A chi-square goodness-of-fit test for continuous distributions against a known alternative

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Received: 15 October 2019 / Accepted: 30 April 2020 / Published online: 14 May 2020 © The Author(s) 2020

Abstract
The chi square goodness-of-fit test is among the oldest known statistical tests, first proposed by Pearson in 1900 for the multinomial distribution. It has been in use in many fields ever since. However, various studies have shown that when applied to data from a continuous distribution it is generally inferior to other methods such as the Kolmogorov-Smirnov or Anderson-Darling tests. However, the performance, that is the power, of the chi square test depends crucially on the way the data is binned. In this paper we describe a method that automatically finds a binning that is very good against a specific alternative. We show that then the chi square test is generally competitive and sometimes even superior to other standard tests.

Keywords Kolmogorov–Smirnov · Anderson–Darling · Zhang tests · Power · Monte carlo simulation

1 Introduction

A goodness-of-fit test is concerned with the question whether a data set may have been generated by a certain distribution. It has a null hypothesis of the form \( H_0 : F = F_0 \), where \( F_0 \) is a probability distribution. For example, one might wish to test whether a data set comes from a standard normal distribution. An obvious and often more useful extension is to test \( H_0 : F \in \mathcal{F}_0 \) where \( \mathcal{F}_0 \) is a family of distributions but without specifying the parameters. So one might wish to test whether a data set comes from a normal distribution but without specifying the mean and standard deviation. If the null distribution is fully specified we have a simple hypothesis whereas if parameters are to be estimated it is called a composite hypothesis.

As described above a goodness-of-fit test is a hypothesis test in the Fisherian sense of testing whether the data is in agreement with a model. The main issue with this
approach is that it does not allow us to decide which of two testing methods is better. To solve this problem Neyman and Pearson in the 1930s introduced the concept of an alternative hypothesis, and most tests done today follow more closely the Neyman–Pearson description, although they often are a hybrid of both. The original Fisherian test survives mostly in the goodness-of-fit problem, because here the obvious alternative is \( H_0 : F \neq \mathcal{F}_0 \), a space so huge as to be useless for power calculations.

However, in almost all discussions of goodness-of-fit testing there is an immediate pivot and a specific alternative is introduced. This is a necessary step in order to be able to say anything regarding the performance of a test. In our method we have taken advantage of this, and describe a way to find a good binning from among a large number. We will show that if such a binning is used the chi-square test can be quite competitive with other tests, and sometimes even better. Moreover it fully automates the choice of bins.

The goodness-of-fit test is one of the oldest and most studied problems in Statistics. For an introduction to Statistics and hypothesis testing in general see Casella and Berger (2002) or Bickel and Doksum (2015). For discussions of the many goodness-of-fit tests available see D’Agostini and Stephens (1986), Raynor et al. (2009), Zhang (2002) and Thas (2010). Chi-square tests are the subject of Watson (1958), Greenwood and Nikulin (1996) and Voinov and Nikulin (2013). Thas (2010) has an extensive list of references on the subject.

2 Chi-square test

The original test by Pearson was designed to see whether an observed set of counts \( O \) was in agreement with a multinomial distribution with parameters \( m, p_1, \ldots, p_k \). This is done by calculating the expected counts \( E_i = mp_i \) and the test statistic \( X = \sum (O - E)^2 / E \). Pearson showed that under mild conditions \( X \sim \chi^2(k - 1) \), a chi-square distribution with \( k - 1 \) degrees of freedom. The test therefore rejects the null at the \( \alpha \) level if \( X \) is larger than the \( (1 - \alpha)100\% \) quantile of said chi-square distribution. Later work showed that this test works well as long as the expected counts are not too small. \( E > 5 \) is often suggested although it has been shown that it can still work well even if some expected counts are smaller. In the context of goodness-of-fit testing for a continuous distribution it is generally possible to insure \( E > 5 \) for all bins, and we will do so in all that follows.

If the test is to be applied to a continuous distribution this distribution has to be discretized by defining a set of bins. In principle any binning (subject to \( E > 5 \)) will work. Two standard methods often used are bins of equal size and bins with equal probabilities under the null hypothesis.

Among Statisticians the use of the chi-square test for continuous distributions has been discouraged for a long time. This is due to its lack of power when compared to other tests. However, it is still the go-to test in many applied fields, and this will be the case for a long time to come. The chi-square test does in fact have one advantage over most other test, namely that it deals with parameter estimation very easily. Fisher (1922) showed that if the parameters are estimated by minimizing the chi-square statistic, \( X \) again has a chi-square distribution, now with \( k - 1 - p \) degrees of freedom.
where \( p \) is the number of parameters estimated. In fact Fisher coined the term degrees of freedom in this seminal paper.

By contrast other standard tests do not easily generalize to allow parameter estimation, and usually the null distribution has to be found via simulation.

A number of alternative test statistics have been proposed, all of which also lead to a limiting chi-square distribution. For a survey of such statistics see D’Agostini and Stephens (1986) and Cressie and Read (1989). In this paper we use six different formulas and again find the one that yields the highest power against a specific alternative. They are:

- Pearson: \( \sum \frac{(O - E)^2}{E} \)
- Freeman–Tukey: \( 4 \sum (\sqrt{O} - \sqrt{E})^2 \)
- \( \lambda_p \): \( 2 \sum (E - O + O \log(O/E)) \)
- loglikelihood \( G^2 \): \( 2 \sum (O \log(O/E)) \)
- Neyman Modified: \( \sum (E^2/O - O) \)
- \( \lambda/3 \): \( \frac{9}{5} \sum (O(O/E)^2/3 - 1) \)

Many of these are members of the Cressie-Read divergence family (Cressie and Read 1989), given by

\[
I^\lambda(q : p) = \frac{1}{\lambda(\lambda + 1)} \sum q [(p/q)^\lambda - 1] \tag{1}
\]

### 3 Parameter estimation

If the test has a composite null hypothesis it is necessary to estimate the parameters from the data. In practice this is often done via maximum likelihood estimation using the unbinned data. That this leads to a test that is anti-conservative was shown long ago by Fisher (1922). As an example consider the following case: We wish to test whether the data comes from a normal mixture, that is

\[
\mathcal{F}_0 = \lambda N(\mu_1, \sigma_1) + (1 - \lambda) N(\mu_2, \sigma_2) \tag{2}
\]

and the parameters \( \lambda, \mu_1, \sigma_1, \mu_2, \sigma_2 \) are to be estimated. For our simulation we will generate 1000 observations with \( \lambda = \frac{1}{3}, \mu_1 = 0, \sigma_1 = 1, \mu_2 = 5, \sigma_2 = 2 \) and use unbinned maximum likelihood to estimate the parameters. Then we apply the chi-square test with 10 equal probability bins at the 5% level. This is repeated 10,000 times. We find a true type I error rate of over 9%, almost double the nominal one of 5%.
This simulation as well as all others discussed in this paper were done using R. An Rmarkdown file with all calculations as well as an R library with all routines is available at https://github.com/wolfgangrolke/chisqalt.

Instead of maximum likelihood with the unbinned data one can use either maximum likelihood with binned data or a method called minimum chi-square. This is just what the name suggests, find the set of values of the parameters that minimizes the chi-square statistic. Using this estimation method in the above simulation yields a correct type I error rate of 5%. The same is true in every simulation study we performed, and our routine uses this estimation method.

This method of estimation has another advantage: by the way it is defined it is clear that if the null hypothesis is rejected, it would also be rejected for any other set of parameter values. Also, Berkson (1980) argues in favor of minimum chi-square.

Watson (1958) discusses this issue and provides alternative formulas for the chi-square statistic when unbinned maximum likelihood estimation is used. This was useful when minimum chi-square was difficult to do in the absence of computers but is no longer necessary today.

4 Other tests

Many other goodness-of-fit methods have been developed over time. The most commonly used are the Kolmogorov–Smirnov (KS) and Anderson–Darling (AD) tests. Zhang (2002) proposed three statistics (ZK, ZA and ZC) based on likelihood ratios and showed that they provided good power in a number of cases. We will employ all of these methods for comparison. For the cases where parameters need to be estimated we will use unbinned maximum likelihood estimation and simulation to find the null distributions of these tests. For discussions of the relative merits of these tests see Massey (1951), Birnbaum (1952), Goodman (1954), Zhang (2002) and Thas (2010).

5 Binning

5.1 Bin types

There are two binning methods that are most commonly used. They are bins of equal size and bins with equal probabilities. In the case of equal size bins often some adjustment is necessary to insure that all expected counts are at least 5.

We will increase the bin types as follows. Let us say that it was decided to use $k$ bins, and the equal probability method yielded bins with endpoints $B^0_i$, whereas the equal size bins have endpoints $B^1_i$, $i = 0, \ldots, k$. Here possibly $B^0_0 = B^1_0 = -\infty$ and $B^0_k = B^1_k = \infty$. We define a new set of bins by interpolating between these, so a $\kappa$ bin set has endpoints

$$B^\kappa_i = (1 - \kappa)B^0_i + \kappa B^1_i \quad (3)$$

for any $0 \leq \kappa \leq 1$. Note that this includes equal probability bins ($\kappa = 0$) as well as equal size bins ($\kappa = 1$).
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25 50 75 100

Number of Bins

51 0 1 5 2 0

Fig. 1

Power

n 100 250 500 1000 2000

Fig. 1 Power of testing uniform versus linear. While power increases as sample size increases, in each case just two bins yield the highest power.

5.2 Number of bins

Many studies in the past have focused on the number of bins to use. A default formula used in many software programs, including R’s hist function, is Sturges’ rule $k = 1 + \log_2(n)$, Sturges (1926), where $n$ is the sample size. One of the first suggestions was Mann and Wald (1942) $k = 4 \left[ 2(n-1)^2 \right]^{1/5}$. Others can be found in D’Agostini and Stephens (1986), Dahiya and Gurland (1973), Bogdan (1995), Harrison (1985), Kallenberg (1985), Kallenberg et al. (1985), Koehler and Gann (1990), Williams (1950), Ooosterhoff (1985) and Quine and Robinson (1985). Mineo (1979) suggests a different binning scheme.

All of these suggestions have in common that the number of bins increases as the sample size increases, although some recommend a small number (6 or 7) independent of sample size. However, a simple example shows that the optimal number of bins does not always increase with the sample size. Say we wish to test $H_0 : F = U[0, 1]$ versus $H_1 : F = \text{Linear}(\text{slope}=0.2)$. Here under the alternative the distribution function is $F(x) = 0.2x^2 + 0.8x; 0 < x < 1$. In this case equal size and equal probability bins are the same. We run simulations for the cases of 2 to 21 bins and sample sizes 100, 250, 500, 1000 and 2000. The resulting powers are shown in Fig. 1. The power increases as the sample size increases but in each case just two bins yields the highest power.
5.3 Finding the optimal bin set

Optimal in the context of hypothesis testing always means having the highest power, and the power of a test can only be found when an alternative is specified. So let us consider the following problem: we wish to test $H_0 : F = F_0$ versus $H_1 : F = F_1$. A standard way to estimate the power would proceed as follows: generate a data set of the desired size from $F_1$, apply the test to the data and see whether it rejects the null at the desired level. Repeat many times, and the percentage of rejections is the power of the test.

In the case of a chi-square test this means one has to find the bin counts for the generated data set. However, we already know that these counts have a multinomial distribution with probabilities $p_i = F_1(B_{i+1}^\kappa) - F_1(B_i^\kappa)$. We can therefore run the simulation by generating variates from a multinomial distribution with these probabilities directly. In our simulation studies we have seen a speedup on the order of 100 and more using this approach. An additional advantage is that we need not be able to generate variates from any $F_1$ directly. This is done in the cases where no parameter estimation is needed.

There is another issue when trying to find an optimal binning. How are we to choose between two binnings that both have a power of 100%? Moreover, using (say) $k$ and $k + 1$ bins will often result in tests with almost equal power, well within simulation error. To always find a single best binning (from among our sets) we will use the idea of a perfect data set. This is an artificial data set that has its observations at the exact right spots, under the alternative. These of course are simply the quantiles of the distribution under the alternative hypothesis. Applying the test to this perfect data set and using $k$, $\kappa$ bins we will use as a figure of merit $M_{k,\kappa,TS} = TS/qchisq(0.95, k - 1 - p)$, where $TS$ is the value of one of the test statistics discussed above and $qchisq(0.95, k - 1 - p)$ is the 95% critical value of a chi-square distribution with $k - 1 - p$ degrees of freedom. 95% was chosen here not because we wish to test at the 5% level but to account (roughly) for the increase in the critical values.

The idea here is simple: the binning that yields the highest value of $M_{k,\kappa,TS}$ would be best in rejecting the null hypothesis for the perfect data set at the 95% level, and one would expect this to be quite good for testing a random data set from that same distribution.

Let us apply this idea to the following case: we wish to test $H_0 : F = \text{Linear}(\text{slope} = -0.5)$ versus $H_1 : F = \text{truncExp}(1)$, an exponential rate 1 truncated to $[0, 1]$.

Assuming a sample size of 10,000, in Fig. 2 we have $M_{k,\kappa,TS}$ for $k = 2, \ldots, 21$, $\kappa = 0, 0.25, 0.5, 0.75, 1$ and using Pearson’s formula. The highest value is achieved for $k = 4, \kappa = 1$. In Fig. 3 we see the actual powers, and indeed (within simulation error) $k = 4, \kappa = 1$ is best.

So our test proceeds as follows: it searches through a grid of number and type of bins as well as the formulas for the test statistics. By default these are $k = (2 + p) : 2(1 + \log_2(n))$ and $\kappa = 0, 0.25, 0.5, 0.75, 1$, but these can be adjusted by the user. It finds the combination that maximizes $M_{k,\kappa,TS}$ and applies the corresponding chi-square test to the data. Therefore the choice of number of bins, type of bins and test statistic is automatic, and independent of the data.

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**Fig. 2** $M_{k,\kappa}$ of a test of linear versus truncated exponential. The maximum value of $M_{k,\kappa}$ is attained for $k = 4, \kappa = 1$

**Fig. 3** Power of a test of linear versus truncated exponential. The maximum power is attained for $k = 4, \kappa = 1$
It is important to note that this searching through many binning schemes will not lead to a problem of multiple testing, and thereby a wrong type I error probability, because the test is done only once, using the chosen binning scheme. As an example, if a data set has 1000 observations, the method searches through 660 different binning schemes and chi-square formulas. This only takes a fraction of a second on a modern PC.

6 Other circumstances

Our routines also allow for two situations sometimes encountered in practice:

6.1 Already binned data

In some fields it is common that the data, although coming from a continuous distribution, is already binned. This is typically the case, for example, in high energy physics experiments because of finite detector resolution. If so our routine finds the optimal binning as described above and then finds the combination of the data bins that comes closest to the optimal one.

6.2 Random sample size

Another feature often encountered is that the sample size itself is random. This is the case, for example, if the determining factor was the time over which an experiment was run. Our routine allows this if the sample size is a variate from a Poisson distribution with known rate $\lambda$, as is often the case.

One consequence of such a random sample size is that the bin counts no longer have a multinomial distribution, but instead are independent Poisson with rates that depend on the bin probabilities and $\lambda$. In turn this implies that the chi-square statistic now has $k - p$ instead of $k - p - 1$ degrees of freedom. Another consequence is that for the Kolmogorov–Smirnov, Anderson–Darling and Zhang tests the null distribution has to be found via simulation, even if no parameters are estimated.

7 Performance

7.1 Type I error

Our method always guarantees that the binning used has expected counts at least five, and so the basic theory of chi-square tests should yield a good approximation to the chi-square distribution. Nevertheless, Table 1 shows the results of a simulation study with a number of null distributions and using $\alpha = 1\%, 5\%$ and $10\%$. As it is based on 10,000 simulation runs we see that the true type I error probabilities are well within the simulation error of the nominal ones.
In the following sections we will discuss a number of cases. For each we will find the power of the Kolmogorov–Smirnov (KS), Anderson–Darling (AD) and Zhang (ZK, ZA and ZC) tests applied to the unbinned data. We also include chi-square tests with equal bin sizes (Equal Size) and equal bin probabilities (Equal Prob) and the number of bins found with the often used formula $k = 1 + \log_2(n)$. A binning often done in real life by practitioners uses the data as it would be used to draw a histogram, that is with a fairly large number of essentially equal size bins. In the examples below we start with 50 bins but may have a little less after combining them to achieve $E > 5$. This binning is denoted Histogram. Finally we include our new test, which is always highlighted in the graphs to make it easier to compare to all others and is called RG.

There are of course many other tests one could use for comparison. There is however none that is generally much superior to those included here. Moreover, among non-statisticians KS, and to already a lesser extend AD, are the most commonly used tests because they are included in most software programs.

### 7.2 Normal(0, 1) versus t(df)

We have $H_0 : F = N(0, 1)$ versus $H_a : F = t(df)$. We use a sample size of $n = 1000$ and $B = 10,000$ simulation runs. This will be the case for all future simulations as well, unless stated otherwise.

The power curves are shown in Fig. 4.

The RG test uses 3 bins, $\kappa = 0.5$ and Pearson’s formula regardless of sample size.

The mean of the powers over the 20 parameter values are, in order: ZC: 44%, RG: 40%, ZK: 34%, Equal Size: 32%, ZA: 25%, Histogram: 24%, AD: 22%, Equal Prob: 18% and KS: 11%, so RG is a close second.

In our studies (not shown here) we always also found the powers of the tests directly and verified that the combination of $k, \kappa$ and test statistic that maximized $M_{k, \kappa, TS}$ also had the highest power, or very close to it.

### 7.3 Normal versus t(df)

Here we have $H_0 : F = \mathcal{N}$ versus $H_a : F = t(df)$, so now the mean and the standard deviation are estimated. For the KS, AD and Zhang tests maximum likelihood estimation is used, and the null distribution is found via simulation.
The power curves are shown in Fig. 5.

RG uses $k = 5$ bins, $\kappa = 0.5$ and Pearson’s formula regardless of sample size. Notice that because two parameters are estimated, four bins is the least possible.

The mean of the powers over the 20 parameter values are, in order: ZC: 31%, AD: 28%, ZK: 25%, KS: 22%, RG: 21%, ZA: 17%, Equal Size: 16%, Histogram: 10%, Equal Prob: 8%. RG does not perform to well but is just about as good as KS.

### 7.4 Uniform[0,1] versus Linear

Next we have $H_0 : F = U[0, 1]$ versus $H_a : F = \text{Linear}(s)$, where the slope changes from 0 (that is the null hypothesis is true) to 0.3.

The power curves are shown in Fig. 6.

RG uses 2 or 3 equal probability bins and the Neyman Modified formula regardless of sample size.

The mean of the powers are: AD: 63%, KS: 60%, ZA: 58%, RG: 57%, ZK: 50%, ZC: 49%, Equal Size: 47%, Equal Prob: 46% and Histogram: 29%. Here the often used histogram binning does especially poorly.

### 7.5 Exponential versus Exponential with normal bump

Here the null hypothesis specifies an exponential with an unknown rate and the alternative is a mixture of 90% exponential rate 1 and 10% normal mean 1.5 and the standard
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Fig. 5 Powers of tests for $H_0 : F_0 = \text{Normal}$ versus $H_a : F_1 = t(d.f)$. ZC performs best, with AD second.

Fig. 6 Powers of tests for $H_0 : F_0 = U[0, 1]$ versus $H_a : F_1 = \text{Linear(slope)}$. AD test performs best, with KS second and RG third.
deviation varies. The normal is truncated to \([0, \infty)\) and the rate of the exponential is estimated. This is a case often encountered in high energy physics, were the normal bump would indicate the presence of a signal, for example a new particle.

The power curves are shown in Fig. 7.

RG uses four bins with the \(\kappa\) depending on the alternative as well as the sample size. Again Neyman Modified is best.

The mean of the powers are: RG: 67\%, AD: 64\%, KS: 58\%, Equal Size: 53\%, Equal Prob: 48\%, Histogram: 42\%, ZC: 31\%, ZK: 25\% and ZA: 21\%.

The power curve of RG has a curious jump at around \(\sigma = 0.75\), which is due to the fact that here \(\kappa\) changes from 0.25 to 0.5. Choosing a large number of \(\kappa\) values would make this jump disappear.

This simulation shows that while the Zhang tests generally do very well, sometimes they perform poorly.

7.6 Uniform\([0,1]\) versus Beta\((1, q)\)

The power curves are shown in Fig. 8.

RG uses three equal probability bins and Neyman Modified.

The mean of the powers are: ZA: 67\%, AD: 64\%, KS: 60\%, ZC: 57\%, RG: 56\%, ZK: 55\%, Equal Prob: 51\%, Equal Size: 51\% and Histogram: 37\%.

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Fig. 8 Powers of tests for $H_0 : F_0 = U[0, 1]$ versus Beta(1, q). ZA is best, with AD second and RG third

7.7 Uniform[0,1] versus Beta(q, q)

The power curves are shown in Fig. 9.

RG uses six equal probability bins and Neyman Modified.

The mean of the powers are: ZC: 44%, RG: 38%, Equal Prob: 38%, Equal Size: 38%, AD: 38%, ZK: 38%, Histogram: 27%, ZA: 26% and KS: 22%

7.8 $N(r, \sqrt{r})$ versus Gamma(r, 1)

The power curves are shown in Fig. 10.

RG uses three equal size bins and Neyman Modified.

The mean of the powers are: RG: 91%, ZC: 91%, Equal Size: 88%, ZK: 77%, Histogram: 64%, Equal Prob: 60%, AD: 58%, KS: 46% and ZA: 12%.

This is of course a very small number of simulation studies. However, in the case of the goodness-of-fit problem no simulation study can ever be exhaustive. The case studies discussed above include a total of 140 power calculations, with powers ranging from the nominal 5% type I error probability to 100%. The mean power for all cases of the RG method is 53.0%, which is higher than any other. Those are: ZC 49.5%, AD 48.1%, Equal Size 46.2%, ZK 43.7%, KS 39.9%, Equal Prob 38.5%, Histogram 33.2% and ZA 32.1%. That RG has the highest overall power is due to the fact that it never performs especially badly.
Fig. 9 Powers of tests for $H_0 : F_0 = U[0, 1]$ versus Beta(q, q). ZC is best, with RG second.

Fig. 10 Powers of tests for $H_0 : F_0 = N(r, \sqrt{r})$ versus Gamma(r, 1). RG is best, with ZC second.
8 Computational issues

All the calculations and simulations discussed in this paper were done using R. An R library with all the routines as well as an RMarkdown file with the routines to do all the simulations discussed here is available at https://github.com/wolfgangrolke/chisqalt. We also created a R Shiny app running online at https://drrolke.shinyapps.io/RGtest/ that allows the user to upload their data and run the test without knowledge of R. It also allows the user to upload a C++ routine for more complicated cases.

9 Conclusions

We have presented a new method for binning continuous data for a chi-square test. Our method uses the idea of a perfect data set to quickly search through a large number of binnings and finds one which can be expected to have the highest power from among the included binnings against a specified alternative. Our simulation studies show that this method is quite competitive with and sometimes better than either the Kolmogorov–Smirnov, the Anderson–Darling or the Zhang tests.

Our results also are of interest if there is no alternative hypothesis. Unlike most published results we find that a small number of bins is generally best, regardless of the sample size. Certainly the practice in many fields to draw a histogram with many bins, and then apply the chi-square test using the same binning leads to a badly underpowered test.

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