

Nonparametric Goodness-of-Fit Tests for Discrete Null Distributions

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Abstract Methodology extending nonparametric goodness-of-fit tests to discrete null distributions has existed for several decades. However, modern statistical software has generally failed to provide this methodology to users. We offer a revision of R's `ks.test()` function and a new `cvm.test()` function that fill this need in the R language for two of the most popular nonparametric goodness-of-fit tests. This paper describes these contributions and provides examples of their usage. Particular attention is given to various numerical issues that arise in their implementation.

Introduction

Goodness-of-fit tests are used to assess whether data are consistent with a hypothesized null distribution. The χ^2 test is the best-known parametric goodness-of-fit test, while the most popular nonparametric tests are the classic test proposed by Kolmogorov and Smirnov followed closely by several variants on Cramér-von Mises tests.

In their most basic forms, these nonparametric goodness-of-fit tests are intended for continuous null distributions, but they have also been adapted for discrete null distributions. Unfortunately, most modern statistical software packages and programming environments have failed to incorporate these discrete versions. As a result, researchers would typically rely upon the χ^2 test or use of a nonparametric test designed for a continuous null distribution. For smaller sample sizes, in particular, both of these choices can produce misleading inferences.

This paper presents a revision of R's `ks.test()` function and a new `cvm.test()` function to fill this void for researchers and practitioners in the R environment. We first present overviews of the theory and general implementation of the discrete Kolmogorov-Smirnov and Cramér-von Mises tests. We discuss the particular implementation of tests in R and provide examples. We conclude with a short discussion, including the state of existing continuous and two-sample Cramér-von Mises testing in R.

Kolmogorov-Smirnov Test

Overview

The most popular nonparametric goodness-of-fit test is the Kolmogorov-Smirnov test. Given the cumu-

lative distribution function $F_0(x)$ of the continuous null distribution and the empirical distribution function $F_{data}(x)$ of the observed data, the test statistic is given by

$$D = \sup_x |F_0(x) - F_{data}(x)|. \quad (1)$$

The distribution of D does not depend on the hypothesized distribution, making this a computationally attractive method. Slakter (1965) offers a standard presentation of the test and its performance relative to other algorithms. The test statistic is easily adapted for one-sided tests. For these, the absolute value in (1) is discarded and the tests are based on either the supremum of the remaining difference (the 'greater' testing alternative) or by replacing the supremum with a negative infimum (the 'lesser' hypothesis alternative). Tabulated p-values have been available for these tests since 1933.

The extension of the Kolmogorov-Smirnov test to non-continuous null distributions is not straightforward. The formula of the test statistic D remains unchanged, but its distribution is much more difficult to obtain; unlike the continuous case, its distribution depends on the null model. It has been known since at least the 1950's that using the tables associated with continuous null distributions results in conservative p-values when the null distribution is discontinuous (see *** or *** or Stephens (1974), for example). In the early 1970's, Conover (1972) developed the method implemented here for computing exact p-values in the case of discrete null distributions.

Implementation

The implementation of the discrete Kolmogorov-Smirnov test involves two steps. First, the particular test statistic is calculated (corresponding to the desired one-sided or two-sided test). Then, the p-value for that particular test statistic may be computed.

The form of the test statistic is the same as in the continuous case; it would seem that no additional work would be required for the implementation, but this is not the case. Consider two non-decreasing functions f and g , where the function f is a step function with jumps on the set $\{x_1, \dots, x_N\}$ and g is continuous (the classical Kolmogorov-Smirnov situation). In order to determine the supremum of the difference between these two functions, notice that

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$$\begin{aligned}
 & \sup_x |f(x) - g(x)| \\
 &= \max_i \left(\max \left\{ |g(x_i) - f(x_i)|, \lim_{x \rightarrow x_i} |g(x) - f(x_{i-1})| \right\} \right) \quad (2) \\
 &= \max_i \left(\max \left\{ |g(x_i) - f(x_i)|, |g(x_i) - f(x_{i-1})| \right\} \right). \quad (3)
 \end{aligned}$$

Computing the maximum over these $2N$ values (with f equal to $F_{data}(x)$ and g equal to $F_0(x)$ as defined above) is clearly the most efficient way to compute the Kolmogorov-Smirnov test statistic for a continuous null distribution. When the function g is not continuous, however, equality (3) does not hold in general because we cannot replace $\lim_{x \rightarrow x_i} g(x)$ with the value $g(x_i)$.

If it is known that g is a step function, it follows that for some small ϵ ,

$$\sup_x |f(x) - g(x)| = \max_i \{ |g(x_i) - f(x_i)|, |g(x_i - \epsilon) - f(x_{i-1})| \} \quad (4)$$

where the discontinuities in g are more than some distance ϵ apart. This, however, requires knowledge that g is a step function as well as of the nature of its support (or break-points). We implement the Kolmogorov-Smirnov test statistic for discrete null distributions by forcing the user to completely specify the null distribution.

Having obtained the test statistic, the p-value must then be calculated. For larger sample sizes, the null distribution can be approximated with the null distribution from the classical Kolmogorov-Smirnov test. When an exact p-value is required for smaller sample sizes, the methodology in [Conover \(1972\)](#) is used. Full details of the calculations are contained in source code of our revised function `ks.test()` and in Conover's original paper.

Cramér-von Mises Tests

Overview

While the Kolmogorov-Smirnov test may be the most popular of the nonparametric goodness-of-fit tests, there is another family of tests which has been shown to be more powerful against a large class of alternatives hypotheses. The original test was developed by Harald Cramér and Richard von Mises ([Cramer, 1928](#); [von Mises, 1928](#)) and further adapted by [Anderson and Darling \(1952\)](#), and [Watson \(1961\)](#). The original test statistic, W^2 , Anderson's A^2 , and Wat-

son's U^2 are:

$$W^2 = n \cdot \int_{-\infty}^{\infty} [F_{data}(x) - F_0(x)]^2 dF_0(x) \quad (5)$$

$$A^2 = n \cdot \int_{-\infty}^{\infty} \frac{[F_{data}(x) - F_0(x)]^2}{F_0(x) - F_0(x)^2} dF_0(x) \quad (6)$$

$$U^2 = n \cdot \int_{-\infty}^{\infty} [F_{data}(x) - F_0(x) - W^2]^2 dF_0(x) \quad (7)$$

As with the original Kolmogorov-Smirnov test statistic, these all have null distributions of their test statistics which are independent of the specified null models.

The W^2 statistic was the original test statistic; it has the benefit of having the simplest form. The A^2 statistic was developed by Anderson in the process of generalizing the test for the two-sample case. Watson's U^2 statistic was developed for distributions which are cyclic (with an ordering to the support but no natural starting point), as it is invariant to cyclic reordering of the support. For example, a distribution on the months of the year could be considered cyclic.

It has been shown that these tests can be more powerful than Kolmogorov-Smirnov tests to certain deviations from the hypothesized distribution. As they all involve integration over the whole range of data, rather than use of a supremum. Thus, they are best-suited for situations where the true alternative distribution deviates a little over the whole support rather than having large deviations over a small section of the support. For a complete analysis of the relative powers of these tests, see [Stephens \(1974\)](#).

Generalizations of the Cramér-von Mises tests to discrete distributions were developed in [V Choulakian \(1994\)](#). As with the Kolmogorov-Smirnov test, the forms of the test statistics are unchanged, and the null distributions of the test statistics are again hypothesis-dependent. The methods do not offer finite-sample results, but rather show that the asymptotic distributions of the test statistics under the null hypothesis each involve consideration of a weighted sum of independent chi-squared variables (with the weights depending on the particular null distribution). We implement the asymptotic distributions here; [Stephens \(1974\)](#) showed that these approximations are conservative and asymptotically equivalent to the true null distributions.

Implementation

Calculation of the three test statistics is done using the matrix algebra given by [V Choulakian \(1994\)](#). The only notable difficulty in the implementation of the discrete form of the tests involves calculating the percentiles of the weighted sum of chi-squares,

$$Q = \sum_{i=1}^p \lambda_i \chi_{i,1df}^2, \quad (8)$$

where p is the number of elements in the support of the hypothesized distribution. Imhof (1961) provides a method for obtaining the distribution of Q , easily adapted for our case because the chi-squared variables have only one degree of freedom. The exact formula given for the distribution function of Q is given by

$$\mathbb{P}\{Q \geq x\} = \frac{1}{2} + \frac{1}{\pi} \int_0^\infty \frac{\sin \theta(u, x)}{u \rho(u)} du \quad (9)$$

for continuous functions $\theta(\cdot, x)$ and $\rho(\cdot)$ depending on the weights λ_i .

There is no analytic solution to the integral in (9), so the integration is accomplished numerically. This seems fine in most situations we considered, but numerical issues appear in the regime of large test statistics x (or, equivalently, small p-values). The function $\theta(\cdot, x)$ is linear in x ; as the test statistic grows the corresponding periodicity of the integrand decreases and the approximation becomes unstable. We resolve this problem by using a simple conservative approximation to avoid the numerical instability. Consider the following inequality:

$$\mathbb{P}\left(\sum_{i=1}^p \lambda_i \chi_1^2 \geq x\right) \leq \mathbb{P}\left(\lambda_{\max} \sum_{i=1}^p \chi_1^2 \geq x\right) \quad (10)$$

$$= \mathbb{P}\left(\chi_p^2 \geq \frac{x}{p \lambda_{\max}}\right) \quad (11)$$

The values for the weighted sum can be bounded using a simple transformation and a chi-squared distribution of a higher degree of freedom. The original formulation is preferable for most p-values, while this approximation is used for smaller p-values (smaller than 0.001, based on our observations of the numerical instability of the original formulation).

Figure 1 shows the non-monotonicity of the numerical evaluation of equation (9) for the null distribution which is uniform on the set $\{1, 2, 3\}$, as well as the behavior of the conservative upper bound given in equation (11).

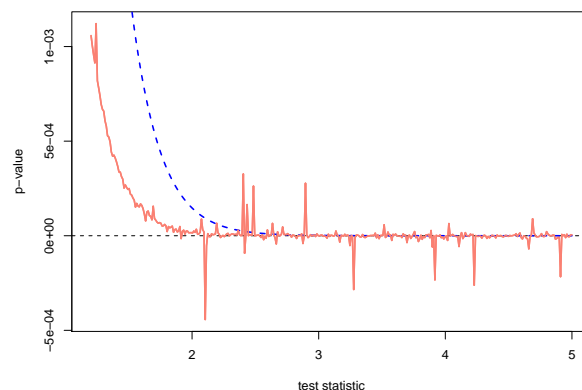


Figure 1: Plot of calculated p-values for given test statistics using numerical integration (pink) compared to the conservative chi-squared bound (dashed blue). The null distribution is uniform on the set $\{1, 2, 3\}$ in this example. The instability in the calculated p-values is a result of numerical instabilities.

Kolmogorov-Smirnov and Cramér-von Mises Tests in R

Functions `ks.test()` and `cvm.test()` are provided for convenience in packages **ks.test** and **cvm.test**, respectively. Function `ks.test()` offers a revision of R's Kolmogorov-Smirnov function `ks.test()` from base package **stats**, while `cvm.test()` is a new function for Cramér-von Mises tests. Both are available from the authors or from R-Forge (https://r-forge.r-project.org/R/?group_id=802); they will be proposed for inclusion in **stats** in late 2010.

The revised `ks.test()` function supports one-sample tests for discrete null distributions by allowing the second argument, `y`, to be an empirical cumulative distribution function (an R function with class `ecdf`) or an object of class `stepfun` specifying a discrete distribution. As in the original version of `ks.test()`, the presence of ties in the data (the first argument, `x`) generates a warning unless `y` describes a discrete distribution. When a discrete distribution is specified, exact p-values are not available for two-sided alternative hypotheses, but the reported p-values will be conservative. For one-sided tests, exact p-values are calculated using Conover's method (when `exact = NULL` or `exact = TRUE`) if the sample size is less than or equal to 30; otherwise, asymptotic distributions are used which are reliable in such cases (CITATION? Is this correct?). When `exact = FALSE` the asymptotic distribution is used which is known to be imprecise but conservative, even for small samples (CITATION).

The function `cvm.test()` is similar to `ks.test()`. Its first two arguments specify the data and null distri-

bution; the only extra option, `type`, specifies the variant of the Cramér-von Mises test:

- `x`: a numerical vector of data values.
- `y`: an `ecdf` or step-function (`stepfun`) for specifying the null model
- `type`: the variant of the Cramér-von Mises test; `W2` is the default and most common method, `U2` is for cyclical data, and `A2` is the Anderson-Darling alternative.

As with `ks.test()`, `cvm.test()` returns an object of class `htest`.

Examples

Consider a toy example, with observed data of length 2 (specifically, the values 0 and 1) and a hypothesized null distribution that places equal probability on the values 0 and 1. With the current `ks.test()` function in R (which, admittedly, doesn't claim to handle discrete distributions), the reported p-value, 0.5, is clearly incorrect:

```
> stats::ks.test(c(0, 1), ecdf(c(0, 1)))

One-sample Kolmogorov-Smirnov test

data:  c(0, 1)
D = 0.5, p-value = 0.5
alternative hypothesis: two-sided
```

Instead, the value of D given in equation (1) should be 0 and the associated p-value should be 1. Our revision of `ks.test()` fixes this problem when the user provides a discrete distribution:

```
> ks.test(c(0, 1), ecdf(c(0, 1)))

One-sample Kolmogorov-Smirnov test

data:  c(0, 1)
D = 0, p-value = 1
alternative hypothesis: two-sided
```

Next, we simulate a sample of 25 from the discrete uniform distribution on the integers $\{1, 2, \dots, 10\}$ and show several variants of the new `ks.test()` implementation. The first is the default two-sided test, where the reported p-value is a conservative upper bound for the actual p-value. In this case, the approximation may not be that tight, but this is irrelevant for such large p-values (for more interesting p-values, the upper bound is very close to the true p-value).

```
> library(ks.test)
> set.seed(1)
> x <- sample(1:10, 25, replace = TRUE)
> x
```

```
[1] 3 4 6 10 3 9 10 7 7 1 3 2 7
[14] 4 8 5 8 10 4 8 10 3 7 2 3
```

```
> ks.test(x, ecdf(1:10))

One-sample Kolmogorov-Smirnov test

data:  x
D = 0.08, p-value = 1
alternative hypothesis: two-sided
```

Next, we conduct the default one-sided test, where Conover's method provides the exact p-value (up to the numerical precision of the implementation):

```
> ks.test(x, ecdf(1:10), alternative = "g")

One-sample Kolmogorov-Smirnov test

data:  x
D^+ = 0.04, p-value = 0.7731
alternative hypothesis:
the CDF of x lies above the null hypothesis
```

In contrast, the option `exact=FALSE` results in the p-value obtained by applying the classical Kolmogorov-Smirnov test, resulting in a conservative p-value:

```
> ks.test(x, ecdf(1:10), alternative = "g",
+         exact = FALSE)

One-sample Kolmogorov-Smirnov test

data:  x
D^+ = 0.04, p-value = 0.9231
alternative hypothesis:
the CDF of x lies above the null hypothesis
```

A different toy example shows the dangers of using R's existing `ks.test()` function:

```
> ks.test(rep(1, 3), ecdf(1:3))

One-sample Kolmogorov-Smirnov test

data:  rep(1, 3)
D = 0.6667, p-value = 0.04938
alternative hypothesis: two-sided
```

If, instead, either `exact=FALSE` is used with the new `ks.test()` function, or if the original `stats::ks.test()` is used, the reported p-value is 0.1389.

Finally, we employ two of the Cramér-von Mises tests. Need short discussion, and we could use a good cyclical example:

```
> library(cvm.test)
> cvm.test(x, ecdf(1:10))

Cramer-von Mises - W2

data:  x
W2 = 0.057, p-value = 0.8114
alternative hypothesis: Two.sided

> cvm.test(x, ecdf(1:10), type = "A2")
```

Cramer-von Mises - A2

```
data: x
A2 = 0.3969, p-value = 0.75
alternative hypothesis: Two.sided
```

Cyclical example:

```
> library(cvm.test)
> x <- sample(1:4, 20, replace=T)
> cvm.test(x, ecdf(1:4), type='U2')
```

Cramer-von Mises - U2

```
data: x
U2 = 0.075, p-value = 0.4027
alternative hypothesis: Two.sided
```

```
> y <- x%%4 + 1
> cvm.test(y, ecdf(1:4), type = 'U2')
```

Cramer-von Mises - U2

```
data: y
U2 = 0.075, p-value = 0.4027
alternative hypothesis: Two.sided
```

Discussion

In the end, for methods such as those presented in this paper where it is possible, there are enough positives to suggest that we attempt to implement exact p -value calculations. This does lead to an interesting direction for future research in non-parametric goodness of fit tests: the methods presented here were historically chosen because they could be shown to have fixed null distributions which could easily be calculated in an era without fast computers for carrying out permutation tests. It is quite possible that variants without the property, which could be easily used today, have greater power to certain alternative distributions.

In the continuous setting, both of the Kolmogorov-Smirnov and the Cramér-von Mises tests have two-sample analogues. Here data are observed from two processes, and the hypothesis tested is whether they came from the same (but unspecified) distribution. There does not exist an analogous theory for discrete distributions. This comes from the fact that the discrete null distributions of the test statistics depend on the exact null distribution; therefore the two-sample case would surely have to depend on the exact distributions used as well which are generally not even stated in the two-sample case.

While we have implemented the two most popular variants of goodness-of-fit tests, there are several more exotic varieties to be found. For further generalizations of tests see the extended study done in de Wet and Venter (1994).

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