

Testing Consistency of Two Histograms*

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Abstract

Several approaches to testing the hypothesis that two histograms are drawn from the same distribution are investigated. We note that single-sample continuous distribution tests may be adapted to this two-sample grouped data situation. The difficulty of not having a fully-specified null hypothesis is an important consideration in the general case, and care is required in estimating probabilities with “toy” Monte Carlo simulations. The performance of several common tests is compared; no single test performs best in all situations.

1. Introduction

Sometimes we have two histograms and are faced with the question: “Are they consistent?” That is, are our two histograms consistent with having been sampled from the same parent distribution. For example, we might have a kinematic distribution in two similar channels that we think should be consistent, and wish to test this hypothesis. Each histogram represents a sampling from a multivariate Poisson distribution. The question is whether the means are bin-by-bin equal between the two distributions. Or, if we are only interested in “shape”, are the means related by the same scale factor for all bins? We investigate this question in the context of frequency statistics.

For example, consider Fig. 1. Are the two histograms consistent or can we conclude that they are drawn from different distributions?

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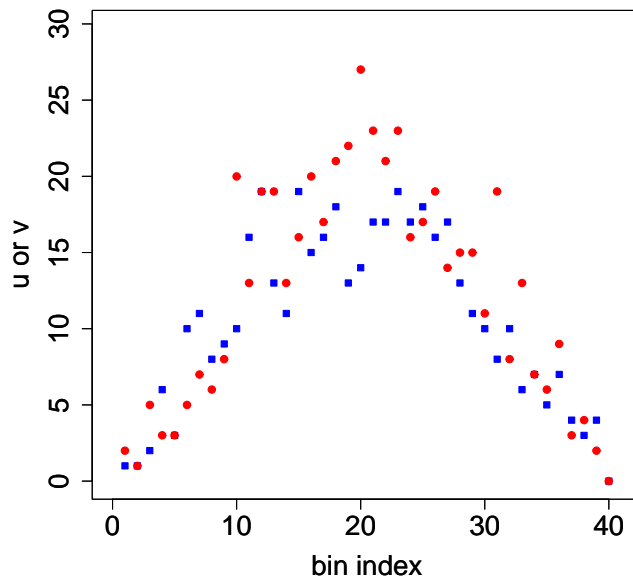


Fig. 1. Two histograms (blue squares and red circles) to be compared for consistency.

There are at least two variants of interest to this question:

1. We wish to test the hypothesis:

H_0 : The means of the two histograms are bin-by-bin equal, against

H_1 : The means of the two histograms are not bin-by-bin equal.

2. We wish to test the hypothesis:

H'_0 : The densities of the two histograms are bin-by-bin equal, against

H'_1 : The densities of the two histograms are not bin-by-bin equal.

In the second case, the relative normalization of the two histograms is not an issue: we only compare the shapes.

It may be noted that there are a large variety of tests that attempt to answer the question of whether a given dataset is consistent with having been drawn from some specified continuous distribution. These tests may typically be adapted to address the question of whether two datasets have been drawn from the same continuous distribution, often referred to as “two-sample” tests. These tests may further be adapted to the present problem, that of determining whether two histograms have

the same shape. This situation is also referred to as comparing whether two (or more) rows of a “table” are consistent. The datasets of this form are also referred to as “grouped data”.

Although we keep the discussion focussed on the comparison of two histograms, it is worth remarking that many of the observations apply also to other situations, such as the comparison of a histogram with a model prediction.

2. Notation

We assume that we have formed our two histograms with the same number of bins, k , with identical bin boundaries. The bin contents of the “first” histogram are given by realization u of random variable U , and of the second by realization v of random variable V . Thus, the sampling distributions are:

$$\begin{aligned} P(U = u) &= \prod_{i=1}^k \frac{\mu_i^{u_i}}{u_i!} e^{-\mu_i}, \\ P(V = v) &= \prod_{i=1}^k \frac{\nu_i^{v_i}}{v_i!} e^{-\nu_i}, \end{aligned} \tag{1}$$

where the vectors μ and ν are the mean bin contents of the respective histograms.

We define:

$$\begin{aligned} N_u &\equiv \sum_{i=1}^k U_i, && \text{total contents of first histogram,} \\ N_v &\equiv \sum_{i=1}^k V_i, && \text{total contents of second histogram,} \\ \mu_T &\equiv \langle N_u \rangle = \sum_{i=1}^k \mu_i, \\ \nu_T &\equiv \langle N_v \rangle = \sum_{i=1}^k \nu_i, \\ t_i &\equiv u_i + v_i, && i = 1, \dots, k. \end{aligned}$$

We are interested in the power of a test, at any given confidence level. The power is the probability that the null hypothesis is rejected when it is false. Of course, the

power depends on the true sampling distribution. In other words, the power is one minus the probability of a Type II error. The confidence level is the probability that the null hypothesis is accepted, if the null hypothesis is correct. Thus, the confidence level is one minus the probability of a Type I error. In physics, we usually don't specify the confidence level of a test in advance, at least not formally. Instead, we quote the P -value for our result. This is the probability, under the null hypothesis, of obtaining a result as “bad” or worse than our observed value. This would be the probability of a Type I error if our observation were used to define the critical region of the test.

Note that we are dealing with discrete distributions here, and exact statements of frequency are problematic, though not impossible. Instead of attempting to construct exact statements, our treatment of the discreteness will be such as to err on the “conservative” side. By “conservative”, we mean that we will tend to accept the null hypothesis with greater than the stated probability. It is important to understand that this is not always the “conservative” direction, for example it could mislead us into accepting a model when it should be rejected.

We will drop the distinction between the random variable (upper case symbols U and V) and a realization (lower case u and v) in the following, but will point out where this informality may yield confusion.

The computations in this note are carried out in the framework of the R statistics package [1].

2.1 Large Statistics Case

If all of the bin contents of both histograms are large, then we may use the approximation that the bin contents are normally distributed.

Under H_0 ,

$$\langle u_i \rangle = \langle v_i \rangle \equiv \mu_i, \quad i = 1, \dots, k.$$

More properly, it is $\langle U_i \rangle = \mu_i$, etc., but we are permitting u_i to stand for the random variable as well as its realization, as noted above. Let the difference in the contents

of bin i between the two histograms be:

$$\Delta_i \equiv u_i - v_i,$$

and let the standard deviation for Δ_i be denoted σ_i . Then the sampling distribution of the difference between the two histograms is:

$$P(\Delta) = \frac{1}{(2\pi)^{k/2}} \left(\prod_{i=1}^k \frac{1}{\sigma_i} \right) \exp \left(-\frac{1}{2} \sum_{i=1}^k \frac{\Delta_i^2}{\sigma_i^2} \right).$$

This suggests the test statistic:

$$T = \sum_{i=1}^k \frac{\Delta_i^2}{\sigma_i^2}.$$

If the σ_i were known, this would simply be distributed according to the chi-square distribution with k degrees of freedom. The maximum-likelihood estimator for the mean of a Poisson is just the sampled number. The mean of the Poisson is also its variance, and we will use the sampled number also as the estimate of the variance in the normal approximation.

We suggest the following algorithm for this test:

1. For σ_i^2 form the estimate

$$\hat{\sigma}_i^2 = (u_i + v_i).$$

2. Statistic T is thus evaluated according to:

$$T = \sum_{i=1}^k \frac{(u_i - v_i)^2}{u_i + v_i}.$$

If $u_i = v_i = 0$ for bin i , the contribution to the sum from that bin is zero.

3. Estimate the P -value according to a chi-square with k degrees of freedom. Note that this is not an exact result.

If it is desired to only compare shapes, then the suggested algorithm is to scale both histogram bin contents:

1. Let

$$N = 0.5(N_u + N_v).$$

Scale u and v according to:

$$\begin{aligned} u_i &\rightarrow u'_i = u_i(N/N_u) \\ v_i &\rightarrow v'_i = v_i(N/N_v). \end{aligned}$$

2. Estimate σ_i^2 with:

$$\hat{\sigma}_i^2 = \left(\frac{N}{N_u}\right)^2 u_i + \left(\frac{N}{N_v}\right)^2 v_i.$$

3. Statistic T is thus evaluated according to:

$$T = \sum_{i=1}^k \frac{\left(\frac{u_i}{N_u} - \frac{v_i}{N_v}\right)^2}{\frac{u_i}{N_u^2} + \frac{v_i}{N_v^2}}.$$

3. Estimate the P -value according to a chi-square with $k - 1$ degrees of freedom.

Note that this is not an exact result.

Due to the presence of bins with small bin counts, we might not expect this method to be especially good for the data in Fig. 1, but we can try it anyway. Table I gives the results of applying this test, both including the normalization and only comparing shapes.

Table I. Results of tests for consistency of the two datasets in Fig. 1. The tests below the χ^2 lines are described in Section 3.

Type of test	T	NDOF	$P(\chi^2 > T)$	P -value
χ^2 Absolute comparison	29.8	40	0.88	0.86
χ^2 Shape comparison	24.9	39	0.96	0.95
Likelihood Ratio Shape comparison	25.3	39	0.96	0.96
Kolmogorov-Smirnov Shape comparison	0.043	39	NA	0.61
Bhattacharyya Shape comparison	0.986	39	NA	0.97
Cramér-Von-Mises Shape comparison	0.132	39	NA	0.45
Anderson-Darling Shape comparison	0.849	39	NA	0.45
Likelihood value shape comparison	79	39	NA	0.91

In the column labeled “ P -value” an attempt is made to compute (by simulation) a more reliable estimate of the probability, under the null hypothesis, that a value for T will be as large as that observed. This may be compared with the $P(\chi^2 > T)$ column, which is the probability assuming T follows a χ^2 distribution with NDOF degrees of freedom.

Note that the absolute comparison yields slightly poorer agreement between the histograms than the shape comparison. The total number of counts in one dataset is 492; in the other it is 424. Treating these as samplings from a normal distribution with variances 492 and 424, we find a difference of 2.2 standard deviations or a two-tailed P -value of 0.025. This low probability is diluted by the bin-by-bin test. Using a bin-by-bin test to check whether the totals are consistent is not a powerful approach. In fact, the two histograms were generated with a 10% difference in expected counts.

The evaluation by simulation of the probability under the null hypothesis is in fact problematic, since the null hypothesis actually isn’t completely specified. The problem is the dependence of Poisson probabilities on the absolute numbers of counts. Probabilities for differences in Poisson counts are not invariant under the total number of counts. Unfortunately, we don’t know the true mean numbers of counts in each bin. Thus, we must estimate these means. The procedure adopted here is to use the maximum likelihood estimators (see below) for the mean numbers, in the null hypothesis. We’ll have further discussion of this procedure below – it does not always yield valid results.

In our example, the probabilities estimated according to our simulation and the probabilities according to a χ^2 distribution are close to each other. This suggests the possibility of using the χ^2 probabilities – if we can do this, the problem that we haven’t completely specified the null hypothesis is avoided. We offer the following conjecture:

Conjecture: Let T be the test statistic described above, for either the absolute or the shape comparison, as desired. Let T_c be a possible value of T (perhaps the critical value to be used in a hypothesis test). Then, for large values of T_c :

$$P(T < T_c) \geq P(T < T_c | \chi^2(T, \text{ndof})) ,$$

where $P(T < T_c | \chi^2(T, \text{ndof}))$ is the probability that $T < T_c$ according to a χ^2 dis-

tribution with ndof degrees of freedom (either k or $k - 1$, according to which test is being performed).

We'll only suggest an approach to a proof, which could presumably also be used to develop a formal condition for T_c to be “large”. The conjecture also appears to be true anecdotally, and for interesting values of T_c , noting that it is large values of T_c that we care most about for an interesting hypothesis test.

We provide some intuition for the conjecture by considering the case of one bin. For simplicity we'll also suppose that $\nu = \mu$ and that μ is small ($\ll 1$, say). Since we are interested in large values of the statistic, we are interested in the situation where one of u, v is large, and the other small (since μ is small). Suppose it is u that is large. Then

$$T = \frac{(u - v)^2}{u + v} \approx u.$$

For given v (0, say), the probability of T is thus

$$P(T) \approx \frac{\mu^T}{T!} e^{-\mu}.$$

This may be compared with the chi-square probability distribution for one degree of freedom:

$$P(T = \chi^2) = \frac{1}{\sqrt{2\pi}} \frac{e^{-T/2}}{\sqrt{T}}.$$

The ratio is, dropping the constants:

$$\frac{P(T)}{P(T = \chi^2)} \propto \frac{\mu^T e^{T/2} \sqrt{T}}{T!} = \frac{\exp [T (\frac{1}{2} + \ln \mu)]}{\sqrt{T} \Gamma(T)},$$

which approaches zero for large T , for any given μ . We conclude that the conjecture is valid in the case of one bin, and strongly suspect that the argument generalizes to multiple bins.

According to the conjecture, if we use the probabilities from a χ^2 distribution in our test, the error that we make is in the “conservative” direction (as long as T_c is large). That is, we'll reject the null hypothesis less often than we would with the correct probability. It should be emphasized that this conjecture is independent of the statistics of the sample, bins with zero counts are fine. In the limit of large statistics, the inequality approaches equality.

Lest we conclude that it is acceptable to just use this great simplification in all situations, we hasten to point out that it isn't as nice as it sounds. The problem is that, in low statistics situations, the power of the test according to this approach can be dismal. That is, we might not reject the null hypothesis in situations where it is obviously implausible.

We may illustrate these considerations with some simple examples, see Fig. 2. The plot for high statistics on the left shows excellent agreement between the actual distribution and the χ^2 distribution. The lower statistics plots in the middle and right, for two different models, show that the chi-square approximation is very conservative in general. Thus, using the chi-square probability lacks power in this case, and is not a recommended approximation.

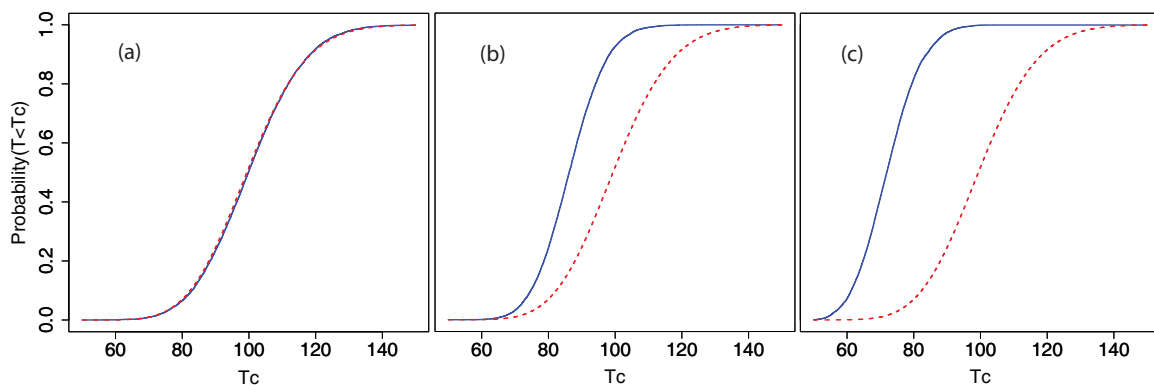


Fig. 2. Comparison of the actual (cumulative) probability distribution for T with the chi-square distribution. The solid blue curves show the actual distributions, and the dashed red curves the chi-square distributions. All plots are for 100 bin histograms. (a) Each bin has mean 100. (b) Each bin has mean 1. (c) Bin j has mean $30/j$.

3. General Case

If the bin contents are not necessarily large, then the normal approximation may not be good enough. There are various approaches we could take in this case. We'll discuss and compare several possibilities.

3.1 Combining Bins

A simple approach is to combine bins until the normal approximation is good enough. In many cases this doesn't lose too much statistical power. It may be necessary to check with simulations that probability statements are valid. Figure 3 shows the results of this approach on the data in Figure 1, as a function of the minimum number of events per bin. The comparison being made is for the shapes. The algorithm is to combine corresponding bins in both histograms until both have at least “minBin” counts in each bin.

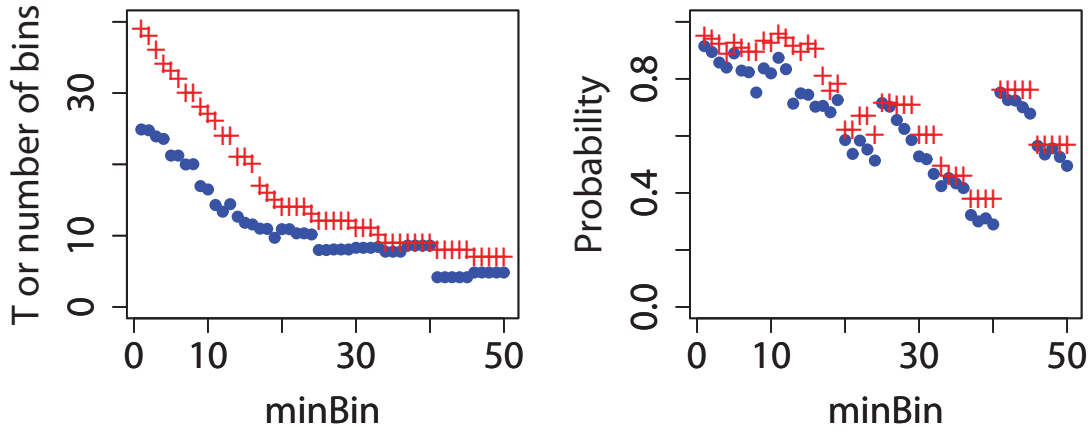


Fig. 3. Left: The blue dots show the value of the test statistic T , and the red pluses shows the number of histogram bins for the data in Fig. 1, as a function of the minimum number of counts per histogram bin. Right: The P -value for consistency of the two datasets in Fig. 1. The red pluses show the probability for a chi-square distribution, and the blue circles show the probability for the actual distribution, with an estimated null hypothesis.

3.2 Testing for Equal Normalization

An alternative is to work with the Poisson distributions. Let us separate the problem of the shape from the problem of the overall normalization. In the case of testing equality of overall normization, there is a well-motivated choice for the test statistic, even for low statistics.

To test the normalization, we simply compare totals over all bins between the

two histograms. Our distribution is

$$P(N_u, N_v) = \frac{\mu_T^{N_u} \nu_T^{N_v}}{N_u! N_v!} e^{-(\mu_T + \nu_T)}.$$

The null hypothesis is $H_0 : \mu_T = \nu_T$, to be tested against alternative $H_1 : \mu_T \neq \nu_T$. We are thus interested in the difference between the two means; the sum is effectively a nuisance parameter. That is, we are interested in

$$\begin{aligned} P(N_v | N_u + N_v = N) &= \frac{P(N | N_v) P(N_v)}{P(N)} \\ &= \frac{\mu_T^{N-N_v} e^{-\mu_T}}{(N-N_v)!} \frac{\nu_T^{N_v} e^{-\nu_T}}{N_v!} \bigg/ \frac{(\mu_T + \nu_T)^N e^{-(\mu_T + \nu_T)}}{N!} \\ &= \binom{N}{N_v} \left(\frac{\nu_T}{\mu_T + \nu_T} \right)^{N_v} \left(\frac{\mu_T}{\mu_T + \nu_T} \right)^{N-N_v}. \end{aligned}$$

This probability now permits us to construct a uniformly most powerful test of our hypothesis (Ref. 2). Note that it is simply a binomial distribution, for given N . The uniformly most powerful property holds independently of N , although the probabilities cannot be computed without N .

The null hypothesis corresponds to $\mu_T = \nu_T$, that is:

$$P(N_v | N_u + N_v = N) = \binom{N}{N_v} \left(\frac{1}{2} \right)^N.$$

For our example, with $N = 916$ and $N_v = 424$, the P -value is 0.027, assuming a two-tailed probability is desired. This may be compared with our earlier estimate of 0.025 in the normal approximation. Note that for our binomial calculation we have “conservatively” included the endpoints (424 and 492). If we try to mimic more closely the normal estimate by subtracting one-half the probability at the endpoints, we obtain 0.025, essentially the normal number we found earlier. The `dbinom` function Ref. 3 in the R package has been used for this computation.

3.3 Shape Comparison Statistics

There are many different possible statistics for comparing the shapes of the histograms. We investigate several choices. Table I summarizes the result of each of these tests applied to the example in Fig. 1. We list the statistics here, and discuss performance in the following sections.

3.3.1 Chi-square test for shape

Even though we don't expect it to follow a χ^2 distribution, we may evaluate the test statistic:

$$\chi^2 = \sum_{i=1}^k \frac{\left(\frac{u_i}{N_u} - \frac{v_i}{N_v}\right)^2}{\frac{u_i}{N_u^2} + \frac{v_i}{N_v^2}}.$$

If $u_i = v_i = 0$, the contribution to the sum from that bin is zero. We have already discussed application of this statistic to the example of Fig. 1.

3.3.2 Geometric test for shape

Another test statistic we could try may be motivated from a geometric perspective. We consider the bin contents of a histogram to define a vector in a k -dimensional space. If two such vectors are drawn from the same distribution (the null hypothesis), then they will tend to point in the same direction (we are not interested in the lengths of the vectors here). Thus, if we represent each histogram as a unit vector with components:

$$\{u_1/N_u, \dots, u_k/N_u\}, \text{ and } \{v_1/N_v, \dots, v_k/N_v\},$$

we may form the test statistic:

$$T_{\text{BDM}} = \sqrt{\frac{u}{N_u} \cdot \frac{v}{N_v}} = \left(\sum_{i=1}^k \frac{u_i v_i}{N_u N_v} \right)^{1/2}.$$

This is known as the ‘‘Bhattacharyya distance measure’’. We'll refer to it as the ‘‘BDM’’ statistic for short. We assume that neither histogram is empty for this statistic. All vectors lie in the positive direction in all coordinates, so there is no issue with taking the square root.

It may be noticed that this statistic is related to the χ^2 statistic – the $\frac{u}{N_u} \cdot \frac{v}{N_v}$ dot product is close to the cross term in the χ^2 expression.

We apply this formalism to the example in Fig. 1. The resulting terms in the sum over bins are shown in Fig. 4. The sum over bins gives 0.986 (See Table I for a summary). According to our estimated distribution of this statistic under the null hypothesis, this gives a P -value of 0.97, similar to the χ^2 test result.

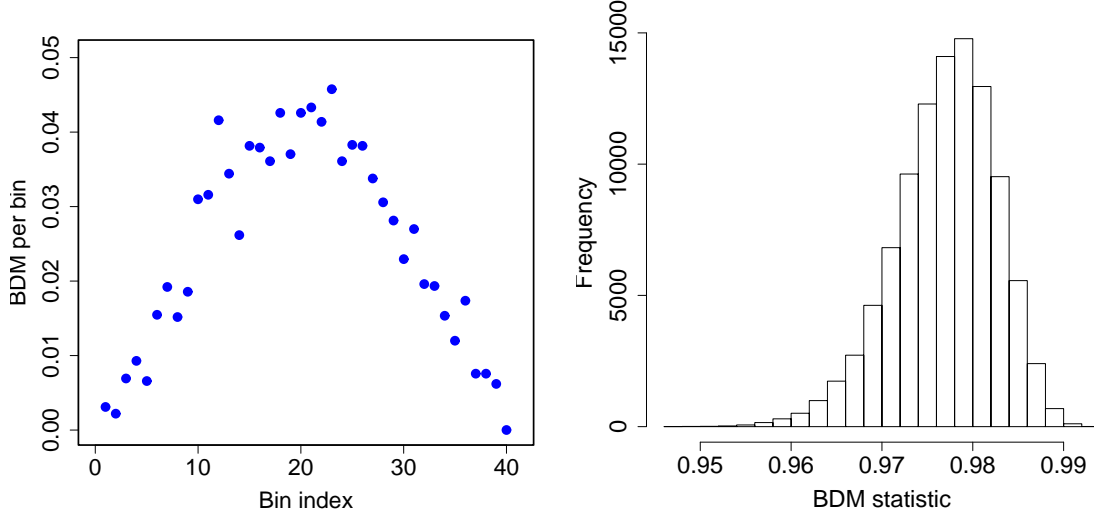


Fig. 4. Left: Bin-by-bin contributions to the geometric (“BDM”) test statistic for the example of Fig. 1. Right: Estimated distribution of the BDM statistic for the null hypothesis in the example of Fig. 1.

3.3.3 Kolmogorov-Smirnov test

Another approach to a shape test may be based on the Kolmogorov-Smirnov (KS) idea. Recall that the idea of the KS test is to estimate the maximum difference between observed and predicted cumulative distribution functions (CDFs) and compare with expectations. We may adapt this idea to the present case. It should be remarked that if we have the actual data points from which the histograms are derived, then we may use the Kolmogorov-Smirnov (“KS”) procedure directly on those points. This would incorporate additional information and yield a potentially more powerful test. However, if the bin widths are small compared with possible structure it may be expected to not make much difference.

We modify the KS statistic to apply to comparison of histograms as follows. We assume that neither histogram is empty. Form the “cumulative distribution histograms” according to:

$$u_{ci} = \sum_{j=1}^i u_j / N_u$$

$$v_{ci} = \sum_{j=1}^i v_j / N_v.$$

Then compute the test statistic:

$$T_{\text{KS}} = \max_i |u_{ci} - v_{ci}|.$$

Test statistics may also be formed for one-tail tests, but we consider only the two-tail test here.

We apply this formalism to the example in Fig. 1. The bin-by-bin distances are shown in Fig. 5. The maximum over bins gives 0.043 (See Table I for a summary). According to our estimated distribution of this statistic under the null hypothesis, this gives a P -value of 0.61, somewhat smaller than for the χ^2 test result, but still indicating consistency of the two histograms. Note that the KS test tends to emphasize the region near the peak of the distribution, that is the region where the largest fluctuations are expected in Poisson statistics.

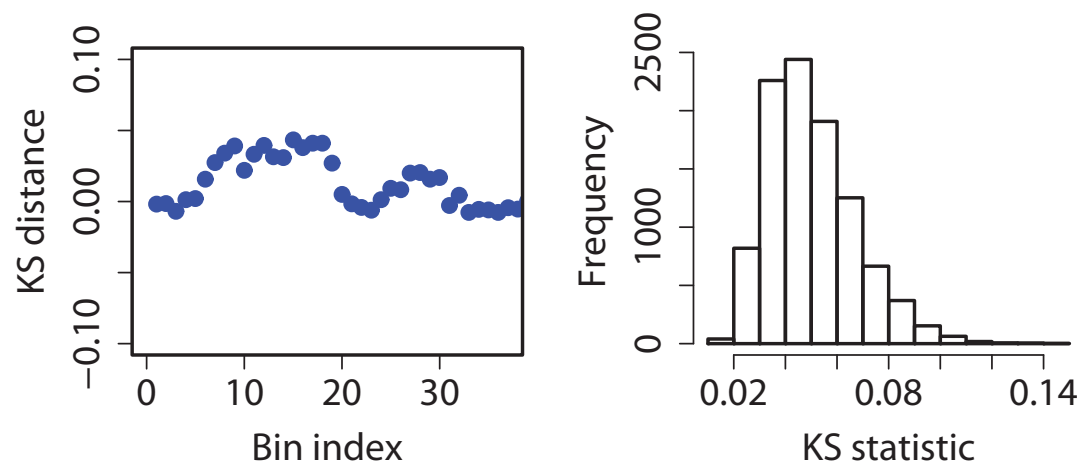


Fig. 5. Left: Bin-by-bin distances for the Kolmogorov-Smirnov test statistic for the example of Fig. 1. Right: Estimated distribution of the Kolmogorov-Smirnov distance for the null hypothesis in the example of Fig. 1.

3.3.4 Cramér-von-Mises test

Somewhat similar to the Kolmogorov-Smirnov test is the Cramér-von-Mises (CVM) test. The idea in this test is to add up the squared differences between the cumulative distributions being compared. Again, this test is usually thought of as a test to compare an observed distribution with a presumed parent continuous probability distribution. However, the algorithm can be adapted to the two-sample comparison, and to the case of comparing two histograms.

The test statistic for comparing the two samples x_1, x_2, \dots, x_N and y_1, y_2, \dots, y_M is [4]:

$$T = \frac{NM}{(N+M)^2} \left\{ \sum_{i=1}^N [E_x(x_i) - E_y(x_i)]^2 + \sum_{j=1}^M [E_x(y_j) - E_y(y_j)]^2 \right\},$$

where E_x is the empirical cumulative distribution for sampling x . That is, $E_x(x) = n/N$ if n of the sampled x_i are less than or equal to x .

We adapt this for the present application of comparing histograms with bin contents u_1, u_2, \dots, u_k and v_1, v_2, \dots, v_k with identical bin boundaries: Let z be a point in bin i , and define the empirical cumulative distribution function for histogram u as:

$$E_u(z) = \sum_{j=1}^i u_j / N_u.$$

Then the test statistic is:

$$T_{\text{CVM}} = \frac{N_u N_v}{(N_u + N_v)^2} \sum_{j=1}^k (u_j + v_j) [E_u(z_j) - E_v(z_j)]^2.$$

We apply this formalism to the example in Fig. 1, finding $T_{\text{CVM}} = 0.132$. The resulting estimated distribution under the null hypothesis is shown in Fig. 6. According to our estimated distribution of this statistic under the null hypothesis, this gives a P -value of 0.45 (See Table I for a summary), somewhat smaller than the χ^2 test result.

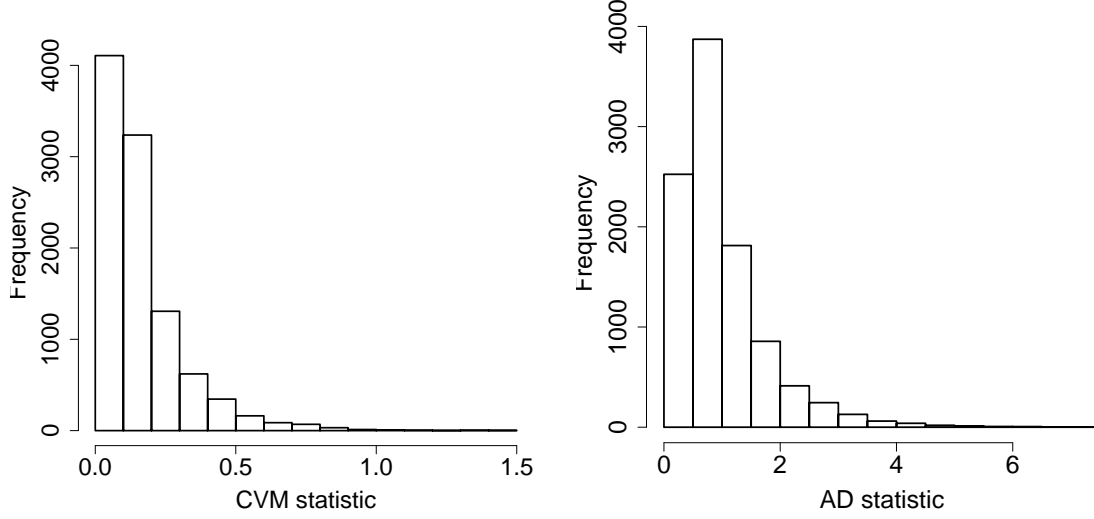


Fig. 6. Estimated distributions of the test statistic for the null hypothesis in the example of Fig. 1 Left: The Cramér-von-Mises statistic. Right: The Anderson-Darling statistic.

3.3.5 Anderson-Darling test for shape

The Anderson-Darling test is another variant on the theme of non-parametric comparison of cumulative distributions. It is similar to the Cramér-von-Mises statistic, but is designed to be sensitive to the tails of the CDF. The original statistic was, once again, designed to compare a dataset drawn from a continuous distribution, with CDF $F_0(x)$ under the null hypothesis:

$$A_m^2 = m \int_{-\infty}^{\infty} \frac{[F_m(x) - F_0(x)]^2}{F_0(x)[1 - F_0(x)]} dF_0(x),$$

where $F_m(x)$ is the empirical CDF of dataset x_1, \dots, x_m . Scholz and Stephens [5] provide a form of this statistic for a k -sample test on grouped data (e.g., as might be used to compare k histograms). Based on the result expressed in their Eq. 6, the expression of interest to us for two histograms is:

$$T_{\text{AD}} = \frac{1}{N_u + N_v} \sum_{j=k_{\min}}^{k_{\max}-1} \frac{t_j}{\Sigma_j (N_u + N_v - \Sigma_j)} \left\{ [(N_u + N_v)\Sigma_{uj} - N_u \Sigma_j]^2 / N_u + [(N_u + N_v)\Sigma_{vj} - N_v \Sigma_j]^2 / N_v \right\},$$

where k_{\min} is the first bin where either histogram has non-zero counts, k_{\max} is the number of bins counting up to the last bin where either histogram has non-zero counts, and

$$\begin{aligned}\Sigma_{uj} &\equiv \sum_{i=1}^j u_i, \\ \Sigma_{vj} &\equiv \sum_{i=1}^j v_i, \quad \text{and} \\ \Sigma_j &\equiv \sum_{i=1}^j t_i = \Sigma_{uj} + \Sigma_{vj}.\end{aligned}$$

We apply this formalism to the example in Fig. 1. The resulting estimated distribution under the null hypothesis is shown in Fig. 6. The sum over bins gives 0.849 (See Table I for a summary). According to our estimated distribution of this statistic under the null hypothesis, this gives a P -value of 0.45, somewhat smaller than the χ^2 test result, but similar with the CVM result.

3.3.6 Likelihood ratio test for shape

We may base a test whether the histograms are sampled from the same shape distribution on the same binomial idea as we used for the normalization test. In this case, however, there is a binomial associated with each bin of the histogram. We start with the null hypothesis, that the two histograms are sampled from the joint distribution:

$$P(u, v) = \prod_{i=1}^k \frac{\mu_i^{u_i}}{u_i!} e^{-\mu_i} \frac{\nu_i^{v_i}}{v_i!} e^{-\nu_i},$$

where $\nu_i = a\mu_i$ for $i = 1, 2, \dots, k$. That is, the “shapes” of the two histograms are the same, although the total contents may differ.

With $t_i = u_i + v_i$, and fixing the t_i at the observed values, we have the multi-binomial form:

$$P(v|u+v=t) = \prod_{i=1}^k \binom{t_i}{v_i} \left(\frac{\nu_i}{\nu_i + \mu_i} \right)^{v_i} \left(\frac{\mu_i}{\nu_i + \mu_i} \right)^{t_i - v_i}.$$

The null hypothesis is that $\nu_i = a\mu_i$ for all values of i . We would like to test this, but there are now two complications:

1. The value of “ a ” is not specified;
2. We still have a multivariate distribution.

For a , we will substitute an estimate from the data, namely the maximum likelihood estimator:

$$\hat{a} = \frac{N_v}{N_u}.$$

Note that this estimate is a random variable; its use will reduce the effective number of degrees of freedom by one.

We propose to use a likelihood ratio statistic to reduce the problem to a single variable. This will be the likelihood under the null hypothesis (with a given by its maximum likelihood estimator), divided by the maximum of the likelihood under the alternative hypothesis. Thus, we form the ratio:

$$\begin{aligned} \lambda &= \frac{\max_{H_0} \mathcal{L}(a|v; u + v = t)}{\max_{H_1} \mathcal{L}(\{a_i \equiv \nu_i/\mu_i\}|v; u + v = t)} \\ &= \prod_{i=1}^k \frac{\left(\frac{\hat{a}}{1+\hat{a}}\right)^{v_i} \left(\frac{1}{1+\hat{a}}\right)^{t_i-v_i}}{\left(\frac{\hat{a}_i}{1+\hat{a}_i}\right)^{v_i} \left(\frac{1}{1+\hat{a}_i}\right)^{t_i-v_i}}. \end{aligned}$$

The maximum likelihood estimator, under H_1 , for a_i is just

$$\hat{a}_i = v_i/u_i.$$

Thus, we rewrite our test statistic according to:

$$\lambda = \prod_{i=1}^k \left(\frac{1 + v_i/u_i}{1 + N_v/N_u} \right)^{t_i} \left(\frac{N_v}{N_u} \frac{u_i}{v_i} \right)^{v_i}.$$

In practice, we'll work with

$$-2 \ln \lambda = -2 \sum_{i=1}^k \left[t_i \ln \left(\frac{1 + v_i/u_i}{1 + N_v/N_u} \right) + v_i \ln \left(\frac{N_v}{N_u} \frac{u_i}{v_i} \right) \right].$$

Before attempting to apply this, we investigate how to handle zero bin contents. It is possible that $u_i = v_i = 0$ for some bin. In this case, $P(v_i|u_i + v_i = t_i) = 1$,

under both H_0 and H_1 , and this bin contributes zero to the sum. It is also possible that $t_i \neq 0$, but $v_i = 0$ or $u_i = 0$. If $v_i = 0$, then

$$P(0|t_i) = \left(\frac{\mu_i}{\nu_i + \mu_i} \right)^{t_i}.$$

Under H_0 , this is

$$\left(\frac{1}{1+a} \right)^{t_i},$$

and under H_1 it is

$$\left(\frac{1}{1+a_i} \right)^{t_i}.$$

The maximum likelihood estimator for a_i is $\hat{a}_i = 0$. Thus, the likelihood ratio for bin i is

$$\lambda_i = \left(\frac{1}{1+\hat{a}} \right)^{t_i},$$

and this contributes to the sum an amount:

$$-2 \ln \lambda_i = -2t_i \ln \left(\frac{N_u}{N_u + N_v} \right).$$

If instead $u_i = 0$, then

$$P(t_i|t_i) = \left(\frac{\nu_i}{\nu_i + \mu_i} \right)^{t_i}.$$

and the contribution to the sum is

$$-2 \ln \lambda_i = -2t_i \ln \left(\frac{N_v}{N_u + N_v} \right).$$

We apply this formalism to the example in Fig. 1. The resulting terms in the sum over bins are shown in Fig. 7. The sum over bins gives 25.3 (See Table I for a summary). This statistic should asymptotically be distributed according to a χ^2 distribution with the number of degrees of freedom equal to one less than the number of bins, or $N_{\text{DOF}} = 39$ in this case. If valid, this gives a P -value of 0.96 in this example. This may be compared with a probability of 0.96 according to the estimated actual distribution. In this example we obtain nearly the same answer as the naive application of the chi-square calculation with no bins combined.

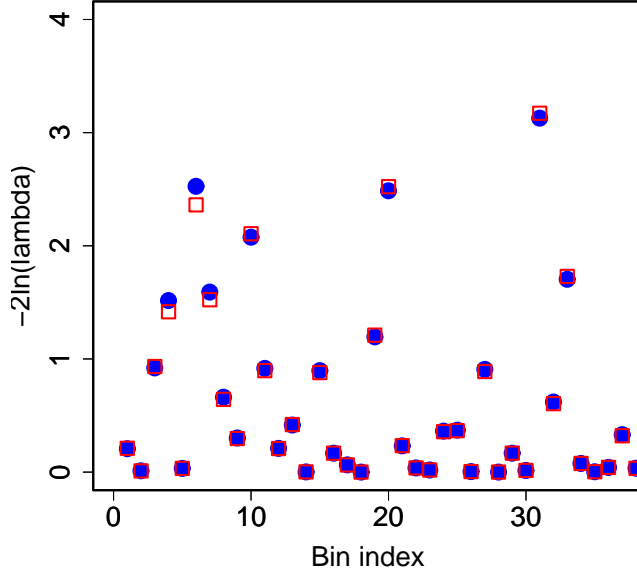


Fig. 7. Value of $-2 \ln \lambda_i$ or χ_i^2 as a function of histogram bin in the comparison of the two distributions of Fig. 1. Blue circles are $-2 \ln \lambda_i$; red squares are χ_i^2 .

We may see that this close agreement is a result of nearly bin-by-bin equality of the two statistics, see Fig. 7. To investigate when this might hold more generally, we compare the values of $-2 \ln \lambda_i$ and χ_i^2 as a function of u_i and v_i , Fig. 8. We observe that the two statistics agree when $u_i = v_i$ with increasing difference away from that point. This observation is readily verified analytically. This agreement holds even for low statistics. However, we shouldn't conclude that the chi-square approximation may be used for low statistics – fluctuations away from equal numbers lead to quite different results when we get into the tails at low statistics. Our example doesn't really sample these tails.

The precise value of the probability should not be taken too seriously, except to conclude that the two distributions are consistent according to these tests. For example, when we combine bins to improve expected χ^2 behavior, we see fairly large fluctuations in the probability estimate just due to the re-binning (Fig. 3).

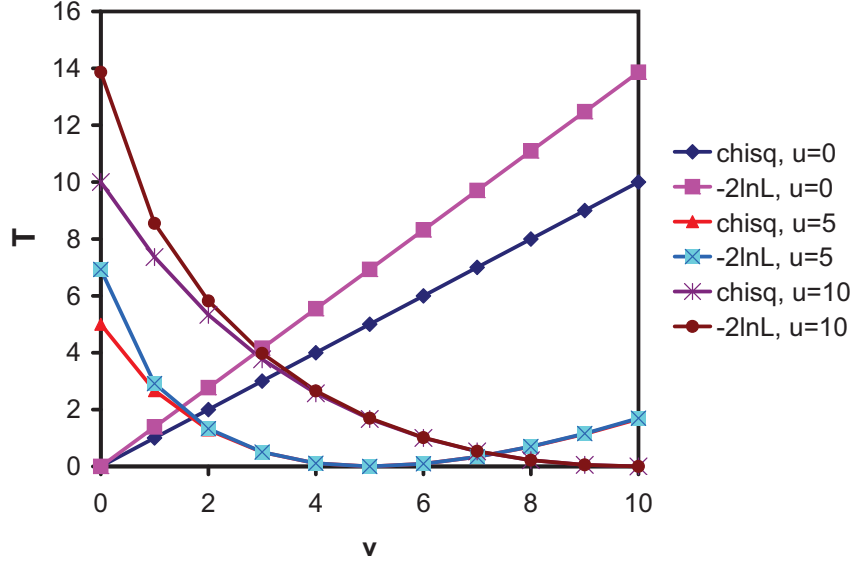


Fig. 8. Value of $-2 \ln \lambda_i$ or χ_i^2 as a function of u_i and v_i bin contents. This plot assumes $N_u = N_v$. The i subscript is dropped, with the understanding that this comparison is for a single bin.

3.3.7 Likelihood value test for shape

An often-used but controversial goodness-of-fit statistic is the value of the likelihood at its maximum value under the null hypothesis. It can be demonstrated that this statistic carries little or no information in some situations. However, in the limit of large statistics it is essentially the chi-square statistic, so there are known situations where it is a plausible statistic to use. We thus look at it here.

Using the results in the previous section, the test statistic is:

$$T = -\ln \mathcal{L} = -\sum_{i=1}^k \left[\ln \left(\frac{t_i}{v_i} \right) + t_i \ln \frac{N_u}{N_u + N_v} + v_i \ln \frac{N_v}{N_u} \right].$$

If either $N_u = 0$ or $N_v = 0$, then $T = 0$.

We apply this formalism to the example in Fig. 1. The resulting estimated distribution under the null hypothesis is shown in Fig. 9. The sum over bins gives 90 (See Table I for a summary). According to our estimated distribution of this statistic under the null hypothesis, this gives a P -value of 0.29, similar to the χ^2 test result. The fact that it is similar may be expected from the fact that our example is reasonably well-approximated by the large statistics limit.

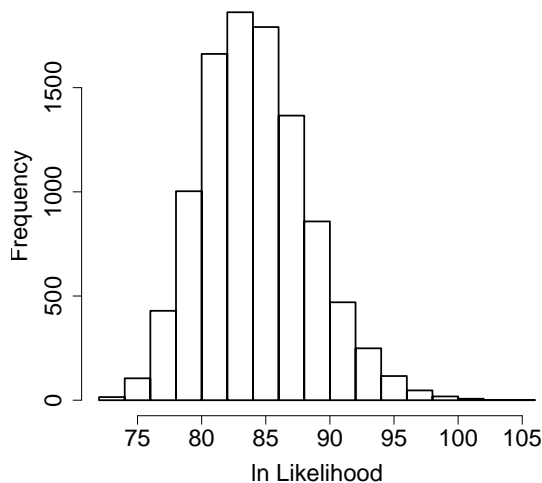


Fig. 9. Estimated distribution of the $\ln \mathcal{L}$ test statistic for the null hypothesis in the example of Fig. 1.

There are many other possible tests that could be considered, for example, schemes that “partition” the χ^2 to select sensitivity to different characteristics [6].

3.4 Distributions Under the Null Hypothesis

For the situation where the asymptotic distribution may not be good enough, we would like to know the probability distribution of our test statistic under the null hypothesis. However, we encounter a difficulty: our null hypothesis is not completely specified! The problem is that the distribution depends on the values of $\nu_i = a\mu_i$. Our null hypothesis only says $\nu_i = a\mu_i$, but says nothing about what μ_i might be. Note that it also doesn’t specify a , but we have already discussed that complication, which appears manageable (although in extreme situations one might need to check for dependence on a).

We turn once again to the data to make an estimate for μ_i , to be used in estimating the distribution of our test statistics. The straightforward approach is to use the maximum likelihood parameter estimators (under H_0):

$$\hat{\mu}_i = \frac{1}{1 + \hat{a}}(u_i + v_i),$$

$$\hat{\nu}_i = \frac{\hat{a}}{1 + \hat{a}}(u_i + v_i),$$

where $\hat{a} = N_v/N_u$. The data is then repeatedly simulated using these values for the parameters of the sampling distribution. For each simulation, a value of the test statistic is obtained. The distribution so obtained is then an estimate of the distribution of the test statistic under the null hypothesis, and P -values may be computed from this. Variations in the estimates for $\hat{\mu}_i$ and \hat{a} may be used to check robustness of the probability estimates obtained in this way.

We have just described the approach that was used to compute the estimated probabilities for the example of Fig. 1. The bin contents in this case are reasonably large, and this approach works well enough for this case.

Unfortunately, this approach does very poorly in the low-statistics realm. We consider a simple test case: Suppose our data is sampled from a flat distribution with a mean of 1 count in each of 100 bins. We test how well our estimated null hypothesis works for any given test statistic, T , as follows:

1. Generate a pair of histograms according to the distribution just described.
 - (a) Compute T for this pair of histograms.
 - (b) Given the pair of histograms, compute the estimated null hypothesis according to the specified prescription above.
 - (c) Generate many pairs of histograms according to the estimated null hypothesis in order to obtain an estimated distribution for T .
 - (d) Using the estimated distribution for T , determine the estimated P -value for the value of T found in step 1a.
2. Repeat step 1 many times and make a histogram of the estimated P -values. Note that this histogram should be uniform if the estimated P -values are good estimates.

The distributions of the estimated probabilities for the seven test statistics under the null hypothesis are shown in the second column of Fig. 10. If the null hypothesis were to be rejected at the estimated 0.01 probability, this algorithm would actually reject H_0 19% of the time for the χ^2 statistic, 16% of the time for the BDM statistic, 24% of the time for the $\ln \lambda$ statistic, and 29% of the time for the \mathcal{L} statistics, all unacceptably larger than the desired 1%. The KS, CVM, and AD statistics are all consistent with the desired 1%. For comparison, the first column of Fig. 10 shows the distribution for a “large statistics” case, where sampling is from histograms with a mean of 100 counts in each bin. We find that all test statistics display the desired flat distribution in this case. Table II summarizes these results.

Table II. Probability that the null hypothesis will be rejected with a cut at 1% on the estimated distribution (see text). H_0 is estimated with the bin-by-bin algorithm in the first two columns, by the uniform histogram algorithm in the third column, and with a Gaussian kernel estimation in the fourth column.

Test statistic	Probability (%)	Probability (%)	Probability (%)	Probability (%)
Bin mean =	100	1	1 (uniform)	1 (kernel)
H_0 estimate	bin-by-bin	bin-by-bin	uniform	kernel
χ^2	0.97 \pm 0.24	18.5 \pm 1.0	1.2 \pm 0.3	1.33 \pm 0.28
BDM	0.91 \pm 0.23	16.4 \pm 0.9	0.30 \pm 0.14	0.79 \pm 0.22
KS	1.12 \pm 0.26	0.97 \pm 0.24	1.0 \pm 0.2	1.21 \pm 0.27
CVM	1.09 \pm 0.26	0.85 \pm 0.23	0.8 \pm 0.2	1.27 \pm 0.28
AD	1.15 \pm 0.26	0.85 \pm 0.23	1.0 \pm 0.2	1.39 \pm 0.29
$\ln \lambda$	0.97 \pm 0.24	24.2 \pm 1.1	1.5 \pm 0.3	2.0 \pm 0.34
$\ln \mathcal{L}$	0.97 \pm 0.24	28.5 \pm 1.1	0.0 \pm 0.0	0.061 \pm 0.061

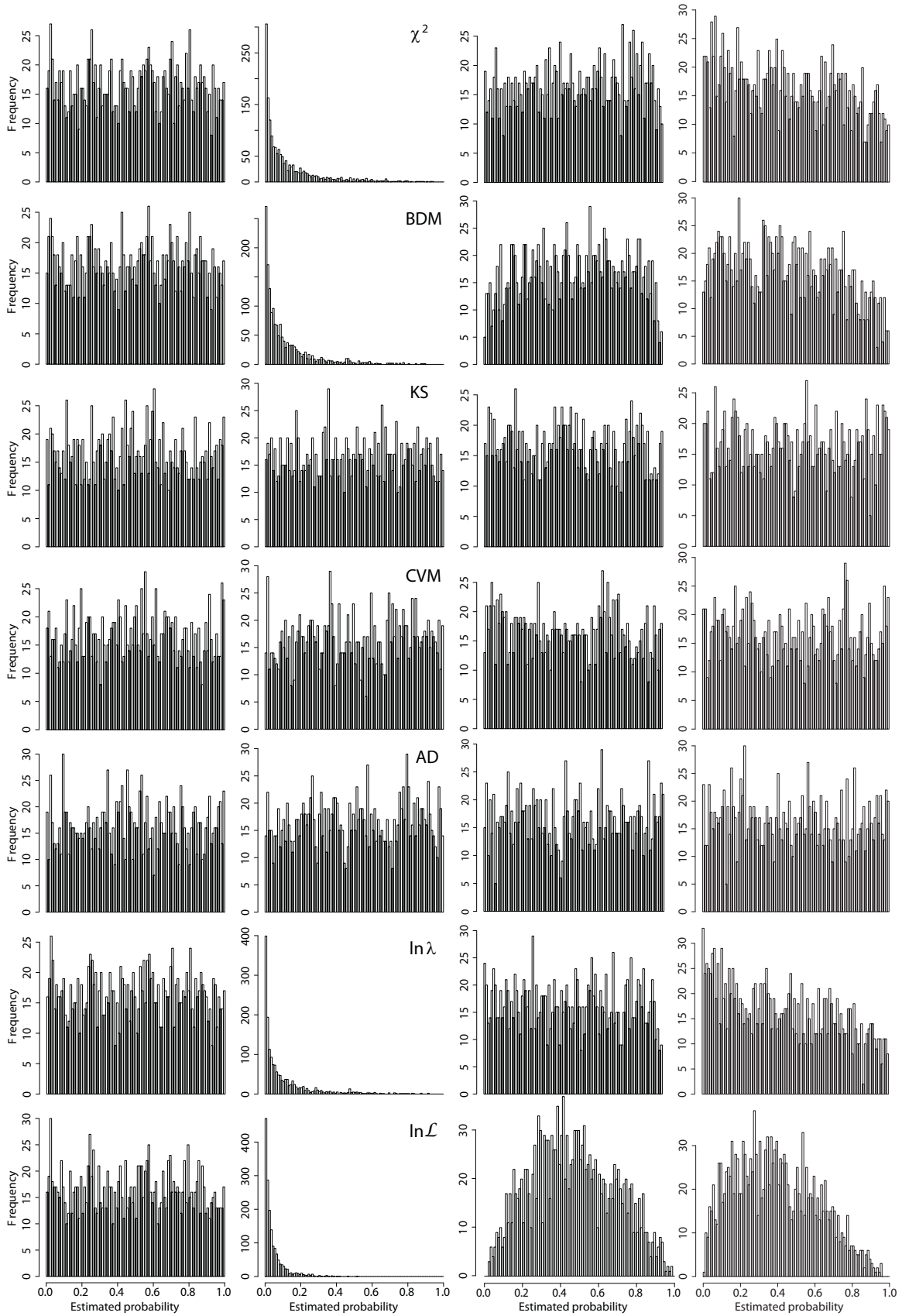


Fig. 10. See caption on next page

Fig. 10. (Figure on previous page) Distribution of the estimated probability that the test statistic is worse than that observed, for seven different test statistics. The data are generated according to the null hypothesis, consisting of 100 bin histograms with a mean of 100 counts (left column) or one count (other columns). The first and second columns are for an estimated H_0 computed as the weighted bin-by-bin average. The third column is for an estimated H_0 where each bin is the average of the total contents of both histograms, divided by the number of bins. The rightmost column is for an estimated H_0 estimated with a Gaussian kernel estimator using the contents of both histograms. The χ^2 is computed without combining bins.

It may be noted that the issue really is one appearing at low statistics. We can give some intuition for the observed effect. Consider the likely scenario at low statistics that some bins will have zero counts in both histograms. In this case our algorithm for the estimated null hypothesis yields a zero mean for these bins. The simulation used to determine the probability distribution for the test statistic will always have zero counts in these bins, that is, there will always be agreement between the two histograms in these bins. Thus, the simulation will find that values of the test statistic are more probable than it should.

If we tried the same study with, say, a mean of 100 counts per bin, we would find that the probability estimates are valid, at least this far into the tails. The left column of Fig. 10 shows that more sensible behavior is achieved with larger statistics. The χ^2 , $\ln \lambda$, and $\ln \mathcal{L}$ statistics perform essentially identically at high statistics, as expected, since in the normal approximation they are equivalent.

The AD, CVM, and KS tests are more robust under our estimates of H_0 than the others, as they tend to emphasize the largest differences and are not so sensitive to bins that always agree. For these statistics, we see that our procedure for estimating H_0 does well even for low statistics, although we caution again that we are not examining the far tails of the distribution.

There are various possible approaches to salvaging the situation in the low statistics regime. Perhaps the simplest is to rely on the typically valid assumption that the underlying H_0 distribution is “smooth”. Then instead of having an unknown parameter for each bin, we only need to estimate a few parameters to describe the smooth distribution, and effectively more statistics are available.

For example, we may repeat the algorithm for our example of a mean of one count per bin, but now assuming a smooth background represented by a uniform distribution. This is cheating a bit, since we perhaps aren't supposed to know that this is really what we are sampling from, but we'll pretend that we looked at the data and decided that this was plausible. As usual, we would in practice want to try other possibilities to evaluate systematic effects.

Thus, we estimate:

$$\begin{aligned}\hat{\mu}_i &= N_u/k, \quad i = 1, 2, \dots, k \\ \hat{\nu}_i &= N_v/k, \quad i = 1, 2, \dots, k.\end{aligned}$$

The resulting distributions for the estimated probabilities are shown in the third column of Fig. 10. These distributions are much more reasonable, at least at the level of a per cent (1650 sample experiments are generated in each case, and the estimated P value is estimated for each experiment with 1650 evaluations of the null hypothesis for that experiment).

It should be remarked that the $\ln \mathcal{L}$ and, perhaps, to a much lesser extent the BDM statistic, do not give the desired 1% result, but now err on the “conservative” side. It may be possible to mitigate this with a different algorithm, but this has not been investigated. We may expect the power of these statistics to suffer under the approach taken here.

Since we aren't supposed to know that our null distribution is uniform, we also try another approach to get a feeling for whether we can really do a legitimate analysis. Thus, we try a kernel estimator for the null distribution, using the sum of the observed histograms as input. In this case, we have chosen a Gaussian kernel, with a standard deviation of 2. The “density” package in R [1] is used for this. An example of such a kernel estimated distribution is shown in Fig. 11. The resulting estimated probability distributions of our test statistics are shown in the rightmost column of Fig. 10. In general, this works pretty well. The bandwidth was chosen here to be rather small; a larger bandwidth would presumably improve the results.

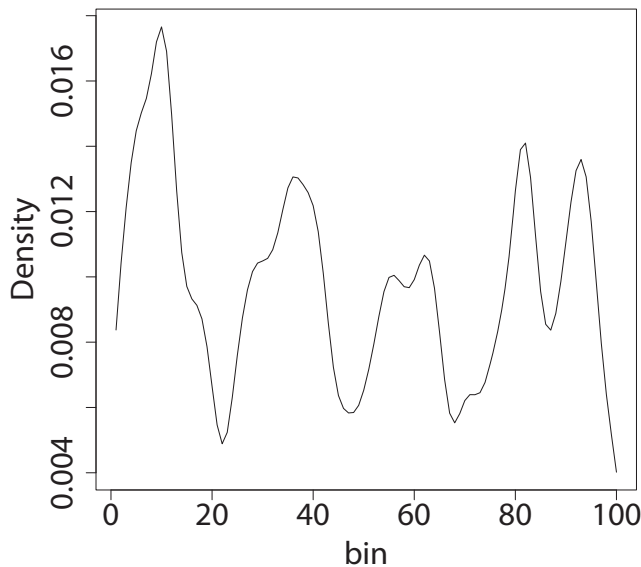


Fig. 11. Sample Gaussian kernel density estimate of the null hypothesis (for sampling from a true null).

3.5 Comparison of Power of Tests

The power depends on what the alternative hypothesis is. Here, we mostly investigate adding a Gaussian component on top of a uniform background distribution. This choice is motivated by the scenario where one distribution appears to show some peaking structure, while the other does not. We also look briefly at a different extreme, that of a rapidly varying alternative.

The data for this study are generated as follows: The background (null distribution) has a mean of one event per histogram bin. The Gaussian has a mean of 50 and a standard deviation of 5, in units of bin number. We vary the amplitude of the Gaussian and count how often the null hypothesis is rejected at the 1% confidence level. The amplitude is measured in percent, for example a 25% Gaussian has a total amplitude corresponding to an average of 25% of the total counts in the histogram, including the (small) tails extending beyond the histogram boundaries. The Gaussian counts are added to the counts from the null distribution. An example is shown in Fig. 12.

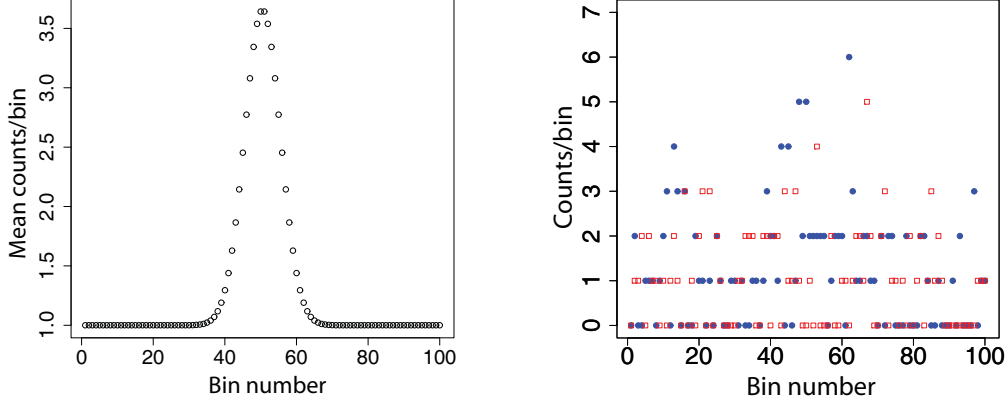


Fig. 12. Left: The mean bin contents for a 25% Gaussian on a flat background of one count/bin (note the suppressed zero). Right: Example sampling from the 25% Gaussian (filled blue dots) and from the uniform background (open red squares).

The distribution of estimated probability, under H_0 , that the test statistic is worse than that observed (i.e., the distribution of P -values) is shown in Fig. 13 for seven different test statistics. Three different magnitudes of the Gaussian amplitude are displayed. The power of the tests to reject the null hypothesis at the 99% confidence level is summarized in Table III and in Fig. 14 for several different alternative hypothesis amplitudes.

Table III. Estimates of power for seven different test statistics, as a function of H_1 . The comparison histogram (H_0) is generated with all $k = 100$ bins Poisson of mean 1. The selection is at the 99% confidence level, that is, the null hypothesis is accepted with (an estimated) 99% probability if it is true.

	H0	12.5	25	37.5	50	-25
Statistic	%	%	%	%	%	%
χ^2	1.2 ± 0.3	1.3 ± 0.3	4.3 ± 0.5	12.2 ± 0.8	34.2 ± 1.2	1.6 ± 0.3
BDM	0.30 ± 0.14	0.5 ± 0.2	2.3 ± 0.4	10.7 ± 0.8	40.5 ± 1.2	0.9 ± 0.2
KS	1.0 ± 0.2	3.6 ± 0.5	13.5 ± 0.8	48.3 ± 1.2	91.9 ± 0.7	7.2 ± 0.6
CVM	0.8 ± 0.2	1.7 ± 0.3	4.8 ± 0.5	35.2 ± 1.2	90.9 ± 0.7	2.7 ± 0.4
AD	1.0 ± 0.2	1.8 ± 0.3	6.5 ± 0.6	42.1 ± 1.2	94.7 ± 0.6	2.8 ± 0.4
$\ln \lambda$	1.5 ± 0.3	1.9 ± 0.3	6.4 ± 0.6	22.9 ± 1.0	67.1 ± 1.2	2.4 ± 0.4
$\ln \mathcal{L}$	0.0 ± 0.0	0.1 ± 0.1	0.8 ± 0.2	6.5 ± 0.6	34.8 ± 1.2	0.0 ± 0.0

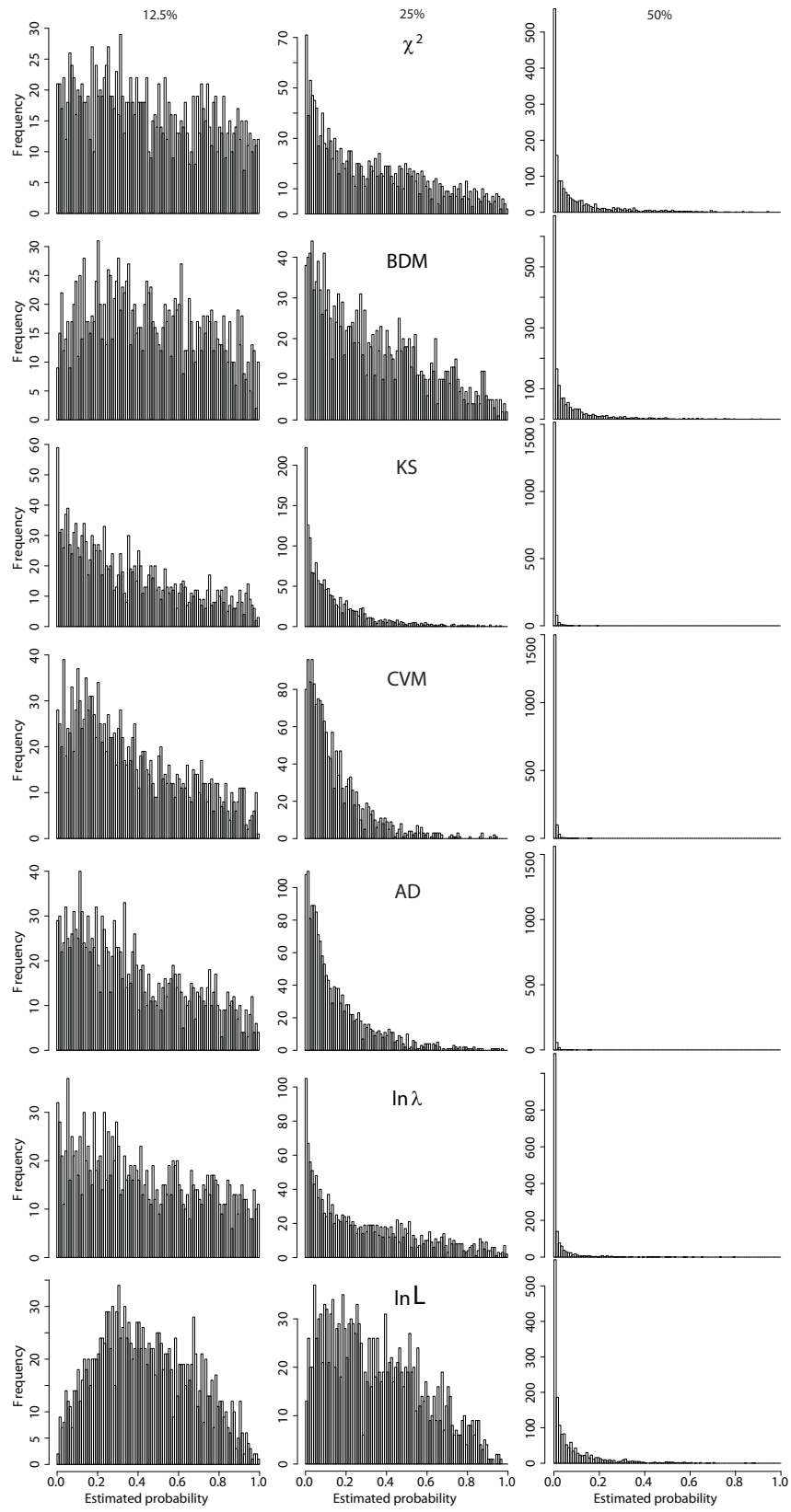


Fig. 13. See caption, next page.

Fig. 13. (Figure on previous page) Distribution of estimated probability, under H_0 , that the test statistic is worse than that observed, for seven different test statistics. The data are generated according to a uniform distribution, consisting of 100 bin histograms with a mean of 1 count, for one histogram, and for the other histogram with a uniform distribution plus a Gaussian of strength 12.5% (left column), 25% (middle column), and 50% (right column). The χ^2 is computed without combining bins.

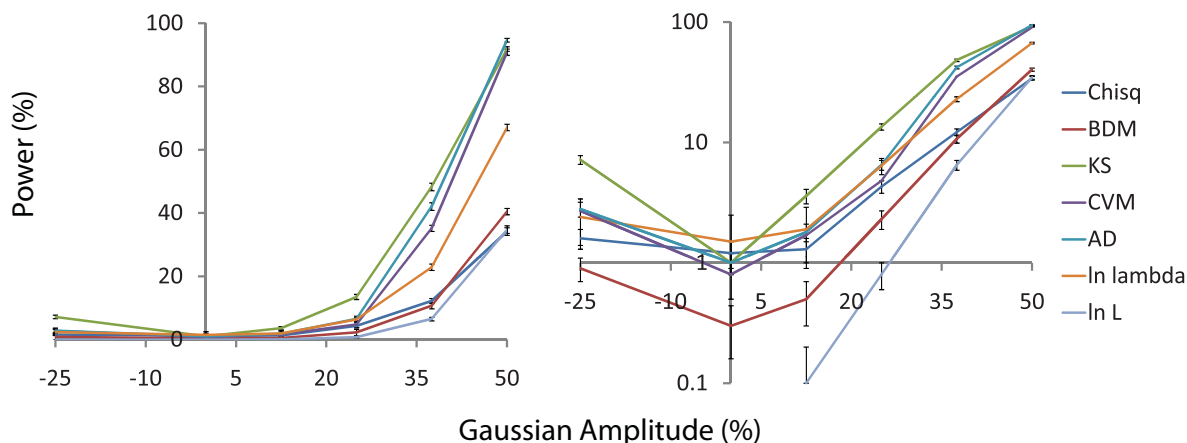


Fig. 14. Summary of power of seven different test statistics, for the alternative hypothesis with a Gaussian bump. Left: linear vertical scale; Right: logarithmic vertical scale. [Best viewed in color. At an amplitude of 35%, the ordering, from top to bottom, of the curves is: KS, AD, CVM, $\ln \lambda$, χ^2 , BDM, $\ln \mathcal{L}$.]

In Table IV we take a look at the performance of our seven statistics for histograms with large bin contents. It is interesting that in this large-statistics case, for the χ^2 and similar tests, the power to reject a dip is greater than the power to reject a bump of the same area. This is presumably because the “error estimates” for the χ^2 are based on the square root of the observed counts, and hence give smaller errors for smaller bin contents. We also observe that the comparative strength of the KS, CVM, and AD tests versus the χ^2 , BDM, $\ln \lambda$, and $\ln \mathcal{L}$ tests in the small statistics situation is largely reversed in the large statistics case.

Table IV. Estimates of power for seven different test statistics, as a function of H_1 . The comparison histogram (H_0) is generated with all $k = 100$ bins Poisson of mean 100. The selection is at the 99% confidence level.

	H0	5	-5
Statistic	%	%	%
χ^2	0.91 ± 0.23	79.9 ± 1.0	92.1 ± 0.7
BDM	0.97 ± 0.24	80.1 ± 1.0	92.2 ± 0.7
KS	1.03 ± 0.25	77.3 ± 1.0	77.6 ± 1.0
CVM	0.91 ± 0.23	69.0 ± 1.1	62.4 ± 1.2
AD	0.91 ± 0.23	67.5 ± 1.2	57.8 ± 1.2
$\ln \lambda$	0.91 ± 0.23	79.9 ± 1.0	92.1 ± 0.7
$\ln \mathcal{L}$	0.97 ± 0.24	79.9 ± 1.0	91.9 ± 0.7

To get an idea of what happens for a radically different alternative to the null distribution, we consider sensitivity to sampling from the “sawtooth” distribution as shown in figure 15. This is to be compared once again to samplings from the uniform histogram. The results are tabulated in Table V. The “percentage” sawtooth here refers to the fraction of the null hypothesis mean. That is, a 100% sawtooth on a 1 count/bin background oscillates between a mean of 0 counts/bin and 2 counts/bin. The period of the sawtooth is always two bins.

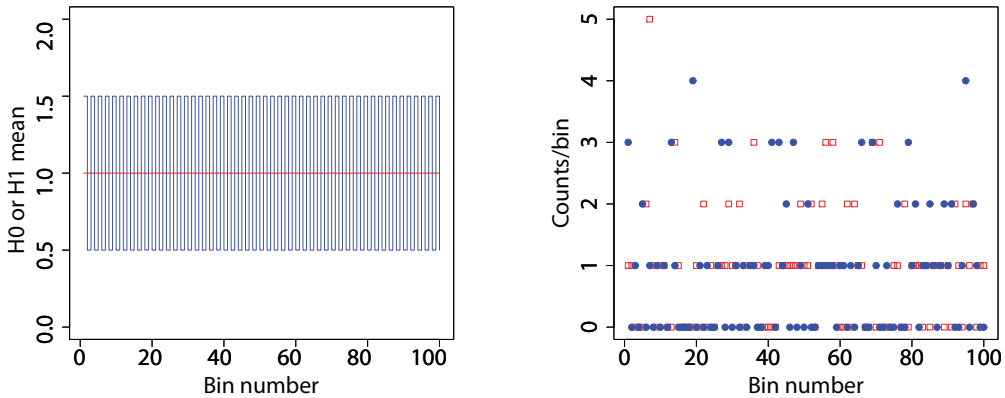


Fig. 15. Left: The mean bin contents for a 50% sawtooth on a flat background of one count/bin (blue), compared with the flat background means (red). Right: Example sampling from the 50% sawtooth (filled blue dots) and from the uniform background (open red squares).

In this example, the χ^2 and likelihood ratio tests are the clear winners, with BDM next. The KS, CVM, and AD tests reject the null hypothesis with the same probability as for sampling from a true null distribution. This very poor performance for these tests is readily understood, as these tests are all based on the cumulative distributions, which average out local oscillations.

Table V. Estimates of power for seven different test statistics, for a “sawtooth” alternative distribution.

	50	100
Statistic	%	%
χ^2	3.7 ± 0.5	47.8 ± 1.2
BDM	1.9 ± 0.3	33.6 ± 1.2
KS	0.85 ± 0.23	1.0 ± 0.2
CVM	0.91 ± 0.23	1.0 ± 0.2
AD	0.91 ± 0.23	1.2 ± 0.3
$\ln \lambda$	4.5 ± 0.5	49.6 ± 1.2
$\ln \mathcal{L}$	0.30 ± 0.14	10.0 ± 0.7

4. Conclusions

These studies have demonstrated some important lessons in “goodness-of-fit” testing:

1. There is no single “best” test for all applications. Statements such as “test X is better than test Y” are empty without giving more context. For example, the Anderson-Darling test is often very powerful in testing normality of data against alternatives with non-normal tails (such as the Cauchy distribution) [7]. However, we have seen that it is not always especially powerful in other situations. The more we know about what we wish to test for, the more reliably we can choose a powerful test. Each of the tests investigated here may be reasonable to use, depending on the circumstance. Even the controversial \mathcal{L} test works as well as the others sometimes. However, there is no known situation where it actually performs better than all of the others, and indeed the situations where

it is observed to perform as well are here limited to those where it is equivalent to another test.

2. Computing probabilities via simulations is a very useful technique. However, it must be done with care. The issue of tests with an incompletely specified null hypothesis is particularly insidious. Simply generating a distribution according to some assumed null distribution can lead to badly wrong results. Where this could occur, it is important to verify the validity of the procedure. Note that we have only looked into the tails to the 1% level. The validity must be checked to whatever level of probability is needed for the results. Thus, we cannot blindly assume the results quoted here at the 1% level will still be true at, say, the 0.1% level.

We have concentrated in this paper on the specific question of comparing two histograms. However, the general considerations apply more generally, to testing whether two datasets are consistent with being drawn from the same distribution, and to testing whether a dataset is consistent with a predicted distribution. The KS, CVM, AD, $\ln \mathcal{L}$, and \mathcal{L} tests may all be constructed for these other situations (as well as the χ^2 and BDM, if we bin the data).

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