A Test for Equality of Distributions in High Dimensions

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Abstract

We present a method which tests whether or not two datasets (one of which could be Monte Carlo generated) might come from the same distribution. Our method works in arbitrarily high dimensions.

Key words: k-nearest neighbor, Kolmogorov-Smirnov test, curse of dimensionality
1 Introduction

Many sciences today rely heavily on the use of Monte Carlo simulation. In High Energy Physics (HEP) for example it is used in practically every stage of an experiment from the design of the detectors to the final analyses. This brings up the question of the precision of the MC simulation. In other words, how close are the probability distributions of the MC to those of the experimental data? Testing whether two datasets come from the same distribution is a classical problem in Statistics, and for one-dimensional datasets a large number of methods have been developed. Tests in higher dimensions have been proposed by Bickel [1] and Friedman and Rafsky [2]. Zech [3] discussed a test based on the concept of minimum energy. The test proposed here belongs to a class of consistent, asymptotically distribution free tests based on nearest neighbors (Narsky [4], Bickel and Breiman [5], Henze [6], and Schilling [7]).

We concentrate in this paper on comparing two datasets, either both real data or one real and one Monte Carlo, but the proposed method also allows us to test whether a dataset comes from a known theoretical distribution as long as we can simulate data from this distribution.
2 The Method

To set the stage, let’s say we have observations (events) $X_1, \ldots, X_n$ from some distribution $F$, and observations $Y_1, \ldots, Y_m$ from some distribution $G$. In the application we have in mind one of these would be MC generated data and the other ”real” data, but this is not crucial for the following. We are interested in testing $H_0 : F = G$ vs $H_a : F \neq G$. The idea of our test is this: let’s concentrate on one of the $X$ observations, say $X_j$. What is its nearest neighbor, that is, the observation closest to it? If the null hypothesis is correct and both datasets were generated by the same probability distribution, then this nearest neighbor is equally likely to be one of the $X$ or $Y$ observations (proportional to $n$ and $m$). If $F \neq G$ there should be regions in space where there are relatively more $X$ or $Y$ observations than could be expected otherwise.

More formally, let $Z_j = 1$ if the nearest neighbor of $X_j$ is from the $X$ data and 0 otherwise. Then, under the null hypothesis, $Z_j$ is a Bernoulli random variable with success probability $(n - 1)/(n + m - 1)$. Therefore $Z = \sum_{j=1}^{n} Z_j$ has an approximate binomial distribution with parameters $n$ and $(n - 1)/(n + m - 1)$. The distribution is only approximately binomial because the $Z_j$’s are not independent, but for datasets of any reasonable size the dependence is very slight and can be ignored.

There is an immediate generalization of the test: instead of just considering the nearest neighbor we can find the k-nearest neighbors. Now $Z_j = (Z_{j1}, \ldots, Z_{jk})$
with \( Z_{ji} = 1 \) if the \( i^{th} \) nearest neighbor of \( X_j \) is from the \( X \) dataset, 0 otherwise. Under the null hypothesis \( Z = \sum_{j=1}^{n} \sum_{i=1}^{k} Z_{ji} \) has again an approximate binomial distribution with parameters \( nk \) and \( (n - 1)/(n + m - 1) \). (Actually, \( \sum_{i=1}^{k} Z_{ji} \) has a hypergeometric distribution, but because we will use a \( k \) much smaller than \( n \) or \( m \) the difference is negligible.)

We can find the p-value of the test with

\[
p = P(V \geq Z)
\]

where \( V \sim \text{Bin}(nk, (n - 1)/(n + m - 1)) \).

Especially if \( n \) and \( m \) are small or if a relatively large \( k \) is desired it would be possible to use a permutation type method to estimate the null distribution. The idea is as follows: under \( H_0 \) all the events come from the same distribution, so any permutation of the events will again have the same distribution. Therefore if we join the \( X \) and \( Y \) events together, shuffle them around and then split them again into \( n \) and \( m \) events \( X' \) and \( Y' \), these are now guaranteed to have the same distribution. Applying the k-nearest neighbor test and repeating the above many times (say 1000 times) will give us an estimate of the null distribution. For more on the idea of permutation tests, see Good [8].

This method will achieve the correct type I error probability by construction, but it also requires a much greater computational effort.

There are a number of choices to be made when using this method. First of all, there is the question of which dataset should be our \( X \) data. Clearly, if \( n = m \),
this does not matter but it might well otherwise. Indeed, in our application of comparing MC data to real data, we have control of the size of the MC data although sometimes there are computational limits on its size.

Next we need to decide on $k$. Again there is no obviously optimal choice here. Finally, we need to decide on a metric to use when finding the nearest neighbor. If the observations differ greatly in "size" in different dimensions, the standard Euclidean metric cannot be expected to work well because small differences in dimensions with a large spread would overwhelm small but significant differences in dimensions with a small spread. This last issue we will deal with by standardizing each dimension separately, using the mean and standard deviation of the combined $X$ and $Y$ data. If the data come from a distribution that is severely skewed, other measures of location and spread (such as the median and the interquartile range) could also be used to standardize the data. In the next section we will show the results of some mini MC studies which give some guidelines for the choices.

3 Performance of this Method

If we use the binomial approximation in our test, we will need to verify that the method works, that is, that it achieves the desired type I error probability $\alpha$. Of course, we are also interested in the power of the test, that is, the probability to reject the null hypothesis if indeed $F \neq G$. In this section we
will carry out several mini MC studies to investigate these questions.

We start with the situation where there exist other methods for this test, namely in one dimension. For comparison we will use a method that is known to have generally very good power, the Kolmogorov-Smirnov (KS) test. In the first simulation we generate $n = m$ observations from 1000 to 20000 in steps of 1000 each for $X$ and $Y$ from the uniform distribution on $[0, 1]$. Because of the probability integral transform this is actually a very general case, and similar conclusions will hold for all other continuous distributions in one dimension. For each of these cases we use our test with $k = 1, 2, 5, 10, 20, 50$ and 100 as well as the KS test. This is repeated 10000 times. Figure 1 shows the results, using a nominal type I error probability of $\alpha = 5\%$.

As we see the true type I error probability is close to nominal but increases slowly as $k$ increases. This is due to the lack of independence between the $Z_j$'s. Especially if $k$ is large relative to $n$ or $m$, the true type I error probability is larger than what is acceptable. Based on this and similar simulation studies, we recommend $k = 10$ if both $n$ and $m$ are at least 1000, otherwise $k = 0.01 \min(n, m)$. Alternatively, one can use the permutation method described above which will have the correct type I error by construction.

Even for $k = 1$ we have a slightly higher than nominal type I error probability, about 5.5% if $\alpha = 5\%$. This is partly due to the dependence between the $Z_j$'s, and partly to the discrete nature of the binomial distribution. For example,
if we defined the p-value as $P(V \geq Z - 1)$ we would get a true type I error probability slightly smaller than the nominal one. In any case, we believe this difference to be acceptable.

Next a simulation to study the power of the test, again in one dimension. We use the uniform on $[0, 1]$ distribution for $F$ and the uniform on $[0, \theta]$ for $G$, where $\theta$ goes from 1 to 1.1 We generate $n = m = 1000$ events and apply our test with $k = 1, 5, 15$ and 25 as well as the KS test. This is repeated 10000 times. The result is shown in Figure 2. Clearly, the higher the $k$ the better the power of the test. In fact, for this example already with $k = 15$ the test has better power than the KS test! Generally speaking, in one dimension, our test has power somewhat inferior to the KS test. However, our test is not meant to be used in one dimension. It is encouraging to find that it does fairly well even in that situation.

How should one choose the size of the Monte Carlo dataset relative to the size of the true data? In the next simulation we generate $n = 1000$ events from a uniform $[0, 1]$ and assume this to be the real data. Then we generate $m$ events from the same distribution, with $m$ going from 50 to 2500. In Figure 3 we show the results which indicate that the MC dataset should have the same size as the real data because in that case the true type I error probability is about the same as the nominal one. This agrees with general statistical experience which suggests that, in two-sample problems, equal sample sizes are often preferable.
Finally we present a multi-dimensional example. We generate $n = m = 1000$ events. The $F$ distribution is a multivariate standard normal in 9 dimensions, and the $G$ distribution a multivariate normal in 9 dimensions with means 0, standard deviations 1 and correlation coefficients $\text{cor}(X_i, X_j) = \rho$ if $|i - j| = 1$ and 0 if $|i - j| > 1$, where $\rho$ goes from 0 to 0.5. This example illustrates the need for a test in higher dimensions. Here all the marginals are standard normals, and any one-dimension-at-a-time method is certain to miss the difference between $F$ and $G$. This is shown in Figure 4 where with $k = 10$ we reject the null hypothesis quite easily (at $\rho = 0.5$) whereas the KS test applied at any of the marginals fails completely.

4 Implementation

A C++ routine that carries out the test is available from one of the authors at [http://math.uprm.edu/~wrolke/](http://math.uprm.edu/~wrolke/) It allows the use of the binomial approximation as well as the permutation method. It uses a simple search for the k-nearest neighbors. k-NN searching is a well known problem in computer science, and more sophisticated and faster routines exist and could also be used in combination with our code. (See, for example, Friedman, Baskett and Shustek [9].)
5 Summary

We describe a test for the equality of distributions of two datasets in higher dimensions. The test is conceptually simple and does not suffer from the curse of dimensionality. Simulation studies show that it approximately achieves the desired type I error probability, or does so exactly at a higher computational cost. They also show that this test is capable to detect differences between the distributions only ”visible” in higher dimensions.

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6 Appendix
Fig. 1. The true type I error probability in a one dimensional example as a function of sample size. $X$ and $Y$ have a uniform distribution on $[0,1]$. $n = m$, and the nominal type I error probability is 5%. Each curve represents a different $k$ value. The KS test gives a flat line at 5%.
Fig. 2. $F = U[0, 1]$, $G = U[0, \theta]$ where $\theta$ goes from 1 to 1.1. We generate $n = m = 1000$ events. $k = 1, 5, 15$ and 25.
Fig. 3. $n = 1000$ from $F = U[0, 1]$, $m$ goes from 50 to 2500, $G = F$. 
Fig. 4. \( n = m = 1000 \). The \( F \) distribution is a multivariate standard normal in 9 dimensions, and the \( G \) distribution a multivariate normal in 9 dimensions with means 0, standard deviations 1 and correlation coefficients \( \text{cor}(X_i, X_j) = \rho \) if \(|i - j| = 1\) and 0 if \(|i - j| > 1\), where \( \rho \) goes from 0 to 0.5. The multidimensional test has much better power than any of the one-dimensional KS tests.