of $-\Delta T$ instead. See text for more discussions.

A. The CL_s Approach Based on the ΔT Statistic

The CL_s approach [13–15] is a popular approach to present searches for new physics beyond the Standard Model. Recent examples of using this approach in neutrino physics can be found in Ref. [25, 26]. Examples of using this approach in LHC super particle search can be found at Ref. [27, 28]. We emphasize that, the CL_s approach is a different way to present statistical results than the traditional approach of setting confidence intervals (CI). The traditional CI approach is appropriate in treating established signals [15]. Whereas the CL_s approach is appropriate in setting exclusion limits, such that models with parameter values beyond the limits are much worse than the Standard Model in fitting the observed data. In this section, we briefly review the principle of the CL_s approach in a two-hypotheses testing problem.

Fig. 2 is a heuristic illustration of the distribution of the log-likelihood ratio $\Delta T(X)$, where X stands for data from a potential repeat of the experiment. The black (red) curve stands for the density function of the expected distribution of $\Delta T(X)$ under the assumption that the null (alternative) hypothesis is true. The green line represents $\Delta T(x)$ calculated from the observed data x . A positive (negative) $\Delta T(x)$ would favor H_0 (H_1) over H_1 (H_0). The CL_s value is then defined as:

$$\text{CL}_s(x) = \frac{1 - p_1}{1 - p_0}, \quad (30)$$

where $1 - p_1$ ($1 - p_0$) is the probability that a potential repeat of the experiment will yield a $\Delta T(X)$ value larger than $\Delta T(x)$ when the alternate (null) hypothesis is true. Hence, the definition of CL_s in Eq. (30) suggests that a CL_s value close to zero would favor H_0 against H_1 . On the other hand, as illustrated in Fig. 3, a CL_s value close to one does not necessarily indicate that H_1 is favored against H_0 . In searching for new physics beyond the Standard Model, H_0 is typically specified to be the Standard Model. The exclusion region of the parameter

FIG. 3. (color online) Same as Fig. 2 except that the null hypothesis H_0 and the alternative hypothesis H_1 are very close to each other.

space is typically defined as the set of parameter values of new physics that corresponds to CL_s value smaller than $\alpha = 0.05$ [24], while other threshold values of the CL_s can be used as well.

Note that the CL_s value is never smaller than $(1 - p_1)$, the p-value used in the corresponding CI approach. Hence, had the exclusion contour at α been used to set a CI, it would have coverage probability over $1 - \alpha$. Nevertheless, the CL_s value appears to be a more reasonable measure of extremeness than $(1 - p_1)$, in situations where H_0 and H_1 are very similar (see Fig. 3). For example, assuming the data x is an “extreme” measurement with respect to H_1 (i.e. small p_1), it will also be disfavored by H_0 (i.e. small p_0). If only a single p-value, either p_0 or p_1 , is examined as in the CI approach, then one would draw the inappropriate conclusion of excluding H_0 or H_1 while favoring the other hypothesis. However, since the hypotheses H_0 and H_1 are similar, the data does not carry enough information to differentiate them. The CL_s value, which is the ratio between $1 - p_1$ and $1 - p_0$ will protect against such situations.

In order to obtain the value of p_0 and p_1 required to calculate the CL_s , one needs to find the distribution of $\Delta T(X)$ under H_0 and H_1 . While Monte Carlo simulations can provide approximations to the distribution of $\Delta T(X)$, simpler methods, such as Gaussian approximations, are desired to lower the computing burden.

B. Setting Exclusion Sets with the Gaussian CL_s Method

In this section, we illustrate the procedure of setting exclusion sets with the Gaussian CL_s method for the neutrino oscillation example from Sec. II.

Here the parameter of interest is $\beta = (\sin^2 2\theta, |\Delta m^2|)$. The mean count for the i th bin is described as $\mu_i(\eta) = m \cdot (a_i(\eta)P_i(\sin^2 2\theta_0, |\Delta m_0^2|) + b_i(\eta))$, where a_i and b_i are coefficients that depend on the vector of nuisance parameters η , and m represents the amount of accumulated data. It is typical to use $\beta_0 = (0, |\Delta m_0^2|)$ as a reference

parameter point, where $|\Delta m_0^2|$ can be any fixed value since it does not enter the model for bin counts when $\sin^2 2\theta = 0$. In this case, the null hypothesis is specified to be $H_0: \beta = \beta_0$ (i.e. the Standard Model with three light neutrinos). Next, for any $\beta_1 = (\sin^2 2\theta_1, |\Delta m_1^2|)$ from the parameter space $\Theta \times M$, specify the alternative hypothesis to be $H_1: \beta = \beta_1$, and perform the following procedure:

1. From the observed data x , obtain

$$\Delta T(x) := T_{H_1}^{\min}(x) - T_{H_0}^{\min}(x).$$

2. From the Asimov data set $x_{H_0}^{\text{Asimov}}$, obtain

$$\overline{\Delta T}_{H_0} = \Delta T(x_{H_0}^{\text{Asimov}}) = T_{H_1}^{\min}(x_{H_0}^{\text{Asimov}})$$

according to Eq. (20). Then according to the main result that we prove in Sec. III B, under H_0 , $\Delta T(X)$ follows approximately a Gaussian distribution with mean $\overline{\Delta T}_{H_0}$ and standard deviation $2\sqrt{|\overline{\Delta T}_{H_0}|}$. This suggests that one can approximate $1 - p_0$ using

$$1 - p_0 \approx \frac{1 + \text{Erf}\left(\frac{\overline{\Delta T}_{H_0} - \Delta T(x)}{\sqrt{8|\overline{\Delta T}_{H_0}|}}\right)}{2}, \quad (31)$$

where $\text{Erf}(s) = \frac{2}{\sqrt{\pi}} \int_0^s e^{-t^2} dt$ is the Gaussian error function for any $s \in (-\infty, \infty)$.

3. Similarly, from the Asimov data set $x_{H_1}^{\text{Asimov}}$, obtain

$$\overline{\Delta T}_{H_1} = \Delta T(x_{H_1}^{\text{Asimov}}) = -T_{H_0}^{\min}(x_{H_1}^{\text{Asimov}}).$$

according to Eq. (21). Then one can approximate $1 - p_1$ using

$$1 - p_1 \approx \frac{1 + \text{Erf}\left(\frac{\overline{\Delta T}_{H_1} - \Delta T(x)}{\sqrt{8|\overline{\Delta T}_{H_1}|}}\right)}{2}. \quad (32)$$

4. According to Eq. (30), the CL_s value at $(\sin^2 2\theta_1, |\Delta m_1^2|)$ can be approximated by

$$\text{CL}_s \approx \frac{1 + \text{Erf}\left(\frac{\overline{\Delta T}_{H_1} - \Delta T(x)}{\sqrt{8|\overline{\Delta T}_{H_1}|}}\right)}{1 + \text{Erf}\left(\frac{\overline{\Delta T}_{H_0} - \Delta T(x)}{\sqrt{8|\overline{\Delta T}_{H_0}|}}\right)}. \quad (33)$$

The point $(\sin^2 2\theta_1, |\Delta m_1^2|)$ is assigned to the 95% CL_s exclusion set if and only if its CL_s value is smaller than 5%.

In terms of the computing effort, the above CL_s procedure requires the calculation of $\Delta T(x)$, $\overline{\Delta T}_{H_1}$, and $\overline{\Delta T}_{H_0}$ at each parameter point in $\Theta \times M$. In comparison, the standard Wilks CI method based on $\Delta\chi^2(x)$ in Eq. (7) requires the calculation of $\Delta\chi^2(x)$ at each parameter point. So the computing cost of the Gaussian CL_s method is about three times that of the Wilks' CI method. In summary, both methods are easily affordable computationally, but the CL_s method is valid under much less restrictive conditions (CD1-CD3).

V. AN EXAMPLE: SEARCH FOR STERILE NEUTRINO

In this section, we introduce an example based on the search for a sterile neutrino. In this example, various methods to carry out the CL_s approach and the CI approach are compared.

A. Model Description

In this model, there are two detectors and one neutrino source. One detector is located at 300 kilo-meters from the neutrino source and is called the near detector. The other detector is located at 1000 kilo-meters from the neutrino source and is called the far detector. As shown in Fig. 4, the neutrino energy E_ν covers from 1 GeV to 9 GeV, and a flat (energy independent) neutrino energy spectrum is assumed. We further assume the detector can measure the spectrum with 20 energy bins equally spaced between 1 GeV and 9 GeV. The mean number of neutrino events seen by the near (far) detector without any oscillation is 10 k (0.9 k) per bin. We consider two types of oscillation measurements: a disappearance measurement with oscillation formula

$$P_{dis} = 1 - \sin^2 2\theta \cdot \sin^2 \left(1.27 \cdot \Delta m^2 \frac{L}{E_\nu} \right), \quad (34)$$

$$T = \sum_{j=n,f} \sum_{i=1}^{20} 2 \left(\mu_i^j(\epsilon, \eta_j, \sin^2 2\theta, \Delta m^2) - N_i^j + N_i^j \log \frac{N_i^j}{\mu_i^j(\epsilon, \eta_j, \sin^2 2\theta, \Delta m^2)} \right) + \frac{\epsilon^2}{0.05^2} + \frac{\eta_n^2}{0.02^2} + \frac{\eta_f^2}{0.02^2}. \quad (36)$$

Here, i represents the bin number and ranges from 1 to 20. j labels the near or the far detector. μ_i^j is the mean number of events in i -th bin and j -th detector. It depends on the oscillation parameters: $\sin^2 2\theta$ and Δm^2 , and the nuisance parameters: ϵ for the detector efficiency and neutrino flux, and η_n (η_f) for the near (far) detector background normalization factors.

B. The Wilks' CI method vs. the MC CI method

For the example mentioned above, the Wilks' method is unsuitable for setting CI for the parameter $\sin^2 2\theta$ because the conditions required are not satisfied as stated in Sec. II. In comparison, the computationally intensive MC CI method need to be used to set CI in this example. The purpose of this section is to demonstrate the practical difference between the two methods. Here, we

and an appearance measurement with oscillation formula

$$P_{app} = \sin^2 2\theta \cdot \sin^2 \left(1.27 \cdot \Delta m^2 \frac{L}{E_\nu} \right), \quad (35)$$

where θ is the neutrino mixing angle, Δm^2 is the neutrino mass squared difference, and L is the distance that neutrino travels.

We further include a background with a linear dependence on E_ν . The number of background events starts from 130 per bin for the first bin to 73 per bin for the last (20th) bin. There are three nuisance parameters, ϵ , η_n , and η_f . The first one is associated with the detector efficiency and the neutrino flux, which is assumed to be accurate to 5%. This uncertainty is assumed to be correlated between the near and the far detectors. The second and the third nuisance parameters are associated with the background normalization factors for the near and the far detectors, respectively. The normalization uncertainty is assumed to be 2% and uncorrelated between the two detectors. Fig. 4 shows the expected neutrino spectra. For the disappearance measurement, we compare the no-oscillation spectrum (the null hypothesis H_0 : $\sin^2 2\theta = 0$) with an oscillation spectrum (an alternative hypothesis H_1 : $\sin^2 2\theta = 0.06$ at $\Delta m^2 = 2.5 \times 10^{-3} \text{ eV}^2$). For the appearance measurement, we compare the no-oscillation spectrum (the null hypothesis H_0 : $\sin^2 2\theta = 0$) with two oscillation spectra (two alternative hypotheses H_1 : $\sin^2 2\theta = 0.008$ or $\sin^2 2\theta = 0.03$ at $\Delta m^2 = 2.5 \times 10^{-3} \text{ eV}^2$). Given a Monte Carlo (MC) sample N_i^j , we use the following test statistic based on the Poisson likelihood, in line of Eq. (15):

examine the distribution of the test statistic in Eq. (37) under the hypothesis H_0 : $\sin^2 2\theta = 0$, where the Wilks' method is especially problematic. To implement the MC CI method, we generate a large number of MC samples assuming that $\sin^2 2\theta = 0$. The MC samples have statistical fluctuations according to Poisson distributions, and systematic variations through randomizing the three nuisance parameters according to normal distributions. While the minimization process in calculating $T^{\min}$ follows the Frequentist's approach, the randomization of the nuisance parameters corresponds to a Bayesian integral over the nuisance parameters. It is a common hybrid Bayesian/Frequentist approach [19]. As a comparison, we also tried a full Frequentist approach as illustrated in Ref. [7, 20]. Results are very similar to that of the hybrid approach. In the latter approach, MCs are generated using the best-fit nuisance parameters obtained in analyzing the data under the $\sin^2 2\theta = 0$ hypothesis.

FIG. 4. (color online) Top panels show the mean number of events seen at the near and far detectors in a disappearance experiment. Bottom panels show the mean number of events seen at near and far detectors in an appearance experiment. Left and right panels show near and far detectors, respectively. See text for more explanations.

For each MC sample, we find $T^{\min}$ and $T_{H_0}^{\min}$, where $T^{\min}$ is the minimum value of T from Eq. (36) in the 5-dimensional parameter space of $(\sin^2 2\theta, \Delta m^2, \epsilon, \eta_n, \eta_f)$, and $T_{H_0}^{\min}$ is the minimum value of T under the restriction, $\sin^2 2\theta_{\text{true}} = 0$. Then we form the test statistic

$$\Delta\chi^2 = T_{H_0}^{\min} - T^{\min}. \quad (37)$$

Fig. 5 shows the distribution of $\Delta\chi^2$, which clearly does not follow a Chi-square distribution with two degrees of freedom. In summary, for this example, the Wilks' method can not be used to correctly set CIs based on the test statistic $\Delta\chi^2$. It is possible to explore alternative formula than that of the Wilks' method, if one takes the hybrid approach in Ref. [19] and finds an analytic approximation to the solution of t_c for the equation $\text{Prob}(\Delta\chi^2 \leq t_c) \geq c$, where the probability is evaluated over the distribution of the nuisance parameters. Otherwise, one can always obtain the distribution of $\Delta\chi^2$ through the computationally intensive MC CI method.

C. Validity of the Gaussian Approximation in the Gaussian CL_s method

For the example in the previous section, there is no known way to set CI without computationally intensive MC simulations. This is the main motivation for using the Gaussian CL_s method as an alternative. In this

FIG. 5. (color online) Distributions of $\Delta\chi^2 = T(\sin^2 2\theta = 0) - T_{\min}$ is plotted for MCs with the true $\sin^2 2\theta = 0$. Distributions based on the hybrid Bayesian/Frequentist and full Frequentist approaches are compared to the Chi-square distribution with two degrees of freedom.

section, we check how closely does the CL_s test statistic $\Delta T = T_{H_1}^{\min} - T_{H_0}^{\min}$ follow the normal distribution $N(\overline{\Delta T}, 4\overline{\Delta T})$. Here, $T_H^{\min}$ is the value of the test statistic T from Eq. (36) under the hypothesis H , minimized over the nuisance parameters $(\epsilon, \eta_n, \eta_f)$. Fig. 6 shows the distribution of ΔT for the disappearance measurement. The null hypothesis H_0 corresponds to $\sin^2 2\theta = 0$. The alternative hypothesis H_1 corresponds to $\sin^2 2\theta = 0.06$

FIG. 6. (color online) The test statistic $\Delta T = T_{H_1}^{\min} - T_{H_0}^{\min}$ is plotted for MCs (disappearance) assuming the hypothesis H_0 or H_1 is true. Here, the null hypothesis H_0 corresponds to $\sin^2 2\theta = 0$. The alternative hypothesis H_1 corresponds to $\sin^2 2\theta = 0.06$ and $\Delta m^2 = 2.5 \times 10^{-3} \text{ eV}^2$.

and $\Delta m^2 = 2.5 \times 10^{-3} \text{ eV}^2$. The histograms on the left (right) are made from the MC samples assuming H_1 (H_0) is true. We also compare them with the expected normal distribution $N(\overline{\Delta T}, 4\overline{\Delta T})$ from the $\overline{\Delta T}_{H_0}$ and $\overline{\Delta T}_{H_1}$ calculated from the Asimov data sets. Good agreements are observed.

Similarly, we also check the appearance measurements. In Fig. 7, the null hypothesis H_0 corresponds to $\sin^2 2\theta = 0$, and the alternative hypothesis H_1 corresponds to $(\sin^2 2\theta, \Delta m^2) = (0.008, 2.5 \times 10^{-3} \text{ eV}^2)$. In Fig. 8, H_0 corresponds to $\sin^2 2\theta = 0$, and H_1 corresponds to $(\sin^2 2\theta, \Delta m^2) = (0.03, 2.5 \times 10^{-3} \text{ eV}^2)$. The agreement between the MCs and expectations in Fig. 7 is slightly worse than that in Fig. 6, but is still reasonably good. However, the difference between the MCs and expectations in Fig. 8 becomes large. This is because the third regularity condition CD3 “when the prediction of two hypotheses (the null hypotheses H_0 and the alternative hypothesis H_1 are relatively close or $|\mu_i - \nu_i| \ll \mu_i \sim \nu_i$ ” is no longer met. In a disappearance search, CD3 can be easily satisfied. However, this may not be true in an appearance experiment as the mean number of signal events is zero when $\sin^2 2\theta = 0$. When H_0 and H_1 are $\sin^2 2\theta = 0$ and $(\sin^2 2\theta, \Delta m^2) = (0.008, 2.5 \times 10^{-3} \text{ eV}^2)$, respectively, CD3 is still reasonably well satisfied with the existence of backgrounds. When H_0 and H_1 are $\sin^2 2\theta = 0$ and $(\sin^2 2\theta, \Delta m^2) = (0.03, 2.5 \times 10^{-3} \text{ eV}^2)$, respectively, CD3 is severely violated. Note that in such situations where H_0 and H_1 are very different, the experimental data is most likely able to exclude one hypothesis easily, making it less interesting to carry out such a statistical test. **Nevertheless, we emphasize it is crucial to validate Gaussian approximation with MCs in practice when any of CD1-CD3 listed in the end of Sec. III are marginally satisfied.**

FIG. 7. (color online) The test statistic $\Delta T = T_{H_1}^{\min} - T_{H_0}^{\min}$ is plotted for MCs (appearance) assuming the hypothesis H_0 or H_1 is true. Here, the null hypothesis H_0 corresponds to $\sin^2 2\theta = 0$. The alternative hypothesis H_1 corresponds to $\sin^2 2\theta = 0.008$ and $\Delta m^2 = 2.5 \times 10^{-3} \text{ eV}^2$.

FIG. 8. (color online) The test statistic $\Delta T = T_{H_1}^{\min} - T_{H_0}^{\min}$ is plotted for MCs (appearance) assuming the hypothesis H_0 or H_1 is true. Here, the null hypothesis H_0 corresponds to $\sin^2 2\theta = 0$. The alternative hypothesis H_1 corresponds to $\sin^2 2\theta = 0.03$ and $\Delta m^2 = 2.5 \times 10^{-3} \text{ eV}^2$.

D. The Gaussian CL_s method vs. the ΔT -based CI method, both based on $\Delta T = T_{H_1}^{\min} - T_{H_0}^{\min}$

Recall that the CL_s approach is based on the test statistic $\Delta T = T_{H_1}^{\min} - T_{H_0}^{\min}$. Although typical methods to form CIs use a different type of test statistic, namely $\Delta\chi^2$ shown in the previous sections, one can in principle also set CIs based on ΔT , which we refer to as the ΔT -based CI method. Below, we use our example to compare the exclusion sets obtained from the Gaussian CL_s method and the CIs obtained from the ΔT -based CI method. For the former method, the exclusion set consists of parameter values that correspond to CL_s values, specifically $(1 - p_1)/(1 - p_0)$, lower than 0.05; and for the latter method, the CI consists of parameter values that correspond to p-values, specifically $(1 - p_1)$, over 0.05. The results are summarized in Fig. 9. In the example, the true $\sin^2 2\theta$ is assumed to be zero. The sensitivity of the Gaussian CL_s method is slightly worse than that of

FIG. 9. (color online) Comparison of the exclusion sets determined by the Gaussian CL_s method vs. the CI, both using the test statistic $\Delta T = T_{H_1}^{\min} - T_{H_0}^{\min}$. The true value of $\sin^2 2\theta$ is 0. For the CI (CL_s) method, the right side of the red (black) line has a p-value (CL_s value) smaller than 0.05. The sensitivity curves are generated from a large number of Monte Carlo samples. At each Δm^2 , 50% (50%) of MC samples will have a better (worse) exclusion limit than the sensitivity curve.

ΔT -based CI method, because the CL_s value is by construction larger than the p-value used in the CI method. Despite the slightly worse sensitivity, the CL_s produces smoother contours that agree better with intuition (not excluding hypotheses that are close to the null hypothesis) than the CI do. As shown in Fig. 9, the region that correspond to $\Delta m^2 \sim 5.5 \times 10^{-2} \text{ eV}^2$ and $\sin^2 2\theta < 0.01$

(also $\Delta m^2 \sim 0.1 \text{ eV}^2$ and $\sin^2 2\theta < 0.01$) is excluded from the 95% CI. This is inconsistent with intuition as the expected spectrum for small $\sin^2 2\theta$ values should be very similar to that of $\sin^2 2\theta = 0$, and we do not expect to exclude regions with small $\sin^2 2\theta$ values. This phenomenon can be understood as follows. With the test statistic ΔT , we compare two hypotheses each time. Therefore, even when the two hypotheses are very similar, the chance of excluding one hypothesis with CI can still be large as illustrated in Fig. 3. As we explained in Sec. IV A, the definition of the CL_s value avoid this problem, giving it an advantage over the traditional CI when test statistic ΔT is used.

E. The Gaussian CL_s method vs. the MC CI method vs. the Raster-Scan MC CI method

The statistical interpretation of (the complement of) exclusion sets obtained using the CL_s method is distinct from that of CIs. Indeed, if an exclusion contour based on thresholding the CL_s value at α is used to set a CI, its coverage probability will be over $1 - \alpha$. Nevertheless, it is still interesting to compare these two kinds of sets in specific physics problems, as seen in many literatures (for example, Ref. [15] and Ref. [29]). Below, we perform such a comparison under the set up of our example. Besides the CL_s approach and the standard $\Delta\chi^2$ -based CI approach, we also include results from another commonly used approach, the so-called raster-scan CI approach. In short, this approach scans through all values of the parameter $|\Delta m^2|$, and at each fixed $|\Delta m^2|$, it checks the compatibility of the other parameter $\sin^2 2\theta$ to the data. A most popular method to carry out the raster scan approach uses the following statistic at each $|\Delta m^2|$,

$$\Delta\chi_{RS}^2(\sin^2 2\theta, |\Delta m^2|; x) \equiv \chi^2(\sin^2 2\theta, |\Delta m^2|, \eta_{\min}(\sin^2 2\theta, |\Delta m^2|); x) - \chi_{RS \min}^2(|\Delta m^2|; x), \quad (38)$$

which is similar to the $\Delta\chi^2$ statistic given in Eq. (7) except that the global minimum $\chi_{\min}^2(x)$ is replaced by the restricted minimum $\chi_{RS \min}^2(|\Delta m^2|; x) = \min_{\sin^2 2\theta, \eta} \chi^2(\sin^2 2\theta, |\Delta m^2|, \eta; x)$. Given a fixed value of $|\Delta m^2|$, the raster scan method examines all $\sin^2 2\theta_1$ values, one at a time, and test the hypothesis $H_0: \sin^2 2\theta = \sin^2 2\theta_1$ based on the statistic $\Delta\chi_{RS}^2(\sin^2 2\theta_1, |\Delta m^2|; x)$. The raster scan approach is usually considered less ideal than the standard CI approach that we described in Sec. II, mainly because it does not make comparisons between hypotheses that have different values of $|\Delta m^2|$ and hence can not distinguish a likely value of this parameter from an unlikely one [6]. In addition, according to Eq. (34) and Eq. (35), when $\sin^2 2\theta = 0$, any value of $|\Delta m^2|$ will result in the same model, namely, the Standard Model. As a consequence, the Standard Model is tested many times against different new physics hypothe-

ses that correspond to different values of $|\Delta m^2|$, which makes it difficult to interpret the test results. Whereas in the standard CI approach, any model is tested only once. Similar to the case of $\Delta\chi^2$, the regularity condition of the Wilks' theorem would also break for $\Delta\chi_{RS}^2$ when the true $\sin^2 2\theta = 0$. Therefore, Monte Carlo is usually necessary to obtain the distribution of $\Delta\chi_{RS}^2$ to compute CIs using the raster scan.

Fig. 10 compares the sensitivity of the Gaussian CL_s method, the standard MC CI method, and the raster-scan MC CI method. We assumed that the true value of $\sin^2 2\theta$ is 0 in generating MC. At each Δm^2 , 50% (50%) of MC samples will have a better (worse) exclusion limit than the sensitivity curve. Sensitivities from these three methods are similar. The sensitivity of the 95% exclusion set from the Gaussian CL_s method is slightly better than that of the 95% CI from the MC CI method, and is in fact

FIG. 10. (color online) Comparison of the sensitivity of the 95% Gaussian CL_s method vs. that of the 95% and the 90% MC CI method. We also added the 95% raster-scan MC CI for comparison. The true value of $\sin^2 2\theta$ is 0. See texts for more explanations.

close to that of the 90% CI from the MC CI method for this setup. This is expected, since the test statistic $\Delta T = T_{H_1}^{\min} - T_{H_0}^{\min}$ used in the Gaussian CL_s method is designed to focus on the differences between the new physics hypotheses ($H_1 : \sin^2 2\theta = \sin^2 2\theta_1$ for some $\sin^2 2\theta_1 > 0$), with the Standard Model ($H_0 : \sin^2 2\theta = 0$). Therefore, when the true value of $\sin^2 2\theta$ is 0, the Gaussian CL_s method has larger power to exclude new physics hypotheses than the MC CI method. In addition, the 95% sensitivity from the Gaussian CL_s method is very close to that from the raster-scan MC CI method. This is actually a coincidence, since the CL_s method and the raster-scan method use the ratios of p-values and p-value to set limits, respectively. The left panel of Fig. 11 shows the difference between the CL_s sensitivity (CL_s value) and raster-scan sensitivity (p-value) at each parameter point. The difference is rather large at small values of $\sin^2 2\theta$, which indicates that the similarity of the 95% lines between the CL_s method and the raster-scan method is a coincidence. The right panel of Fig. 11 shows the sensitivity difference between the raster-scan MC CI method and the standard MC CI method. The sensitivity are also different, since the choice of test statistics are different between the raster-scan MC CI method and the standard MC CI method.

When the new physics is indeed true, the standard MC CI method has clear advantage in constraining the parameter space over the other two methods. This is shown in Fig. 12. The MC sample is generated with $\sin^2 2\theta_{\text{true}} = 0.1$ and $\Delta m_{\text{true}}^2 = 2.5 \times 10^{-3} \text{ eV}^2$ with statistical fluctuations and systematic variations. The 90% CI of the MC CI method were able to identify a small region close to the true value. In comparison, the 95% CL_s limit

successfully excluded the region on the right, but failed to exclude regions (on the left of line) far away from the true value. This again is due to the choice of the test statistic (ΔT in the Gaussian CL_s method vs. $\Delta\chi^2$ in the MC CI method). The proposed test statistic ΔT focuses on the difference between the new physics hypothesis and the Standard Model, while the test statistic $\Delta\chi^2$ takes into account all the likely values of $(\sin^2 2\theta, \Delta m^2)$. Therefore, we confirm the conclusion from Ref. [15]: “the CL_s technique for setting limits is appropriate for determining exclusion sets while the determination of CIs advocated by the Feldman-Cousins method is more appropriate for treating established signals”. For comparison, we also display the 95% raster-scan MC CI. Since the raster scan can not distinguish likely and unlikely values of the parameter $|\Delta m^2|$, it also failed to exclude some regions of the parameter space that are far away from the truth.

VI. DISCUSSION

In order to use the Gaussian CL_s method, it is important that the CD1-CD3 listed in the end of Sec. III are met. The first condition CD1 is continuity of the parameter space for the nuisance parameters, under both the null and the alternative hypotheses. This requirement is easier to achieve compared to the first regularity condition required by the Wilks’ theorem, since it concerns the nuisance parameters only, not the parameters of interest, $(\sin^2 2\theta, |\Delta m^2|)$. The second condition CD2 concerns large enough data size, which is also easier to reach compared to that required by the Wilks’ theorem. This is because in the Gaussian CL_s method tests a simpler pair of hypotheses, in which the values of $(\sin^2 2\theta, |\Delta m^2|)$ are fixed, and one automatically avoids the situation shown in Fig. 1b that involves minimization over a large range of $|\Delta m^2|$ in calculating the test statistic. The third condition CD3 is that the difference between the predictions of two hypotheses is small comparing to the predictions themselves. In searching for new physics with precision measurements, the signal from the Standard Model is usually much larger than the potential signal from new physics. Therefore, CD3 is generally satisfied. In the case that CD3 is violated or marginally satisfied (see Fig. 8), one should use Monte Carlo simulation to derive the distribution of the test statistic.

Similar to the Wilks’ CI method based on the test statistic $\Delta\chi^2$ and predefined constants, the Gaussian CL_s method also allows easy combination of multiple independent experimental results that probe the same parameter space. The CL_s value at each alternative hypothesis H_1

FIG. 11. (color online) Left panel: the difference between the CL_s sensitivity and the raster-scan sensitivity is shown at each parameter point. Right panel: the difference between the raster-scan sensitivity and the standard CI sensitivity is shown at each parameter point.

FIG. 12. (color online) Comparison of the 90% CIs from the MC method vs. 95% Gaussian CL_s limit for a MC sample generated with $\sin^2 2\theta = 0.1$ and $\Delta m^2 = 2.5 \times 10^{-3} \text{ eV}^2$. The 95% raster-scan MC CI is shown for comparison. See texts for more explanations.

from experiments ($k = 1, 2, \dots, m$) can be calculated with

$$\begin{aligned} \Delta T(x) &= \sum_{k=1}^m \Delta T(x_k), \\ \overline{\Delta T(x_{H_1}^{\text{Asimov}})} &= \sum_{k=1}^m \overline{\Delta T(x_{H_1}^{\text{Asimov } k})}, \\ \overline{\Delta T(x_{H_0}^{\text{Asimov}})} &= \sum_{k=1}^m \overline{\Delta T(x_{H_0}^{\text{Asimov } k})}, \end{aligned}$$

with $x = \sum_{k=1}^m$ is the combined data from all experiments. This can be easily achieved if each experiment releases their maps of T_{x_k} , $\overline{\Delta T(x_{H_1}^{\text{Asimov}})}$, and $\overline{\Delta T(x_{H_0}^{\text{Asimov}})}$. In practice, the main challenge in combining multiple experiment results arise from the potential correlation among different experiments and requires careful examinations.

So far, we have argued that, in practice, the CL_s method is often simple to use and allows easy combination of multiple results. But it is important to remind the readers that the CL_s is a limited method that aims at setting boundaries only. The CL_s based on ΔT does not directly address the question “do we see new physics or not”, nor does it provide estimate of parameters. To help address the first question, we recommend reporting the p-value based on the test statistic $\Delta\chi^2$ assuming the Standard Model is true, in addition to the obtained exclusion sets. To address the second question, the standard CI approach is needed. Indeed, the standard CI approach is the preferred approach to take whenever one can afford to carry it out correctly, because the standard CI approach is a unified approach to set limits in the absence of new physics signals and to estimate parameters after the discovery of new physics [6].

VII. SUMMARY

In this paper, we describe a method to present results in searching for new physics in a continuous parameter space. This method takes the CL_s approach to obtain exclusion sets for parameters. Specifically, the method consists of testing many pairs of hypotheses. Each time, a new physics model is tested against the Standard Model

using the log-likelihood ratio test statistic, or certain variations of it, denoted by ΔT . We provide a mathematical proof to show that the distribution of ΔT follows a Gaussian distribution at large data limit under either hypothesis, when the two hypotheses are relatively close. This result allows a simple alternative to the computationally intensive Monte Carlo method to calculate CL_s values, and thus to set exclusion limits in one or multiple dimensional parameter spaces. This method can also be used to conveniently combine results from multiple experiments.

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APPENDICES

A. A few basic properties of the fitted models under H_0 and H_1

Suppose H_0 is the correct hypothesis, that is, the data X came from H_0 . Having observed the data, the best

fitting models under H_0 and H_1 have estimated nuisance parameters $\hat{\eta}$ and $\hat{\zeta}$ respectively, as defined in Sec. IV. The corresponding per unit mean counts are denoted $\hat{\pi}$ and $\hat{\tau}$ respectively.

We show below that there is a unique limit of $\hat{\zeta}$ as the data size increases, and that it leads to the model $\nu(\zeta)$ that is the closest model under H_1 to the true model μ^0 under a certain criteria. Indeed, let $t_m(\zeta) = \chi_{H_1}^2(\zeta)/m = \sum_i \frac{(p_i - \tau_i(\zeta))^2}{\tau_i(\zeta)}$, and let $t(\zeta) = \sum_i \frac{(\pi_i^0 - \tau_i(\zeta))^2}{\tau_i(\zeta)}$. Since p converges almost surely (a.s.) to π^0 as m increases, we have $t_m(\zeta)$ converges a.s. to $t(\zeta)$. Then under regularity conditions, such as t_m being twice differentiable and convex in ζ , $\hat{\zeta}^m = \arg \min_{\zeta} t_m(\zeta)$ also converges a.s. to $\arg \min_{\zeta} t(\zeta)$ as m increases. By denoting the limit of $\hat{\zeta}^m$ by ζ^0 , we have $mt(\zeta^0) = \min_{\zeta} mt(\zeta)$. That is, ζ^0 and $\nu^0 := \nu(\zeta^0)$ are such that $\sum_{i=1}^n \frac{(\mu_i^0 - \nu_i^0)^2}{\nu_i^0} = \min_{\nu} \sum_{i=1}^n \frac{(\mu_i^0 - \nu_i)^2}{\nu_i}$.

We list a few more properties that are useful in the proof of Lemma 1 and the proof of the result in Eq. (26). It is well-known that $\hat{\eta} - \eta^0$ and $\hat{\pi} - \pi^0$ are both of order $O_p(m^{-\frac{1}{2}})$. And $\hat{\zeta} - \zeta^0$ and $\hat{\tau} - \tau^0$ are also both of order $O_p(m^{-\frac{1}{2}})$ according to Ref. [30].

B. Lemma 1

Lemma 1. *Assuming [A0], we have*

$$\sqrt{m} \begin{pmatrix} p - \pi^0 \\ \hat{\tau} - \tau^0 \end{pmatrix} = \begin{pmatrix} I \\ E^* \end{pmatrix} \sqrt{m} (p - \pi^0) + O_p(m^{-\frac{1}{2}}), \quad (39)$$

where

$$E^* = B^* \left(B^{*T} \text{diag} \left\{ \frac{(\pi^0)^2}{(\tau^0)^3} \right\} B^* \right)^{-1} B^{*T} \text{diag} \left\{ \frac{\pi^0}{(\tau^0)^2} \right\} \quad \text{and} \quad B_{n \times q^*}^* = \frac{\partial \tau^0}{\partial \zeta}.$$

Further,

$$B^{*T} \text{diag} \left\{ \frac{(\pi^0 + \tau^0)}{(\tau^0)^2} \right\} \delta = 0. \quad (40)$$

Proof. By definition, $\hat{\zeta}$ is such that

$$\frac{\partial \chi_{H_1}^2(\hat{\zeta})}{\partial \zeta_j} = 0 \quad \text{for } j = 1, \dots, q^*.$$

That is,

$$2 \sum_{i=1}^n \frac{N_i + \hat{\nu}_i}{\hat{\nu}_i^2} \frac{\partial \hat{\nu}_i}{\partial \zeta_j} (N_i - \hat{\nu}_i) = 0$$

$$\sum_{i=1}^n \frac{N_i + \hat{\nu}_i}{\hat{\nu}_i^2} \frac{\partial \hat{\nu}_i}{\partial \zeta_j} (N_i - \nu_i^0) = \sum_{i=1}^n \frac{N_i + \hat{\nu}_i}{\hat{\nu}_i^2} \frac{\partial \hat{\nu}_i}{\partial \zeta_j} (\hat{\nu}_i - \nu_i^0)$$

$$\sum_{i=1}^n \frac{p_i + \hat{\tau}_i}{\hat{\tau}_i^2} \frac{\partial \hat{\tau}_i}{\partial \zeta_j} (p_i - \pi_i^0 + \pi_i^0 - \tau_i^0) = \sum_{i=1}^n \frac{p_i + \hat{\tau}_i}{\hat{\tau}_i^2} \frac{\partial \hat{\tau}_i}{\partial \zeta_j} (\hat{\tau}_i - \tau_i^0). \quad (41)$$

Note by delta's method

$$\hat{\tau}_i = \tau_i^0 + \sum_k \frac{\partial \tau_i^0}{\partial \zeta_k} (\hat{\zeta}_k - \zeta_k^0) + O_p(m^{-1}) \quad \text{and} \quad \frac{\partial \hat{\tau}_i}{\partial \zeta_j} = \frac{\partial \tau_i^0}{\partial \zeta_j} + \sum_k \frac{\partial^2 \tau_i^0}{\partial \zeta_j \partial \zeta_k} (\hat{\zeta}_k - \zeta_k^0) + O_p(m^{-1}),$$

and

$$\frac{p_i + \hat{\tau}_i}{(\hat{\tau}_i)^2} - \frac{\pi_i^0 + \tau_i^0}{(\tau_i^0)^2} = \frac{1}{(\tau_i^0)^2} (p_i - \pi_i^0) - \frac{1}{(\tau_i^0)^2} (2 \frac{\pi_i^0}{\tau_i^0} + 1) (\hat{\tau}_i - \tau_i^0) + O_p(m^{-1}).$$

Hence, the lhs of Eq. (41) becomes

$$\begin{aligned} lhs &= \sum_{i=1}^n \left(\frac{\pi_i^0 + \tau_i^0}{(\tau_i^0)^2} + \frac{1}{(\tau_i^0)^2} (p_i - \pi_i^0) - \frac{1}{(\tau_i^0)^2} (2 \frac{\pi_i^0}{\tau_i^0} + 1) (\hat{\tau}_i - \tau_i^0) + O_p(m^{-1}) \right) \left(\frac{\partial \tau_i^0}{\partial \zeta_j} \right) (p_i - \pi_i^0 + \delta_i) \\ &= \sum_{i=1}^n \left(\frac{\pi_i^0 + \tau_i^0}{(\tau_i^0)^2} \right) \frac{\partial \tau_i^0}{\partial \zeta_j} \delta_i + \sum_{i=1}^n \left[\frac{\pi_i^0 + \tau_i^0}{(\tau_i^0)^2} + \frac{\delta_i}{(\tau_i^0)^2} \right] \frac{\partial \tau_i^0}{\partial \zeta_j} (p_i - \pi_i^0) - \sum_{i=1}^n \frac{1}{(\tau_i^0)^2} (2 \frac{\pi_i^0}{\tau_i^0} + 1) (\hat{\tau}_i - \tau_i^0) \left(\frac{\partial \tau_i^0}{\partial \zeta_j} \right) \delta_i + O_p(m^{-1}) \\ &= \sum_{i=1}^n \left(\frac{\pi_i^0 + \tau_i^0}{(\tau_i^0)^2} \right) \frac{\partial \tau_i^0}{\partial \zeta_j} \delta_i + \sum_{i=1}^n \frac{2\pi_i^0}{(\tau_i^0)^2} \frac{\partial \tau_i^0}{\partial \zeta_j} (p_i - \pi_i^0) - \sum_{i=1}^n \frac{2\pi_i^0 + \tau_i^0}{(\tau_i^0)^3} \delta_i \left(\frac{\partial \tau_i^0}{\partial \zeta_j} \right) (\hat{\tau}_i - \tau_i^0) + O_p(m^{-1}) \\ &= \sum_{i=1}^n \left(\frac{\pi_i^0 + \tau_i^0}{(\tau_i^0)^2} \right) \frac{\partial \tau_i^0}{\partial \zeta_j} \delta_i + \sum_{i=1}^n \frac{2\pi_i^0}{(\tau_i^0)^2} \frac{\partial \tau_i^0}{\partial \zeta_j} (p_i - \pi_i^0) - \sum_{i=1}^n \frac{2\pi_i^0 + \tau_i^0}{(\tau_i^0)^3} \delta_i \left(\frac{\partial \tau_i^0}{\partial \zeta_j} \right) \left(\sum_k \frac{\partial \tau_i^0}{\partial \zeta_k} (\hat{\zeta}_k - \zeta_k^0) + O_p(m^{-1}) \right) + O_p(m^{-1}) \\ &= \sum_{i=1}^n \left(\frac{\pi_i^0 + \tau_i^0}{(\tau_i^0)^2} \right) \frac{\partial \tau_i^0}{\partial \zeta_j} \delta_i + \sum_{i=1}^n \frac{2\pi_i^0}{(\tau_i^0)^2} \frac{\partial \tau_i^0}{\partial \zeta_j} (p_i - \pi_i^0) - \sum_k (\hat{\zeta}_k - \zeta_k^0) \sum_{i=1}^n \frac{2\pi_i^0 + \tau_i^0}{(\tau_i^0)^3} \delta_i \frac{\partial \tau_i^0}{\partial \zeta_j} \frac{\partial \tau_i^0}{\partial \zeta_k} + O_p(m^{-1}) \end{aligned}$$

The rhs of Eq. (41) becomes

$$\begin{aligned} rhs &= \sum_{i=1}^n \frac{p_i + \hat{\tau}_i}{\hat{\tau}_i^2} \frac{\partial \hat{\tau}_i}{\partial \zeta_j} (\hat{\tau}_i - \tau_i^0) \\ &= \sum_{i=1}^n \frac{p_i + \hat{\tau}_i}{\hat{\tau}_i^2} \frac{\partial \hat{\tau}_i}{\partial \zeta_j} \left(\sum_k \frac{\partial \tau_i^0}{\partial \zeta_k} (\hat{\zeta}_k - \zeta_k^0) + O_p(m^{-1}) \right) \\ &= \sum_k (\hat{\zeta}_k - \zeta_k^0) \sum_{i=1}^n \frac{p_i + \hat{\tau}_i}{\hat{\tau}_i^2} \frac{\partial \hat{\tau}_i}{\partial \zeta_j} \frac{\partial \tau_i^0}{\partial \zeta_k} + O_p(m^{-1}) \\ &= \sum_k (\hat{\zeta}_k - \zeta_k^0) \sum_{i=1}^n \left(\frac{\pi_i^0 + \tau_i^0}{(\tau_i^0)^2} + O_p(m^{-\frac{1}{2}}) \right) \left(\frac{1}{\tau_i^0} + O_p(m^{-\frac{1}{2}}) \right) \left(\frac{\partial \tau_i^0}{\partial \zeta_j} + O_p(m^{-\frac{1}{2}}) \right) \frac{\partial \tau_i^0}{\partial \zeta_k} + O_p(m^{-1}) \\ &= \sum_k (\hat{\zeta}_k - \zeta_k^0) \sum_{i=1}^n \frac{\pi_i^0 + \tau_i^0}{(\tau_i^0)^2} \frac{\partial \tau_i^0}{\partial \zeta_j} \frac{\partial \tau_i^0}{\partial \zeta_k} + O_p(m^{-1}) \end{aligned}$$

Hence, equating lhs and rhs leads to, for $j = 1, \dots, q^*$,

$$\begin{aligned} &\sum_{i=1}^n \left(\frac{\pi_i^0 + \tau_i^0}{(\tau_i^0)^2} \right) \frac{\partial \tau_i^0}{\partial \zeta_j} \delta_i + \sum_{i=1}^n \frac{2\pi_i^0}{(\tau_i^0)^2} \frac{\partial \tau_i^0}{\partial \zeta_j} (p_i - \pi_i^0) - \sum_k (\hat{\zeta}_k - \zeta_k^0) \sum_{i=1}^n \frac{2\pi_i^0 + \tau_i^0}{(\tau_i^0)^3} \delta_i \frac{\partial \tau_i^0}{\partial \zeta_j} \frac{\partial \tau_i^0}{\partial \zeta_k} + O_p(m^{-1}) \\ &= \sum_k (\hat{\zeta}_k - \zeta_k^0) \sum_{i=1}^n \frac{\pi_i^0 + \tau_i^0}{(\tau_i^0)^2} \frac{\partial \tau_i^0}{\partial \zeta_j} \frac{\partial \tau_i^0}{\partial \zeta_k} + O_p(m^{-1}) \end{aligned} \quad (42)$$

Note that, under assumption [A0], all the terms are $O_p(m^{-\frac{1}{2}})$ or smaller except for the first term on the lhs. Letting m grow to infinity in Eq. (42) implies that

$$\sum_{i=1}^n \left(\frac{\pi_i^0 + \tau_i^0}{(\tau_i^0)^2} \right) \left(\frac{\partial \tau_i^0}{\partial \zeta_j} \right) \delta_i = 0 \quad \text{for all } j,$$

which in matrix notation becomes

$$B^{*T} \text{diag} \left\{ \frac{\pi^0 + \tau^0}{\tau^{02}} \right\} \delta = 0,$$

which proves Eq. (40) of Lemma 1. Plugging this result back into Eq. (42), we have

$$0 + 2B^{*T} \text{diag} \left\{ \frac{\pi^0}{(\tau^0)^2} \right\} (p - \pi^0) = B^{*T} \text{diag} \left\{ \frac{(\pi^0 + \tau^0)\tau^0 + (2\pi^0 + \tau^0)(\pi^0 - \tau^0)}{(\tau^0)^3} \right\} B^* (\hat{\zeta} - \zeta^0) + O_p(m^{-1}).$$

That is

$$2B^{*T} \text{diag} \left\{ \frac{\pi^0}{(\tau^0)^2} \right\} (p - \pi^0) = 2B^{*T} \text{diag} \left\{ \frac{(\pi^0)^2}{(\tau^0)^3} \right\} B^* (\hat{\zeta} - \zeta^0) + O_p(m^{-1}).$$

Hence

$$\begin{aligned} \sqrt{m}(\hat{\zeta} - \zeta^0) &= (B^{*T} \text{diag} \left\{ \frac{(\pi^0)^2}{(\tau^0)^3} \right\} B^*)^{-1} B^{*T} \text{diag} \left\{ \frac{\pi^0}{(\tau^0)^2} \right\} \sqrt{m} (p - \pi^0) + O_p(m^{-\frac{1}{2}}) \\ &=: P^* \sqrt{m} (p - \pi^0) + O_p(m^{-\frac{1}{2}}). \end{aligned} \quad (43)$$

Therefore

$$\begin{aligned} \sqrt{m}(\hat{\tau} - \tau^0) &= \left(\frac{\partial \tau^0}{\partial \zeta} + O_p(m^{-\frac{1}{2}}) \right) P^* \sqrt{m} (p - \pi^0) + O_p(m^{-\frac{1}{2}}) \\ &= B^* P^* \sqrt{m} (p - \pi^0) + O_p(m^{-\frac{1}{2}}) \\ &=: E^* \sqrt{m} (p - \pi^0) + O_p(m^{-\frac{1}{2}}). \end{aligned} \quad (44)$$

Hence

$$\sqrt{m} \begin{pmatrix} p - \pi^0 \\ \hat{\tau} - \tau^0 \end{pmatrix} = \begin{pmatrix} I \\ E^* \end{pmatrix} \sqrt{m} (p - \pi^0) + O_p(m^{-\frac{1}{2}}).$$

□

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