Calculating $p$-values and their significances with the
Energy Test for large datasets

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ABSTRACT: The energy test method is a multi-dimensional test of whether two samples are consistent with arising from the same underlying population, through the calculation of a single test statistic (called the $T$-value). The method has recently been used in particle physics to search for samples that differ due to CP violation. The generalised extreme value function has previously been used to describe the distribution of $T$-values under the null hypothesis that the two samples are drawn from the same underlying population. We show that, in a simple test case, the distribution is not sufficiently well described by the generalised extreme value function. We present a new method, where the distribution of $T$-values under the null hypothesis when comparing two large samples can be found by scaling the distribution found when comparing small samples drawn from the same population. This method can then be used to quickly calculate the $p$-values associated with the results of the test.

KEYWORDS: Analysis and statistical methods; Computing (architecture, farms, GRID for recording, storage, archiving, and distribution of data)

ArXiv ePrint: 1801.05222

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1 Introduction

A key problem in data science is determining if two samples, measured in multi-dimensional spaces, are consistent with having arisen from the same underlying population. This can be alternatively phrased as asking whether there exists evidence for differences between two samples. One area where this question is crucial is in searches for direct CP violation, which can appear as local differences of event yields in the multi-dimensional phase space between samples of matter and anti-matter data. Several different approaches have been suggested to address this question. One approach that has recently been developed and used in the context of CP violation is that of the Energy Test Method [1–6]. This method calculates a single test statistic, the energy or $T$-value, from the distribution of the data in the two samples. The value of this quantity can then be used to determine the consistency of the two samples by comparing to the expected distribution of the $T$-value under the null hypothesis that the two samples are drawn from the same population. We will label this the $T_0$ distribution. However, the analytic form that this distribution takes is not clearly understood. Understanding this distribution better will enable further application of the energy test method in the coming years, in samples containing a large number of events.

Within the energy test method the $T$-value is calculated as

$$T = \frac{1}{2} \sum_{i \neq j}^{n} \psi_{ij} + \left( \frac{1}{2} \sum_{i \neq j}^{\overline{n}} \psi_{ij} \right) - \left( \frac{1}{n^{2}} \sum_{i,j}^{n} \psi_{ij} \right),$$

where the first sum is over pairs of points (or events) in the first sample, the second sum is over pairs of points in the second sample, and the final sum is over both samples. There are $n$ events in the first sample and $\overline{n}$ events in the second sample. The value $\psi$ is a weighting function, commonly taken as a Gaussian of some scaled Euclidean distance squared ($d^2$) between two points in the (potentially multidimensional) phase space, $\psi_{ij} = e^{-d^2/(2\delta^2)}$, where $\delta$ is a length-scale that is optimised for the problem under consideration. However, other choices have been made for this weighting function (for example logarithms of the Euclidean distance between points). The energy test essentially calculates the mean of the $\psi$ distribution using pairs of events taken from each...
sample independently (the first two terms), and then considers cross-terms between the two samples (the final term), with the added consideration that since the same events are used many times to calculate distances, the different terms in the sums that calculate these means are correlated. In the case where the two samples are drawn from the same population the expected $T$-value is 0. A large, positive $T$-value indicates differences between the samples. The method has recently been extended to also enable comparison of samples containing impurities [4].

Estimating the $T_0$ distribution is an important open question that we consider in this article. This question lies at the heart of interpreting whether the computed test statistic is significant, and whether the two samples are consistent with being drawn from the same underlying population. To date, the typical approach to find this distribution when analysing data is to randomly assign the data to be tested to two samples, and calculate the $T$-value of these permuted samples, which are created, by definition, under the null hypothesis (taking a ‘permutation approach’). By repeating this process multiple times the $T_0$ distribution of $T$-values under the null hypothesis can be found, and used to determine the $p$-value associated with the nominal test, by counting how often the permutations return a more extreme $T$-value than the true data. The key criterion in particle physics for announcing a discovery is that the probability of getting such a result under the null hypothesis is smaller than that of finding a result 5 Gaussian standard deviations (with 5σ significance) from an expected central value. This corresponds to determining whether the $T$-value has a probability ($p$-value) of less than $6 \times 10^{-7}$. If the $T_0$ distribution is not known, then one may need to produce and analyse permutations over 1.7 million times to determine such a $p$-value. Indeed, for reasonable accuracy in determining this $p$-value even more permutations may be required.

The use of this permutation approach raises a problem when considering large samples. The calculation of the $T$-value is computationally intensive, and scales as $O(n^2)$, where $n$ is the number of events in the sample (since $O(n^2)$ distances must be calculated, used to determine some weighting function, and then summed). As noted above, this computation must be performed many times when testing for large significances. This increases the time taken in data analysis, and potentially makes the energy test significantly less useful as a data analysis method as sample sizes get larger and if a large number of permutations are required. A clear understanding of the $T_0$ distribution will therefore allow the use of the energy-test to analyse the largest data samples, making its use tractable in cases where it was not before.

It has been suggested [2] that the $T_0$ distribution seems to follow a generalised extreme value distribution when the energy test is used as a goodness of fit test.\footnote{The article that introduced this approach [2] noted that no proof exists that the GEV function describes the distribution in question and that the behaviour must be verified for each specific case.} However, this property has subsequently been used when the energy test is used as a two sample test [3–6], despite no suggestion that the $T_0$ distribution takes this form in the initial paper [2]. The assumption of this property has allowed quick calculations of $p$-values and significances, since a generalised extreme value (GEV) function can be fit to the $T_0$ distribution found from a limited number of permuted samples, and used to determine the significance of the $T$-value obtained when analysing the two samples present in the data. This is particularly useful if the sample sizes are too large to generate a large number of permutations quickly, since it allows a small number of permutations to be used to determine the free parameters of the GEV distribution, from which large significances can then be determined.
This method has been used to determine \(p\)-values, often alongside direct computation using the permutation approach [3–6]. With more studies using the energy test expected in the future, we investigate here whether the GEV function adequately describes the tail of the \(T_0\) distribution in a test case of the two sample comparison problem, and address this question of how to model the distribution of \(T\)-values found under the null hypothesis. Formal mathematical proofs are not presented in this article. Instead, two different models are considered and used in toy studies to demonstrate the shortcomings and power of different methods. These models are presented in the next section. Following this, the use of the GEV function and a new approach are both presented.

2 Data samples

Two different toy models are considered for these studies:

1. **Model 1:** this model is a very simple model, where events in each sample are generated according to a uniform distribution in three dimensions, with the allowed region of phase space being located between 0 and 1 in all dimensions. Here the probability density of a point in phase space is independent of the location in the space. The Euclidean distance \(d_{ij}\) is defined by
   \[
   d_{ij}^2 = \Delta x_{ij}^2 + \Delta y_{ij}^2 + \Delta z_{ij}^2,
   \]
   where \(\Delta x_{ij}, \Delta y_{ij}\) and \(\Delta z_{ij}\) are the differences in the coordinates of points \(i\) and \(j\).

2. **Model 2:** we also use the more complicated, physically-motivated model, first set out in ref. [7], and also studied in the context of the energy test in ref. [3] and ref. [4]. This model considers the decay of a particle \(X\) to a three-body final state. The axes considered in this problem are formed from the three different invariant mass squared combinations of pairs of the final state particles, and are labelled as \(x_i, y_i\) and \(z_i\), with the Euclidean distance again defined as
   \[
   d_{ij}^2 = \Delta x_{ij}^2 + \Delta y_{ij}^2 + \Delta z_{ij}^2.
   \]
   The presence of intermediate resonances mean that the density of events depends on the location in the phase space. This model is generated using the Laura++ package [8].

In both cases two different choices of the function \(\psi_{ij}\) are used: a Gaussian, as set out above, and a logarithmic function \(-\log |d + \epsilon|\), where \(\epsilon\), like \(\delta\) above, is a parameter to be chosen by the analyst, and which can be optimised for the study in question.

3 Using the generalised extreme value function

The generalised extreme value function takes three free parameters, \(\mu, \sigma\) and \(\xi\), and describes the distribution of a variable, labelled here as \(x\). For \(\xi < 0\) the value is non-zero for \(-\infty < x < \mu - \sigma / \xi\), while for \(\xi > 0\) it is non-zero for \(\mu - \sigma / \xi < x < +\infty\). In the special case where \(\xi = 0\) it is non-zero for all values of \(x\) on the real axis. The cumulative distribution is given by

\[
\text{CDF}(x) = \exp\left(-\left(1 + \xi \left(\frac{x - \mu}{\sigma}\right)\right)^{-1/\xi}\right), \quad (3.1)
\]

\(2\)The literature also uses the parameter \(c = -\xi\).
in the relevant ranges defined above, for \( \xi \neq 0 \). In the case where \( \xi = 0 \), the cumulative distribution is
\[
\text{CDF}(x) = \exp(-\exp(-(x - \mu)/\sigma)).
\] (3.2)

It is not obvious whether the GEV function should be used to describe the \( T_0 \) distribution. If we take a weighting function for the energy test that can only take values between 0 and 1, such as the Gaussian function discussed above, then the \( T_0 \) distribution must be contained in the range \(-1 \) to \( 1 \), given the form of equation (1.1). However, any form of the GEV function must contain either a finite probability for a \( T \)-value above 1 if \( \xi \geq 0 \), and/or below -1 if \( \xi \leq 0 \). Therefore, regardless of the value of \( \xi \), with the GEV function the cumulative distribution is never solely defined in the range \( -1 < T < 1 \); it is therefore possible to find a \( T \)-value where the significance is either underestimated or overestimated.

We perform empirical studies to determine whether this poses problems when seeking to describe reasonable \( T_0 \) distributions that can be generated, or if the GEV function is never-the-less sufficient to describe the distribution at a level needed within particle physics studies. We generate two samples in Model 1, each containing 1000 points (or events), and calculate the \( T \)-value. This is done twice: once for the Gaussian weighting function and once for the logarithmic function. This is repeated 5 million times in order to create a distribution of \( T \)-values for each weighting function (a permutation approach is not used, since ‘toy’ data can be quickly generated to find the distribution of \( T \)-values). With both samples generated from the same underlying distribution, the distributions of \( T \)-values found are the relevant \( T_0 \) distributions for each weighting function. For both the Gaussian weighting function and the logarithmic function we use \( \delta = \epsilon = 0.5 \). The \( T_0 \) distributions are shown in figures 1 and 2. A GEV function is fit to the distributions in both cases using the binned maximum likelihood method, with the fit also shown on the same figures, alongside the cumulative distribution and the cumulative distribution associated with the best fit. In these fits a normalisation, and the three parameters \((\mu, \sigma, \xi)\), are left unconstrained. It is clear for both weighting functions that the fit function does not describe the data. In addition, further cross-checks are made to see if the GEV function can be used to describe the data. First, \( \chi^2 \) fits are performed, and no good \( \chi^2 \) value is returned. Second, the parameters in the GEV function left unconstrained in the fit are reduced to a normalisation and a value of \( \xi \). This is achieved by fixing \( \mu \) using the relation that the cumulative probability is \( 1/e \) when \( x = \mu \), and that the median value \((x = x_{1/2})\) can be used to fix \( \sigma \) and \( \xi \) through \( \sigma = \xi (x_{1/2} - \mu)/(\log(2))^{-\xi} - 1 \). Once again, in this case no good fit is observed. As a cross-check, rather than generating new samples of data repeatedly, the permutation approach is taken to determine the \( T_0 \) distribution. This does not change our conclusions. In the simple model studied here the fit returns a value for the parameter \( \xi > 0 \), and we find that the p-value tends to be overestimated in the tail of the distribution at large \( T \). In this case the discovery of a new effect might be missed. If the fit returns a value of \( \xi < 0 \), the p-value tends to be underestimated, and such a discovery may be incorrectly claimed. We reach similar conclusions when studying other models (including the second model we set out above, Model 2). However, we also find that the fit quality varies with the choice of distance parameter, improving for the much smaller distance parameters considered in ref. [3].

This finding represents an important note in the application of the energy test method: the GEV function has already been used in the literature to fit the \( T_0 \) distribution, and to determine \( p \)-values by extrapolating the fit results. This toy model is a simple case where this method is not
valid: in this case, the use of the GEV function leads to the over-estimation of the $p$-value for large $T$-values, and a new effect or discovery might be missed. We therefore turn our attention to a novel approach to efficiently determining the $T_0$ distribution.

### 4 Scaling the T-values

The energy test (as set out in equation (1.1)) corresponds to the calculation of the mean values of the weighting function $\psi$, using correlated inputs (since the same event is used many times to calculate many distances), with $O(n^2)$ terms (or similar) in each sum. Increasing the sample sizes by a factor $k$ increases the number of terms in each sum by a factor $k^2$; if we neglect that each event is used multiple times when calculating these means (while still considering $O(k^2n^2)$ terms in each sum, but assuming that each term in each sum is statistically independent of all the others), then this increase in sample size would simply scale each mean, and scale the resulting $T_0$ distribution, with the width of the $T_0$ distribution decreasing by a factor of $\sqrt{k^2} = k$ (about a constant central value, since, if the null hypothesis applies, $\langle T \rangle = \frac{1}{2}\langle \psi \rangle + \frac{1}{2}\langle \psi \rangle - \langle \psi \rangle = 0$). In such a scenario,
The distribution of $kT$ would be independent of the sample size (for sufficiently large samples). We investigate empirically whether this property holds here for the energy test, where the same events are used multiple times to calculate the means, as in equation (1.1).

We first test using model 1, by repeating the previous studies, but using two samples of 500 events (as opposed to the 1000 event samples set out above). This is repeated 30 million times to find the $T_0$ distribution. The calculated $T$-values are scaled by a factor of $500/1000 = 0.5$, and overlaid on figures 1 and 2. This gives a much better description of the $T$-values in the 1000 event samples than the GEV function.

We make further studies by generating a sample using model 2 containing 1 000 000 events. We use this sample to investigate the $T_0$ distribution further: we randomly assign events to two smaller sub-samples (here taken to contain an equal number of events, $n$) and calculate the $T$-value and the value of $nT$ associated with running the energy test to compare these sub-samples. This is performed 30 million times for each value of $n$ considered. The distribution of $nT$ is shown in figures 3 and 4 for different values of $n$, for the Gaussian and logarithmic weighting functions (in both cases we use $\delta = \epsilon = 0.5$). Also shown are the values of the $nT$ distribution where the $p$-value for getting such a result corresponds to 1, 2, 3, 4, and 5 $\sigma$ evidence for differences between the samples respectively, for different values of $n$.

It is clear that in these cases the value of $nT$ associated with a particular level of significance is independent of $n$ for sufficiently large n (typically around 100 events, for the levels of significance...
Figure 4. The figure contains similar information to figure 3 but using the logarithmic weighting function, and with $n_{\text{max}} = 2000$. The smaller value of $n_{\text{max}}$ is used here owing to the significant computing time taken to calculate 30 million $T$-values for large $n$.

we have investigated). We have also applied this method to additional models, and used different weighting functions ($\psi$) and have found no evidence for the breaking of this scaling property. We also find that this scaling property does not rely on the sample sizes being equal, so that if the sizes of the samples being compared are increased by a factor $k$, the distribution of $kT$ under the null hypothesis is invariant (for large sample sizes). However, we note that we have no formal proof of this property. Indeed, for the Gaussian weighting function, the distribution of the value of $nT$ must lie in the range $-n < nT < n$. Therefore the use of this scaling property to estimate $p$-values will also provide incorrect coverage for some large (positive or negative) value of $T$. However, in the cases we have examined, this effect appears negligible for $n$ larger than about 100 points when considering significances of around $5\sigma$ and smaller. We recommend similar tests are performed for each specific case where the method is used.

This scaling property means that the $T_0$ distribution can be generated using a small value of $n$, and then scaled to determine the appropriate $T_0$ distribution for the sample sizes under consideration in the main test. This speeds up the computation of the significance of $T$-values when the $p$-value is small: with this method the calculation of the distribution of the null hypothesis no longer requires the generation of over one million permuted samples of the same size as the initial samples to claim a $p$-value smaller than 5 Gaussian standard deviations. Instead, the $T_0$ distribution can be quickly generated using small samples; only the one calculation of the $T$-value of the main data sample remains computationally intensive, and uses the full event yield in the calculation. Consequently it is with the biggest datasets that the impact of this scaling property is most significant.

5 Conclusions

The energy test is a standard method within data science that measures whether two samples are consistent with arising from the same underlying population. The method has recently been used
for studies in particle physics. The small $p$-values necessary to claim a discovery in particle physics require understanding rare $T$-values returned by the energy test method under the null hypothesis that the two samples are identical. Problems arise if the datasets under study are so large that the distribution under the null hypothesis cannot be simulated quickly with a permutation method, so the tail of this distribution cannot be studied sufficiently. In the existing literature the generalised extreme value distribution has been fit to the distribution, with an extrapolation of the fit then used to determine the $p$-values associated with large $T$-values [3–6] (often alongside a straightforward ‘counting method’ of determining the $p$-value from how often tests of the permuted samples return $T$-values larger than that in the test of the true samples). However, we have shown here for a simple test case that the $T_0$ distribution is not sufficiently well described by the generalised extreme value function. We have therefore also presented a new method where small sub-samples of the data, which can be analysed quickly, can be used to find the distribution of $T$-values expected under the null hypothesis for large sample sizes. In this way, the tail of the distribution under the null hypothesis can be probed. This allows the accurate determination of small $p$-values associated with claims of discovery of new physical phenomena.

Acknowledgments

We wish to thank Roger Barlow, Igor Babuschkin, Jolanta Brodzicka, Shanzhen Chen, Giulio Dujany, Marco Gersabeck, Gediminas Sarpis, Mike Williams, and Günter Zech for illuminating discussions. We also thank Günter Zech for the clarification that if the GEV function describes the distribution when used for goodness-of-fit studies (as considered in ref. [2]) this does not imply it also describes the distribution for two sample tests, despite its subsequent use in such studies. This work was supported by STFC grant number ST/N000374/1.

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