

Appendix A

Statistical Hypothesis Testing Using the Frequentist Method

This appendix describes how to test the hypothesis that the measured dijet angular distribution agrees with a theoretical prediction, which is either the Standard Model or a new physics model. This hypothesis test is done by defining a χ^2 test variable. In the next section we derive this variable in the absence of systematic uncertainties in the data, and we describe how to test the null hypothesis of the Standard Model (no new physics). Since measurements are prone to systematic errors, we generalize in Sect. A.2 the method to account for them. Finally Sect. A.3 describes how to set limits on new physics models. The method described in this appendix is referred to as the *frequentist hypothesis test* and is explained in [1].

A.1 Null Hypothesis Testing Using Method of Maximum Likelihood

We assume that Poisson statistics apply on the dijet distributions. We have k bins labeled by the index i running from 1 to k . We let n_i be the number of events in the i th bin, with $\mathbf{n} = (n_1, n_2, \dots, n_k)$ and $N = \sum_i n_i$.

Without systematic uncertainties, the mean number of entries is predicted by

$$E[n_i] = \mu_i s_i + b_i, \quad (\text{A.1})$$

with μ_i the strength parameter ($\mu_i = 1$ for the expected signal), b_i the theoretical prediction of the background and s_i the prediction of the signal. Furthermore, we use the notation that $\boldsymbol{\mu} = (\mu_1, \mu_2, \dots, \mu_k)$. Our task is to test the hypothesis that $\boldsymbol{\mu} = 0$, which can be done using the method of maximum likelihood ratios. For Poisson distributed data, the likelihood L is given by the product of Poisson distributions for each bin:

$$L(\boldsymbol{\mu} : \mathbf{n}) = \prod_i \frac{[(\mu_i s_i + b_i)]^{n_i} \exp[-(\mu_i s_i + b_i)]}{n_i!}, \quad (\text{A.2})$$

From this we can derive the likelihood ratio $\lambda(\boldsymbol{\mu})$:

$$\lambda(\boldsymbol{\mu}) = \frac{L(\boldsymbol{\mu} : \mathbf{n})}{L(\hat{\boldsymbol{\mu}} : \mathbf{n})}, \quad (\text{A.3})$$

with $\hat{\boldsymbol{\mu}} = (\hat{\mu}_1, \hat{\mu}_2, \dots, \hat{\mu}_k)$ the values of μ_i that maximize the likelihood. Maximizing the likelihood gives the best estimate for the parameters μ_i , and is equivalent to maximizing the likelihood ratio or to minimizing $\chi^2(\boldsymbol{\mu})$ defined by

$$\chi^2(\boldsymbol{\mu}) = -2 \ln \lambda = -2 \ln L(\boldsymbol{\mu} : \mathbf{n}) + 2 \ln L(\hat{\boldsymbol{\mu}} : \mathbf{n}) \quad (\text{A.4})$$

The likelihood ratio test theorem says that χ^2 asymptotically obeys a chi-square distribution with the number of degrees of freedom equal to the independent number of parameters being tested, i.e. $(k - 1)$ [1]. Note that the second term of the right hand side of Eq. A.4 is independent of $\boldsymbol{\mu}$ so that the minimization of χ^2 is entirely equivalent to the maximization of the likelihood function L .

For Poisson distributed data, we may replace the unknown values of $\hat{\mu}_i$ by their bin-by-bin model-independent maximum likelihood estimations, which can be easily found by taking the derivatives of $L(\boldsymbol{\mu} : \mathbf{n})$ with respect to μ_i , and solving them for μ_i , giving:

$$n_i s_i [(\mu_i s_i + b_i)]^{n_i-1} \frac{\exp[-(\mu_i s_i + b_i)]}{n_i!} - s_i [(\mu_i s_i + b_i)]^{n_i} \frac{\exp[-(\mu_i s_i + b_i)]}{n_i!} = 0 \quad (\text{A.5})$$

$$\iff n_i - (\mu_i s_i + b_i) = 0 \quad (\text{A.6})$$

So that:

$$\hat{\mu}_i = (n_i - b_i) / s_i \quad (\text{A.7})$$

Suppose we want to test the null hypothesis H_0 that $\boldsymbol{\mu} = 0$. We can use $\chi^2(\boldsymbol{\mu} = 0)$ (Eq. A.4) as a test statistic to test whether to accept or reject H_0 . Inserting Eq. A.7 into Eq. A.4:

$$\begin{aligned} \chi^2(0) &= -2 \sum_i \ln \left(\frac{b_i^{n_i} \exp(-b_i)}{n_i!} \right) + 2 \sum_i \ln \left(\frac{n_i^{n_i} \exp(-n_i)}{n_i!} \right) \\ &= 2 \sum_i (n_i \ln(n_i/b_i) + (b_i - n_i)) \approx \sum_i \frac{(n_i - b_i)^2}{n_i} \end{aligned} \quad (\text{A.8})$$

In the above expression, the following approximation was used:

$$n_i \ln \left(\frac{n_i}{b_i} \right) = -n_i \ln \left(1 + \frac{b_i - n_i}{n_i} \right) \approx n_i \left[\frac{n_i - b_i}{n_i} + \frac{1}{2} \left(\frac{n_i - b_i}{n_i} \right)^2 \right] \quad (\text{A.9})$$

We now use $\chi^2(\boldsymbol{\mu} = 0)$ (Eq. A.4) to derive the *p-value*:

$$p = \int_{\chi^2(\mu=0)}^{\infty} f(z; n_d) dz, \quad (\text{A.10})$$

with $f(z; n_d)$ the probability density function of the chi-square statistic with n_d degrees of freedom [here $n_d = (k - 1)$]. The p -value can be understood as the probability, under the assumption of a hypothesis H_0 , of obtaining data at least as incompatible with H_0 as is actually observed. Values for p can be found in standard math references.

The p -value can be related to the *significance*, which is defined as the number of standard deviations Z at which a Gaussian random variable of zero mean would give a one-sided tail area equal to the p -value:

$$p = \int_Z^{\infty} \frac{1}{\sqrt{2\pi}} e^{-x^2(\mu=0)/2} = 1 - \Phi(Z), \quad (\text{A.11})$$

where Φ is the cumulative distribution for the standard (zero mean, unit variance) Gaussian. Often in HEP, a significance of $Z = 3$ is regarded as evidence, and $Z = 5$ is taken as discovery. These values correspond to p -values of 1.35×10^{-3} and 2.87×10^{-7} respectively.

A.2 Systematic Uncertainties in the Data

Assume now that we have a systematic uncertainty α_i in each bin, which modifies the expectation of the mean in each bin (Eq. A.1):

$$E[n_i] = (\mu_i s_i + b_i)(1 + \alpha_i), \quad (\text{A.12})$$

with α_i typically called the *nuisance parameter*. Assume that α_i is modeled by a Gaussian with mean zero and σ_{α_i} . For example, if the jet energy scale is established with a 5% uncertainty, then $\sigma = 0.05$.

The likelihood is given by:

$$\begin{aligned} L(\mu : \alpha) &= \prod_i \frac{[(\mu_i s_i + b_i)(1 + \alpha_i)]^{n_i} \exp[-(\mu_i s_i + b_i)(1 + \alpha_i)]}{n_i!} \frac{1}{\sqrt{2\pi}\sigma_{\alpha_i}} \exp\left(-\frac{\alpha_i^2}{2\sigma_{\alpha_i}^2}\right), \end{aligned} \quad (\text{A.13})$$

with $\alpha = (\alpha_1, \dots, \alpha_k)$. This changes the expression for $\chi^2(\mu = 0)$:

$$\chi^2(\mu = 0) = -2 \ln \frac{L(\mu = 0 : \hat{\alpha}(\mu = 0))}{L(\hat{\mu} : \hat{\alpha})}, \quad (\text{A.14})$$

with $\hat{\alpha}_i(\mu_i)$ the value of α_i that maximizes the likelihood for a given μ_i . The value of $\hat{\mu}_i$ can be found by maximizing the likelihood $L(\boldsymbol{\mu} : \hat{\boldsymbol{\alpha}}(\boldsymbol{\mu}))$ and furthermore, $\hat{\alpha}_i = \hat{\alpha}_i(\hat{\mu}_i)$. The calculation of $\hat{\alpha}_i(\mu_i)$ is done by taking the derivative in terms of α_i :

$$\frac{\partial L(\boldsymbol{\mu} : \boldsymbol{\alpha})}{\partial \alpha_i} = 0 \Leftrightarrow \frac{\partial}{\partial \alpha_i} (1 + \alpha_i)^{n_i} \exp \left[-(\mu_i s_i + b_i)(1 + \alpha_i) - \frac{\alpha_i^2}{2\sigma_{\alpha_i}^2} \right] = 0, \quad (\text{A.15})$$

giving:

$$\Leftrightarrow n_i - \left(\mu_i s_i + b_i - \frac{\alpha_i}{\sigma_{\alpha_i}^2} \right) (1 + \alpha_i) = 0 \quad (\text{A.16})$$

To solve this, we make the approximation that σ_{α_i} and therefore most likely α_i are small, meaning that $1 + \alpha_i \approx 1$. This gives:

$$\hat{\alpha}_i(\mu_i) = (n_i - (\mu_i s_i + b_i)) \sigma_{\alpha_i}^2 \quad (\text{A.17})$$

Using again $1 + \alpha_i \approx 1$:

$$L(\boldsymbol{\mu} : \hat{\boldsymbol{\alpha}}(\boldsymbol{\mu})) \approx \prod_i \frac{(\mu_i s_i + b_i)^{n_i} \exp \left[-(\mu_i s_i + b_i) - \frac{1}{2}(n_i - (\mu_i s_i + b_i))^2 \sigma_{\alpha_i}^2 \right]}{n_i! \sqrt{2\pi} \sigma_{\alpha_i}} \quad (\text{A.18})$$

We now set the derivative of Eq. A.18 with respect to μ_i equal to zero and solve the result for μ_i :

$$\begin{aligned} 0 &= n_i s_i [(\mu_i s_i + b_i)]^{n_i-1} \frac{\exp \left[-(\mu_i s_i + b_i) - \frac{1}{2}(n_i - (\mu_i s_i + b_i))^2 \sigma_{\alpha_i}^2 \right]}{n_i!} \\ &\quad - \left(s_i - s_i (n_i - (\mu_i s_i + b_i)) \sigma_{\alpha_i}^2 \right) \\ &\quad \times [(\mu_i s_i + b_i)]^{n_i} \frac{\exp \left[-(\mu_i s_i + b_i) - \frac{1}{2}(n_i - (\mu_i s_i + b_i))^2 \sigma_{\alpha_i}^2 \right]}{n_i!} \\ &\Leftrightarrow 0 = n_i - (\mu_i s_i + b_i) \left[1 - (n_i - (b_i + \mu_i s_i)) \sigma_{\alpha_i}^2 \right], \end{aligned} \quad (\text{A.19})$$

giving:

$$\hat{\mu}_i \approx \frac{n_i - b_i}{s_i} \quad (\text{A.20})$$

We can now calculate χ^2 (Eq. A.14):

$$\begin{aligned}
\chi^2(0) &= -2 \sum_i \ln \left(\frac{b_i^{n_i} \exp \left[-b_i - \frac{1}{2}(b_i - n_i)^2 \sigma_{\alpha_i}^2 \right]}{n_i!} \right) + 2 \sum_i \ln \left(\frac{n_i^{n_i} \exp(-n_i)}{n_i!} \right) \\
&= 2 \sum_i \left(n_i \ln(n_i/b_i) + (b_i - n_i) + \frac{1}{2}(b_i - n_i)^2 \sigma_{\alpha_i}^2 \right) \\
&\approx \sum_i \left[\frac{(n_i - b_i)^2}{n_i} + \frac{(b_i - n_i)^2 n_i \sigma_{\alpha_i}^2}{n_i} \right] \\
&\approx \sum_i \frac{(n_i - b_i)^2}{n_i(1 + n_i \sigma_{\alpha_i}^2)} = \sum_i \frac{(n_i - b_i)^2}{(n_i + n_i^2 \sigma_{\alpha_i}^2)} \tag{A.21}
\end{aligned}$$

The interpretation of the above formula is rather straightforward; the presence of a systematic uncertainty, characterized by $\sigma_{\alpha_i}^2$, reduces the χ^2 -value so that it becomes more difficult to reject the null hypothesis. The denominator can be interpreted as the addition of the statistical and systematic uncertainties in quadrature.

A.3 Limits

The previous sections describe how to use data to exclude the null hypothesis of the Standard Model. But data can also be used in a different way, namely for the exclusion of new physics models, i.e. for setting limits on new physics model parameters. We then need to test the hypothesis that $\mu = \mathbf{I}$. We can derive $\chi^2(1)$ in a similar way as was done for $\chi^2(0)$, and the result is similar to Eq. (A.21) but with b_i replaced by $b_i + s_i$. Once we have calculated the χ^2 value, we can obtain the p -value. For those model parameters for which the p -value is sufficiently small, we can exclude them, i.e. set limits on the theory. A common choice is to let the critical p -value correspond to a significance of $Z = 2$. In that case $p = 0.05$ and we obtain so called 95 % Confidence Level (C. L.) limits.

Reference

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Curriculum Vitae

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