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vsgoftest: An R Package for Goodness-of-Fit Testing Based on Kullback-Leibler Divergence

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Abstract

The R package **vsgoftest** performs goodness-of-fit (GOF) tests, based on Shannon entropy and Kullback-Leibler divergence, developed by Vasicek (1976) and Song (2002), of various classical families of distributions. The so-called Vasicek-Song (VS) tests are intended to be applied to continuous data – typically drawn from a density distribution, even including ties. Their excellent properties – they exhibit high power in a large variety of situations, make them relevant alternatives to classical GOF tests in any domain of application requiring statistical processing.

The theoretical framework of VS tests is summarized and followed by a detailed description of the different features of the package. The power and computational time performances of VS tests are studied through their comparison with other GOF tests. Application to real datasets illustrates the easy-to-use functionalities of the **vsgoftest** package.

Keywords: R statistical computing environment, goodness-of-fit tests, Shannon entropy, Kullback-Leibler divergence, sample spacing based estimation.

1. Introduction

Goodness-of-fit (GOF) tests constitute a classical tool in deciding of the compatibility of data with a theoretical (probability) distribution. The present work proposes a package for the R statistical computing environment (R Core Team 2020) performing GOF tests based on Shannon entropy and Kullback-Leibler divergence, together with a methodological guide and applications.

Precisely, we consider fitting numeric (real valued) data either to a unique distribution, the so-called simple null hypothesis test

$$H_0: P = P_0(\theta)$$
 against $H_1: P \neq P_0(\theta)$, (1)

or to a parametric family, the so-called composite null hypothesis test

$$H_0: P \in \mathcal{P}_0(\Theta)$$
 against $H_1: P \notin \mathcal{P}_0(\Theta)$. (2)

The set $\mathcal{P}_0(\Theta) = \{P \in \mathcal{D} : P = P_0(\theta), \theta \in \Theta\}$, with $\Theta \subset \mathbb{R}^d$, is a parametric subfamily of the set \mathcal{D} of all probability distributions absolutely continuous with respect to Lebesgue measure on \mathbb{R} , i.e., probability distributions with a density function. Decision is to be taken from the observation $x_1^n = (x_1, \dots, x_n)$ of a sample $X_1^n = (X_1, \dots, X_n)$ of size n of independent and identically distributed random variables drawn from $P \in \mathcal{D}$.

Classically, a GOF test procedure is derived by computing some distance-like functional between the observations and the null distribution, or family of distributions, the null hypothesis being rejected when the distance is larger than a critical value. Kolmogorov-Smirnov, Cramérvon Mises and Anderson-Darling tests constitute some of the most commonly used GOF tests. Their test statistics measure discrepancy between the empirical cumulative distribution function (EDF) of the sample and the cumulative distribution function of the null distribution; these tests are referred to as EDF tests in the following; see Stephens (1974). The tests in the present work are based on the Kullback-Leibler (KL) divergence of the density of the sample with respect to the null density.

GOF tests based on KL divergence have been introduced by Vasicek (1976) for testing normality. Vasicek normality test relies on the maximum entropy property satisfied by the normal distribution: among all distributions with density and given finite variance, Shannon entropy is maximized by the normal distribution. Vasicek test statistic is a monotone transformation of the entropy difference between the null normal distribution and the observed one. This has been subsequently extended to GOF tests of uncategorical data for numerous families of distributions satisfying a maximum entropy property – say maximum entropy (ME) distributions; see Section 2 for references. Song (2002) considers GOF tests based on KL divergence, for a large class of distributions including all classical distribution families. The test statistic is an estimate of the KL divergence between the sample and the null distributions. It is asymptotically normally distributed. When applied to ME distributions, it is equal to the difference between the entropies of the null distribution and the sample one, yielding the same decision rule as Vasicek test. This paper presents the implementation of Vasicek and Song (VS) tests for various families of distributions: uniform, normal, log-normal, exponential, gamma, Weibull, Pareto, Fisher, Laplace and Beta distributions. For further details on the theoretical aspects of VS tests, see Girardin and Lequesne (2017) in which a unifying framework for tests based on entropy difference and KL divergence is provided.

Numerous R packages perform GOF tests for various families of distributions. The functions chisq.test, ks.test and shapiro.test of the stats package (R Core Team 2020) perform respectively the chi-squared test of adequacy to a discrete distribution, the Kolmogorov-Smirnov GOF test for any theoretical continuous distribution and the Shapiro-Wilk normality test. The packages goftest developed in Faraway, Marsaglia, Marsaglia, and Baddeley (2019) and goft in Gonzalez-Estrada and Villasenor-Alva (2020) perform respectively Cramér-von Mises and Anderson-Darling GOF tests, and tests based on the ratios of variance and other moment estimators. KScorrect in Novack-Gottshall and Wang (2019) performs the Lilliefors-corrected Kolmogorov-Smirnov GOF test. Numerous GOF tests of the exponential or two-parameter Weibull distributions are available in EWGoF (Krit 2019) while nortest (Gross and Ligges 2015) and normtest (Gavrilov and Pusev 2014) are dedicated to testing normality. The dbEmpLikeGOF package developed in Miecznikowski, Vexler, and Shepherd (2013) proposes

GOF normality and uniformity tests based on empirical likelihood ratio. These tests are closely related with VS tests; similarities and differences between them are highlighted in the following sections.

The performances of VS tests have been extensively studied in literature. Particularly, numerous references – see Section 4.1 for details, point out that VS tests exhibit higher power than other GOF tests in many situations. Still, they have had not been made available for R users until now.

The test procedure implemented in **vsgoftest** (Lequesne and Regnault 2020) uses either the asymptotic distribution of the test statistic or Monte-Carlo simulation, depending on sample size or user's choice. Optional arguments are included for handling particular situations such as samples with numerous ties. They also contribute to make the procedure flexible and fully parameterizable. Besides these practical aspects, the paper presents a comprehensive review of the literature dealing with power properties of VS tests. Monte Carlo simulations are conducted to illustrate their performance when applied to discriminate between close distributions.

The paper is organized as follows. The theoretical framework of GOF tests based on Shannon entropy difference and KL divergence is briefly presented in Section 2. The functionalities of **vsgoftest** are presented in Section 3. The tests performed by **vsgoftest** are compared to other GOF tests in Section 4. More precisely, power comparisons to classical GOF tests are presented in Section 4.1; Section 4.2 focuses on the comparison of **vsgoftest** and **dbEmpLikeGOF** test procedures, which rely on very close theoretical frameworks but significantly differ in some of their features. Finally, applications to real data in Section 5 illustrate the usage of the proposed functionalities.

2. Entropy difference and KL divergence based GOF tests

The Shannon entropy of a distribution P with density function p on \mathbb{R} has been defined in Shannon (1948) as

$$S(P) := -\int_{\mathbb{R}} p(x) \log p(x) dx.$$
 (3)

Entropy measures the uncertainty or variability of a distribution. The maximum entropy principle under moment constraints, or ME method, favors distributions with highest entropy for their highest degree of uncertainty; see Shannon (1948) and Jaynes (1957). Among all distributions supported by a given finite length interval I in \mathbb{R} , entropy is maximum and equals $\log |I|$ for the uniform distribution, where |I| denotes the length of I. Hence, the entropy difference $\log |I| - \mathbb{S}(P)$ can be thought as a distance-like measure between P and the uniform distribution.

Similarly, among all continuous distributions supported within \mathbb{R} with mean μ and variance σ^2 , Shannon entropy is maximum for the normal distribution $\mathcal{N}(\mu, \sigma^2)$ and equals

$$S(\mathcal{N}(\mu, \sigma^2)) = \ln(\sigma\sqrt{2\pi e}). \tag{4}$$

The entropy difference $\mathbb{S}(\mathcal{N}(\mu, \sigma^2)) - \mathbb{S}(P)$ is nonnegative and thus defines a distance-like measure between any distribution with mean μ and variance σ^2 and the $\mathcal{N}(\mu, \sigma^2)$ distribution. Based on this property, Vasicek (1976) derives a normality test, with a test statistic expressed

in terms of entropy differences, defined as follows

$$K_{mn} := \frac{n}{2mS} \left\{ \prod_{i=1}^{n} (X_{(i+m)} - X_{(i-m)}) \right\}^{1/n} = \sqrt{2\pi e} \exp\left(V_{mn} - \mathbb{S}\left(\mathcal{N}\left(\overline{X}, S^2\right)\right)\right),$$

where

$$\overline{X} := \frac{1}{n} \sum_{i=1}^{n} X_i$$
 and $S^2 := \frac{1}{n} \sum_{i=1}^{n} (X_i - \overline{X})^2$

are the empirical estimators of respectively the mean and the variance of the sample $X_1^n := (X_1, \dots, X_n), X_{(1)} \le \dots \le X_{(n)}$ denotes the order statistics associated to X_1^n and

$$V_{mn} := \frac{1}{n} \sum_{i=1}^{n} \log \left(\frac{n}{2m} \left[X_{(i+m)} - X_{(i-m)} \right] \right)$$
 (5)

is the non-parametric Vasicek estimator of $\mathbb{S}(P)$ based on spacings, with $X_{(i)} = X_{(1)}$ if i < 1 and $X_{(i)} = X_{(n)}$ if i > n; the window size $m \in \mathbb{N}^*$ is smaller than n/2.

The test statistic has been adapted to various families of ME distributions under moment constraints; see Dudewicz and Van Der Meulen (1981), Ebrahimi, Habibullah, and Soofi (1992), Choi and Kim (2006), Mergel (1999), Mudholkar and Tian (2002), among many others. A unifying framework for any exponential family of distributions is proposed in Girardin and Lequesne (2017), with asymptotic properties, consistency and application to biology; see also Lequesne (2013), Lequesne (2015b) and Lequesne (2015a) for power properties, GOF tests of Pareto distributions and extension to generalized entropies.

The Kullback-Leibler (KL) divergence of a distribution P with respect to another one Q, is defined as

$$\mathbb{K}(P \mid Q) := \int_{\mathbb{R}} p(x) \log \frac{p(x)}{q(x)} dx,$$

if P is absolutely continuous with respect to Q, with respective densities p and q, and as $+\infty$ if not; see Kullback and Leibler (1951). The KL divergence is linked to Shannon entropy through the relation

$$\mathbb{K}(P \mid Q) = -\mathbb{S}(P) - \int_{\mathbb{R}} p(x) \log q(x) dx. \tag{6}$$

The KL divergence is not a mathematical distance because of lack of both symmetry and triangular inequality, but it satisfies $\mathbb{K}(P \mid Q) \geq 0$, with $\mathbb{K}(P \mid Q) = 0$ if and only if P = Q, and thus constitutes a natural measure of discrepancy for GOF tests. Song (2002) proposes GOF tests based on KL divergence for either simple (1) or composite (2) null hypothesis. Precisely, thanks to (6), the test statistic I_{mn} is the estimator of $\mathbb{K}(P \mid P_0(\theta))$, defined by

$$I_{mn} := -V_{mn} - \frac{1}{n} \sum_{i=1}^{n} \log p_0(X_i, \hat{\theta}_n),$$

where V_{mn} is the Vasicek estimator (5) of $\mathbb{S}(P)$, and $\widehat{\theta}_n$ is either the maximum likelihood estimator (MLE) of θ satisfying

$$\frac{1}{n}\sum_{i=1}^{n}\log p_0(X_i,\widehat{\theta}_n) = \max_{\theta \in \Theta} \frac{1}{n}\sum_{i=1}^{n}\log p_0(X_i,\theta),$$

or θ itself in case of a simple null hypothesis (1).

The KL divergence $\mathbb{K}(P \mid Q)$ for a maximum entropy distribution Q under moment constraints reduces to the entropy difference $\mathbb{S}(Q) - \mathbb{S}(P)$ for all P satisfying the same moment constraints; see Csiszár (1975). This Pythagorean equality allowed Girardin and Lequesne (2017) to establish that entropy difference GOF tests for ME distributions coincide with Song tests – we will refer to these tests as Vasicek-Song tests and keep on denoting them by VS tests. Especially, Vasicek and Song normality test statistics are linked through the equality

$$K_{mn} = \sqrt{2\pi e} \exp(-I_{mn}),$$

yielding identical decision rules.

Based on the asymptotic properties of V_{mn} proven by Dudewicz and Van Der Meulen (1981) for testing uniformity, Song (2002) establishes the asymptotic behavior of I_{mn} , independently of the null hypothesis: I_{mn} is consistent and asymptotically normally distributed provided the null distribution belongs to the class

$$\mathcal{F} = \left\{ P \in \mathcal{D} : \sup_{x: \ 0 < F(x) < 1} \frac{|p'(x)|}{p^2(x)} F(x) [1 - F(x)] < \gamma, \ \gamma > 0 \right\},\tag{7}$$

where F is the cumulative distribution function of P and p its density with derivative p' (almost everywhere). The class \mathcal{F} contains the most classical distributions such as uniform $(\gamma = 0)$, normal, exponential and gamma $(\gamma = 1)$, Fisher $(\gamma = (2 + \nu_2)/\nu_2)$ where ν_2 is the second degree of freedom), Pareto $(\gamma = (\mu + 1)/\mu)$, where μ is the shape parameter), etc. For $\mathcal{P}_0(\Theta) \subset \mathcal{F}$, if

$$m/\log n \xrightarrow[n \to \infty]{} 0 \quad \text{and} \quad m(\log n)^{2/3}/n^{1/3} \xrightarrow[n \to \infty]{} 0,$$
 (8)

then

$$\sqrt{6mn}[I_{mn} - \log(2m) + \psi(2m)] \xrightarrow{\mathcal{D}} \mathcal{N}(0, 1), \tag{9}$$

where $\psi(m)$ is the digamma function. The asymptotic bias $\log(2m) - \psi(2m)$ of I_{mn} is that of $-V_{mn}$. Song (2002) suggests a bias correction in the asymptotic distribution (9) for moderate sample sizes:

$$\sqrt{6mn} \left[I_{mn} - b_{mn} \right] \xrightarrow{\mathcal{D}} \mathcal{N}(0, 1), \tag{10}$$

where

$$b_{mn} := \log(2m) - \log(n) - \psi(2m) + \psi(n+1) + \frac{2m}{n} R_{2m-1} - \frac{2}{n} \sum_{i=1}^{m} R_{i+m-2},$$

with $R_m := \sum_{j=1}^m 1/j$. From (10), an asymptotic p value for the related VS test is given by

$$p = 1 - \Phi^{-1} \left(\sqrt{6mn} \left[I_{mn}(x_1^n) - b_{mn} \right] \right), \tag{11}$$

where $I_{mn}(x_1^n)$ denotes the value of the statistic I_{mn} for the observations $x_1^n=(x_1,\ldots,x_n)$, and Φ denotes the cumulative distribution function of the normal distribution. According to Song (2002), the asymptotic p value (11) provides accurate results for sample sizes n larger than 80. For small sample sizes, Monte Carlo simulations should be preferred. A large number N of replications of X_1^n drawn from $P_0(\widehat{\theta}_n)$ (or $P_0(\theta)$ in case of simple null hypothesis) are generated. The test statistic I_{mn}^i is computed for each replication $i, 1 \leq i \leq N$. The p value is then given by the empirical mean $(\sum_{i=1}^N \mathbb{1}_{\{I_{mn}^i > I_{mn}(x_1^n)\}})/N$.

For choosing m, Song (2002) proposes to minimize I_{mn} – that is to maximize V_{mn} , with respect to m, yielding the most conservative test. The KL divergence $\mathbb{K}(P \mid P_0(\theta))$ being nonnegative, values of m for which I_{mn} is negative are excluded, leading to choose m subject to the constraint

$$V_{mn} \le -\frac{1}{n} \sum_{i=1}^{n} \log p_0\left(.; \widehat{\theta}_n\right). \tag{12}$$

Finally, the window size proposed by Song (2002) – say the optimal window size, is

$$\widehat{m} := \min \left\{ m^* \in \operatorname*{argmax}_{m \in \mathbb{N}^*} \left\{ V_{mn} : V_{mn} \leq -\frac{1}{n} \sum_{i=1}^n \log p_0 \left(X_i, \widehat{\theta}_n \right) \right\} : 1 \leq m^* < \lfloor n^{1/3 - \delta} \rfloor \right\}, \tag{13}$$

for some $\delta < 1/3$ and the VS test statistic is then

$$I_{\widehat{m}n} = -V_{\widehat{m}n} - \frac{1}{n} \sum_{i=1}^{n} \log p_0 \left(X_i; \widehat{\theta}_n \right). \tag{14}$$

The upper bound $n^{1/3-\delta}$ for the window size m is chosen so that conditions (8) are fulfilled and hence that asymptotic normality (9) holds. No optimal choice of δ exists; it depends on the family of distributions of the null hypothesis; see Section 3 for details.

The package **vsgoftest** presented below performs VS tests for several parametric families of ME distributions: uniform, normal, log-normal, exponential, Pareto, Laplace, Weibull, Fisher, gamma and beta distributions. These families of distribution, all included in the class \mathcal{F} given by (7), have been chosen so that the package covers a large variety of applications. Note that the package **dbEmpLikeGOF** performs uniformity and normality VS tests, with an alternative choice for the window size. Precisely, the test statistic is $nI_{mn} + 1/2$, and the window m is chosen, between 1 and $n^{1/2}$, minimizing nI_{mn} . The constraint (12) is not considered. The asymptotic distribution of nI_{mn} is not used, p values being computed from a pre-calculated table for small sample sizes or via Monte-Carlo simulation; see Miecznikowski, Vexler, and Shepherd (2013) and Vexler and Gurevich (2010). This alternative methodological approach leads to different decisions that may be less reliable, particularly when applied to heavy tailed samples. Other differences in the coding structure make **vsgoftest** faster than **dbEmpLikeGOF**, especially when Monte-Carlo simulation is performed. These points will be detailed in Section 4.2.

3. The package content

The **vsgoftest** package provides functions for estimating Shannon entropy of absolutely continuous distributions and testing the goodness-of-fit of some theoretical family of distributions to a vector of real numbers. It also provides functions for computing the density, cumulative density and quantile functions of Pareto and Laplace distributions, as well as for generating samples from these distributions.

Package **vsgoftest** is available from the Comprehensive R Archive Network (CRAN) at https://CRAN.R-project.org/package=vsgoftest and can be installed by executing the command

R> install.packages("vsgoftest")

Alternatively, the latest (under development) version of the **vsgoftest** package is also available and can be installed in R from the GitHub repository of the project as follows (requires the **devtools** package, Wickham, Hester, and Chang 2020, to be installed):

```
R> devtools::install_github(repo = "pregnault/vsgoftest")
```

The package is structured around two functions, entropy.estimate and vs.test; the first one computes the spacing based estimator (5) from a numeric sample, the second one performs Vasicek-Song GOF test for usual parametric families of distributions based on the test statistic (14). A comprehensive presentation of their usage is proposed in Sections 3.1 and 3.2, with numerous examples. Section 3.3 provides further technical information about the structure of the package.

3.1. Estimating Shannon entropy

The function entropy.estimate computes the spacing based estimate (5) of Shannon entropy (3) from a numeric sample. Two arguments have to be provided:

- x: the numeric sample;
- window: an integer between 1 and half of the sample size, specifying the window size of the spacing-based estimator (5).

It returns the estimate of Shannon entropy of the sample. Here is an example for a sample drawn from a normal distribution with parameters $\mu = 0$ and $\sigma^2 = 1$. The last instruction of the code chunk returns the exact value of the entropy of this normal distribution.

```
R> library("vsgoftest")

Loading required package: fitdistrplus
Loading required package: MASS
Loading required package: survival

R> set.seed(2)
R> samp <- rnorm(n = 100, mean = 0, sd = 1)
R> entropy.estimate(x = samp, window = 8)

[1] 1.394728

R> log(2 * pi * exp(1))/2

[1] 1.418939
```

The estimate returned by entropy.estimate obviously depends on the window size selected by the user, as illustrated by the following chunk.

R> sapply(1:10, function(w) entropy.estimate(x = samp, window = w))

- [1] 1.205018 1.346352 1.378732 1.387337 1.391691 1.393512 1.394428
- [8] 1.394728 1.394486 1.392669

One may select the window size that maximizes the entropy estimate, as follows.

```
R > n < -100

R > V < -sapply(1:(n/2 - 1), function(w) entropy.estimate(x = samp, + window = w))

R > which.max(V)
```

[1] 8

Let us consider a sample of size n = 100 drawn from a Pareto distribution with density

$$p(x; c, \mu) = \frac{\mu c^{\mu}}{x^{\mu+1}}, \quad x \ge c,$$

where c > 0 and $\mu > 0$, which can be obtained by making use of the function rpareto as illustrated below. Its Shannon entropy is

$$\mathbb{S}(p(.; c, \mu)) = -\ln \mu + \ln c + \frac{1}{\mu} + 1.$$

```
R> set.seed(5)
```

R > samp < - rpareto(n, c = 1, mu = 2)

R > entropy.estimate(x = samp, window = 3)

[1] 0.8480204

$$R > -\log(2) + 3/2$$

[1] 0.8068528

3.2. Testing GOF of a distribution or family of distributions

The function vs.test performs the VS test, as described in Section 2; setting two non-optional arguments is required:

- x: the numeric sample;
- densfun: a character string specifying the theoretical family of distributions of the null hypothesis. Supported families of distributions are: uniform, normal, log-normal, exponential, gamma, Weibull, Pareto, Fisher and Laplace distributions. They are referred to by the symbolic name in R of their density function. For example, set densfun = "dnorm" to test GOF of the family of normal distributions; see Table 1 for details.

Distribution	Call	Parameters	Density	Default
	$(\mathtt{densfun})$			δ
Uniform	"dunif"	a < b	$\frac{1}{b-a}1_{[a,b]}(x)$	1/12
Normal	"dnorm"	$\mu \in \mathbb{R}, \sigma \in \mathbb{R}_+$	$\frac{1}{b-a} 1_{[a,b]}(x)$ $\frac{1}{\sqrt{2\pi}\sigma} \exp\left(-\frac{1}{2\sigma^2}(x-\mu)^2\right)$	1/12
Log-normal	"dlnorm"	$\mu \in \mathbb{R}, \sigma \in \mathbb{R}_+$	$\frac{1}{x\sqrt{2\pi}\sigma}\exp\left(-\frac{(\log x-\mu)^2}{2\sigma^2}\right)1_{\mathbb{R}_+}(x)$	1/12
Exponential	"dexp"	$\lambda \in \mathbb{R}$	$\lambda \exp(-\lambda x) 1_{\mathbb{R}_+}(x)$	1/12
Pareto	"dpareto"	$c \in \mathbb{R}, \mu \in \mathbb{R}_+$	$\mu c^{\mu} \frac{1}{r^{\mu+1}} 1_{[c,\infty[}(x)$	1/12
Laplace	"dlaplace"	$\mu \in \mathbb{R}, \sigma \in \mathbb{R}_+$	$\mu c^{\mu} \frac{1}{x^{\mu+1}} 1_{[c,\infty[}(x)$ $\frac{1}{2\sigma} \exp\left(-\frac{ x-\mu }{\sigma}\right)$	1/12
Weibull	"dweibull"	$a, b \in \mathbb{R}_+$	$\frac{a}{b^a}x^{a-1}\exp\left[-\left(\frac{x}{b}\right)^a\right]1_{\mathbb{R}_+}(x)$	2/15
Fisher	"df"	$ u_1, u_2 \in \mathbb{R}_+ $	$\frac{\left(\frac{d_1x}{d_1x+d_2}\right)^{d_1/2} \left(1 - \frac{d_1x}{d_1x+d_2}\right)^{d_2/2}}{xB(d_1/2, d_2/2)} 1_{\mathbb{R}_+}(x)$	2/15
Gamma	"dgamma"	$\alpha, \beta \in \mathbb{R}_+$	$\frac{\beta^{\alpha}}{\Gamma(\alpha)} x^{\alpha-1} \exp(-\beta x) 1_{\mathbb{R}_{+}}(x)$	2/15
Beta	"dbeta"	$\alpha, \beta \in \mathbb{R}$	$\frac{x^{\alpha-1}(1-x)^{\beta-1}}{B(\alpha,\beta)}1_{\mathbb{R}_+}(x)$	2/15

Table 1: Families of distributions supported as the null by the **vsgoftest** package. The column denoted "Default δ " corresponds to the default setting for the parameter δ ; see (13). Note that $B(a,b) = \int_0^1 x^{a-1} (1-x)^{b-1} dx$ is the Beta function.

It returns an object of class 'htest', i.e., a list whose main components are:

- statistic: the value of VS test statistic (14) for the sample, with optimal window size defined by (13);
- parameter: the optimal window size;
- estimate: the maximum likelihood estimate of the parameters of the null distribution (for the test (2) with composite null hypothesis);
- p.value: the p value associated to the sample.

By default, vs.test performs the composite VS test of the family of distributions densfun for the sample x. The p value is estimated by means of Monte-Carlo simulation if the sample size is smaller than 80, or through the asymptotic distribution (9) of the VS test statistic otherwise.

In the following example, a normally distributed sample is simulated. VS test rejects the null hypothesis that this sample is drawn from a Laplace distribution, but does not reject the normality hypothesis (for a significant level set to 0.05).

```
R> set.seed(5)
R> samp <- rnorm(50, 2, 3)
R> vs.test(x = samp, densfun = "dlaplace")
```

Vasicek-Song GOF test for the Laplace distribution

For performing a simple null hypothesis GOF test, the additional argument param has to be set to a numeric vector, consistent with the parameter requirements for the null distribution. In such case, the MLE of the parameter(s) of the null distribution has not to be computed and hence the component estimate in results is not available.

If param is not consistent with the specified distribution – e.g., standard deviation for testing a normal distribution is missing or negative, the execution is stopped and an error message is returned.

```
R> set.seed(2)
R> samp <- rnorm(50, -2, 1)
R> vs.test(samp, densfun = "dnorm", param = -2)

Error in vs.test(samp, densfun = "dnorm", param = -2) :
    "param": invalid parameter (not consistent with the specified distribution)
```

One can estimate the p value of the sample by Monte-Carlo simulation, even when sample size is larger than 80, by setting the optional argument simulate.p.value to TRUE (NULL by default). The number of Monte-Carlo replicates can be fixed through the optional argument B (default is B = 5000).

Vasicek's estimates V_{mn} are computed for all m from 1 to $n^{1/3-\delta}$, where $\delta < 1/3$; the test statistic is $I_{\widehat{m}n}$ for \widehat{m} the optimal window size, as defined in (13). The choice of δ depends on the family of distributions of the null hypothesis. Precisely, for Weibull, Pareto, Fisher, Laplace and Beta, δ is set by default to 2/15, while for uniform, normal, log-normal, exponential and gamma, it is set to 1/12. These default settings result from numerous experimentations. Still, the user can choose another value through the optional argument delta.

```
R> set.seed(63)
R> vs.test(samp, densfun = "dexp", delta = 5/30)

Vasicek-Song GOF test for the exponential distribution
data: samp
Test statistic = 0.16517, Optimal window = 2, p-value = 0.1538
sample estimates:
   Rate
1.15047
```

Note that upper-bounding the window size by $n^{1/3-\delta}$ is only required when the asymptotic normality of I_{mn} is used to compute asymptotic p values from (9). When the p values are computed by means of Monte-Carlo simulation, this upper-bound can be extended to n/2 by adding extend = TRUE, which may lead to a more reliable test, as illustrated below.

sample estimates:
Location Scale
-2.162290 1.683868

Enlarging the range of m is also pertinent if ties are present in the sample. Indeed, the presence of ties is particularly inappropriate for performing VS tests, because some spacings $X_{(i+m)} - X_{(i-m)}$ can be null. The window size m has thus to be greater than the maximal number of ties in the sample. Hence, if the upper-bound $n^{1/3-\delta}$ is less than the maximal number of ties, the test statistic can not be computed. Setting extend to TRUE can avoid this behavior, as illustrated below (ties are added to the previous sample drawn from the exponential distribution).

```
R> samp <- c(samp, rep(4, 3))
R> vs.test(x = samp, densfun = "dexp")
```

Warning in vs.estimate(x, densfun, ESTIM, extend, delta, relax): Ties should not be present for Vasicek-Song test

Error in vs.estimate(x, densfun, ESTIM, extend, delta, relax) : Too many ties to compute Vasicek estimate.

```
R> vs.test(x = samp, densfun = "dexp", extend = TRUE)
```

Warning in vs.estimate(x, densfun, ESTIM, extend, delta, relax): Ties should not be present for Vasicek-Song test

Vasicek-Song GOF test for the exponential distribution

```
data: samp
Test statistic = 0.025702, Optimal window = 16, p-value = 0.9052
sample estimates:
    Rate
```

1.683785

Finally, Vasicek's estimate V_{mn} may exceed the parametric estimate of the entropy of the null distribution for all m between 1 and $n^{1/3-\delta}$. Then, no window size exists satisfying (13), as illustrated below.

```
R> set.seed(84)
R> ech <- rpareto(20, mu = 1/2, c = 1)
R> vs.test(x = ech, densfun = "dpareto", param = c(1/2, 1))
```

```
Error in vs.estimate(x, densfun, ESTIM, extend, delta, relax):

The sample entropy is greater than empirical maximal entropy for all possible window sizes; the sample may be too small or is unlikely to be drawn from the null distribution.
```

Enlarging the possible window sizes by setting extend to TRUE may enable Vasicek estimates to be smaller than empirical entropy.

Note that when computing the p value by Monte-Carlo simulation, the constraint (12) may not be satisfied for some replicates, whatever be the window size. These replicates are then ignored and the p value is computed from the remaining replicates. A warning message is added to the output, informing on the number of ignored replicates.

A large proportion of such ignored replicates may indicate that the original sample is too small or the null distribution obviously does not fit it.

The function vs.test also allows to avoid the constraint (12) when computing the optimal window size, by setting the optional argument relax to TRUE. This however should be used with special care, even when the p value is computed by Monte-carlo simulation, because it may lead to spurious conclusions. Some examples will be discussed in Section 5. This option is to recover the non-parametric likelihood ratio GOF test developed by Vexler and Gurevich (2010) and performed by dbEmpLikeGOF; see Section 4.2.

3.3. Technical information on the internal structure of the package

While entropy.estimate is a stand-alone function – depending only on the base and stats packages, vs.test is supported by a set of internal functions – not available for users; the structure of the package and connections between functions are described in the organizational chart presented in Figure 1. Functions available for users are depicted by rectangles while internal functions are depicted by ellipses. An arrow connecting a function to another means that the first function (say master function) calls the second (slave) during execution. When such a call is optional (depending on arguments given in the master function), the arrow is dashed and annotated with the corresponding argument settings. The function

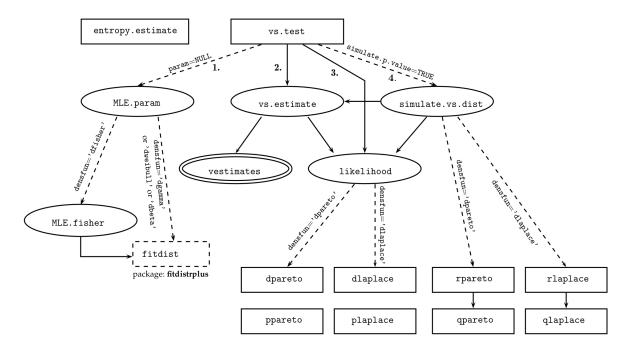


Figure 1: Organizational chart of the structure of the package and connections between functions available for users (depicted by rectangles) and internal functions (depicted by ellipses).

fitdist depicted by a dashed rectangle is a function implemented in the **fitdistrplus** package (Delignette-Muller and Dutang 2015). The double-lined ellipse depicts a C++ encoded function that has been integrated via the package **Rcpp** (Eddelbuettel and Francois 2011).

The vsgoftest package is structured in such a way so as to:

- Allow easy access to the code source. Especially, the master function vs.test calls four slave functions corresponding to the following tasks (enumerated according to the organizational chart of Figure 1):
 - 1. computing the MLE of the parameter θ of the null distribution through the function MLE.param.
 - 2. Computing Vasicek estimate $V_{\widehat{m}n}$ of Shannon entropy for the sample with the optimal window \widehat{m} given by (13).
 - 3. Computing the VS test statistic $I_{\widehat{m}n}$.
 - 4. Computing the p value associated to the sample. If the sample size is either greater than 80 or the optional argument simulate.p.value is TRUE, then the p value is estimated by means of Monte-Carlo simulation performed by the internal function simulate.vs.dist.
- Limit dependence to other packages. In this aim, density, cumulative density and quantile functions as well as random generators for Pareto and Laplace distributions have been encoded, even if they are available in other R packages such as **VGAM** in Yee (2010), **POT** in Ribatet and Dutang (2019) and **smoothmest** in Hennig (2012). The

MLE $\widehat{\theta}_n$ of the parameter of the null distribution is computed thanks to the function fitdist of the fitdistrplus package only if no closed form expression is known for it, i.e., for Gamma, Weibull, Beta and Fisher distributions. Otherwise, the closed form expression is used.

• Optimize time and resources, especially for Monte-Carlo simulation. To this end, the most time-consuming part of the procedure – namely, the computation of Vasicek estimate for all possible window sizes, has been converted to C++ and integrated to the package via **Rcpp**, in the internal function **vestimates**.

4. Performance of Vasicek-Song tests

First, a review of power studies of VS tests available in literature is presented in Section 4.1. Then, power comparisons of VS tests and classical GOF tests are proposed when applied to discriminate between close distributions, such as Pareto versus shifted log-normal and Exponential versus Weibull. Finally, the features of packages **vsgoftest** and **dbEmpLikeGOF** are compared in Section 4.2; the methodological differences are highlighted, the higher performance of **vsgoftest** both in terms of power and computational time is pointed out and illustrated.

4.1. Power computation

Comparisons of the power properties of VS tests are widely discussed in literature. Various choices of null and alternative distribution families are considered. VS tests are shown to generally outperform classical GOF tests. A comprehensive list of these references is given in this section, with main conclusions summarized in Table 2. Especially, power properties of the VS test for normality have been discussed by Vasicek (1976), Arizono and Ohta (1989) and Gurevich and Davidson (2008) among many others. Compared with many tests, including Kolmogorov-Smirnov (KS), Cramér-von Mises (CvM), Anderson-Darling (AD) and Shapiro-Wilk (SW), the VS test exhibits higher power for most of alternative distributions. When the null distribution is an exponential distribution, the VS test is also shown in Ebrahimi, Habibullah, and Soofi (1992) to be more powerful than the Van-Soest and Finkelstein and Schafer tests, which are modified versions of respectively CvM and KS tests, for various alternative distributions such as Weibull, gamma and log-normal. Choi and Kim (2006) for Laplace and Lequesne (2015b) for Pareto show that the VS test is more powerful than EDF tests, for various alternative distributions. The uniform VS test is shown to outperform many other tests for alternative distributions having most of their mass near 0.5, but remains less powerful than CvM and Watson tests for other alternative distributions. On the basis of power computation in literature, we choose to compare the power of the VS test to the KS, CvM and AD tests, for close null and alternative distributions. In particular, difficulties in distinguishing a Pareto tail from that of a log-normal is an issue; see for example Malevergne, Pisarenko, and Sornette (2011). For illustration, we estimate through Monte-Carlo simulation the power of VS, KS, CvM and AD for null Pareto distributions applied to samples drawn from a (shifted) log-normal distribution. We simulate 10000 replicates x_1^n of a random sample X_1^n drawn from a shifted log-normal distribution $\mathcal{LN}(0,\sigma)$ with support $[1,\infty[$ and $\sigma=1,1.25,$ for $n \in \{20, 30, 50, 100\}$. Then, we apply the tests for the simple null hypothesis $H_0: P =$

Reference	Null	Alternative	VS compared with	Most powerful	
	distribution	distribution			
Vasicek (1976)	Normal	Exponential, gamma, uniform, beta, Cauchy	KS, CvM, Kuiper, Watson, AD, SW	AD (for Cauchy), VS (for others)	
Arizono and Ohta (1989)		Log-normal, uniform, χ^2 , student	KS, CvM, χ^2	VS	
Gurevich and Davidson (2008)		Log-normal, χ^2 , Student, uniform, exponential, gamma, beta, Cauchy	KS	KS (for Student and Cauchy), VS (for others)	
Ebrahimi et $al.$ (1992)	Exponential	Weibull, gamma, log- normal	Van-Soest, Finkelstein and Schafer	VS	
Dudewicz and Van Der Meulen (1981)	Uniform	Distributions defined on $[0,1]$	KS, CvM, Kuiper, Watson, AD, log-statistic, χ^2	VS (for alternative having most of its mass near 0.5), CvM or Watson (for others)	
Choi and Kim (2006)	Laplace	Normal, Student, logistic, Cauchy, uniform, chi-squared, Weibull, lognormal, extreme value and inverse Gaussian	KS, CvM, AD, Kuiper and Wat- son	VS	
Lequesne (2015b)	Pareto	Weibull, gamma, log- normal, two-parameter exponential	KS, AD	VS	
Mudholkar and Tian (2002)	Inv. Gaussian	Exponential, uniform, Weibull and log-normal	KS	VS (uniform and Weibull)	
Alizadeh Noughabi, Al- izadeh Noughabi, and Ebrahimi Moghaddam Behabadi (2014)	Rayleigh	Weibull, gamma, log- normal, half-normal, uniform, modified extreme value, linear increasing failure rate law, Dhillon's law and Chen's distribu- tion	KS, CvM, AD, Kuiper and Wat- son	VS (for uniform) and AD (for other alternatives)	
Perez-Rodriguez, Vaquera-Huerta, and Villaseñor- Alva (2009)	Gumbel	Weibull, log-normal, normal, logistic, Cauchy, Student, gamma and Fréchet	KS, CvM, AD, Kuiper and Kinni- son	AD (for heavy tails), VS (for others)	
Tsujitani, Ohta, and Kase (1980)	Extreme value	Normal and 3-parameter log-Weibull	KS, CvM, AD, Kuiper, Mann et modified Mann test	VS	
Lund and Rao Jammalamadaka (2000)	von Mises	Mixtures of Von Mises distributions (bimodal, skewed, long-tailed and half), the cardoid and triangular distributions	Watson and integrated squared error test	Watson (for long-tailed), VS (for half) and fairly equal for other alternatives	

Table 2: Power studies of VS tests performed in literature.

	VS	KS	AD	CvM	VS	KS	AD	CvM
	$H_0: \mathcal{P}(1,1); H_1: 1 + \mathcal{LN}(0,1)$				$H_0: \mathcal{P}(1,0.8); H_1: 1 + \mathcal{LN}(0,1.25)$			
n = 20	59.79	8.93	6.72	7.02	40.62	16.36	13.44	16.21
n = 30	77.66	15.79	22.83	16.61	55.50	27.05	26.54	26.98
n = 50	94.02	37.39	68.02	46.86	76.83	50.70	58.87	52.36
n = 100	99.99	85.90	99.83	96.36	98.42	89.22	97.58	92.07
	$H_0: \mathcal{E}(1)$	$(2); H_1: V$	V(1.2, 2)		$H_0: \mathcal{E}(1)$	$(2); H_1: V$	V(1.3, 2)	
n = 20	9.97	5.06	3.65	4.63	14.67	5.27	3.28	4.41
n = 30	12.05	6.10	4.29	5.19	19.93	7.40	5.65	6.45
n = 50	13.47	7.37	6.50	6.80	25.86	11.28	11.30	10.53
n = 100	38.55	11.17	13.91	11.21	67.14	21.91	34.67	24.60

Table 3: Power (expressed as percentage of true rejection) of VS, KS, CvM and AD tests for testing Pareto and exponential distributions against shifted log-normal (top) and Weibull distributions (bottom).

 $\mathcal{P}ar(1,\mu)$, for $\mu=1$ when $\sigma=1$ and $\mu=0.8$ when $\sigma=1.25$; the power is estimated by the proportion of rejections of the null hypothesis among the 10000 replicates. The following code chunk illustrates the procedure, for $\sigma=\mu=1$ and n=20, using the VS test. This procedure immediately adapts to other values of σ , μ and n and to other tests¹. Results are presented in Table 3 (top).

```
R > N < -10000

R > n < -20

R > mu < -1

R > set.seed(54)

R > res.pow < -replicate(n = N, expr = vs.test(x = 1 + rlnorm(n, meanlog = 0, sdlog = 1), densfun = "dpareto", param = c(1, 1), simulate.p.value = TRUE, B = 1000)$p.value)
```

The power of VS, KS, CvM and AD tests is similarly computed for null exponential and alternative Weibull distributions. The Weibull distribution W(a, b) reduces to an exponential distribution $\mathcal{E}(1/a)$ when b=1. The main aim is thus to determine which test better discriminates between these distributions when the shape parameter of the Weibull distribution is close to 1, precisely b=1.2 and b=1.3. Results are given in Table 3 (bottom), clearly showing that the VS test outperforms EDF tests.

Note that the above procedure for comparing the power of GOF tests adapts easily to other sets of null and alternative distributions.

¹The seed of the pseudo-random number generator has been changed for each couple of μ and n; the whole procedure yielding Table 3 is available in the file vsgoftest_performances.R, in the directory inst/doc of the package source file.

	VS	ELR	VS	ELR	
	$H_1: A$	$\mathcal{L}(0,1)$	$H_1:\mathcal{S}(4)$		
n = 50	17.8	16.0	16.1	14.6	
n = 200	86.2	64.9	71.2	35.8	

Table 4: Power comparisons between VS and ELR normality tests for samples drawn from a Laplace distribution (left) and a Student distribution (right). Power is estimated by means of Monte-Carlo simulation based on 1000 replicates of the samples.

4.2. Testing uniformity and normality: vsgoftest versus dbEmpLikeGOF

The package **dbEmpLikeGOF** in Miecznikowski *et al.* (2013) performs uniformity and normality tests based on empirical likelihood ratios (ELR) – say ELR tests. These tests are strongly linked to VS tests. Precisely, for testing the normality of a sample $X_1, \ldots X_n$, the ELR test statistic is $\log V_n$, where

$$V_n = \min_{1 \le m < n^{1/2}} \left[(2\pi e \check{S}^2)^{n/2} \prod_{i=1}^n \frac{2m}{n \left[X_{(i+m) - X_{(i-m)}} \right]} \right] \text{ and } \check{S}^2 = \frac{1}{n-1} \sum_{i=1}^n \left(X_i - \frac{1}{n} \sum_{j=1}^n X_j \right)^2.$$

Mere algebra yields

$$\log V_n = nI_{\widetilde{m}n} + \frac{1}{2},$$

with $\widetilde{m} \in \operatorname{argmax}_{1 \leq m < n^{1/2}} V_{mn}$. Hence, ELR and VS tests differ only in the window size choice: the upper bound is $n^{1/2}$ for the ELR test while it is (by default) $n^{1/4}$ for the VS test and the constraint (12) is not taken into account by the EL test. Enlarging the upper bound from $n^{1/4}$ to $n^{1/2}$ may lead to a more powerful decision rule, as mentioned and illustrated in Section 3.2. Still, practically, the normality VS test tends to outperform the ELR test when applied to heavy tailed samples, as illustrated by Table 4^2 . Moreover, the upper bound $n^{1/4}$ legitimates the use of the asymptotic distribution of $I_{\widehat{m}n}$ in vs.test, which is not performed by dbEmpLikeGOF. As previously mentioned in Section 3.2, disabling the constraint (12) may lead to spurious conclusions. The ELR test can be performed using vs.test, by suitably setting its arguments, as illustrated by the following code chunk 3 .

```
R> set.seed(1)
R> samp <- rnorm(50)
R> res.vs <- vs.test(x = samp, densfun = "dnorm", delta = -1/6, relax = TRUE)
R> res.vs$statistic * 50 + 1/2
```

Test statistic 7.970748

²The comparison procedure is available in the file vsgoftest_performances.R, in the directory inst/doc of the package source file.

³Some slight difference remains between the two computed values, due to numerical inaccuracy in computation procedures: the estimated entropy of the null distribution is computed from the closed form expression (4) in dbEmpLikeGOF while it is computed as the empirical mean of the log-likelihood of the sample in vs.test.

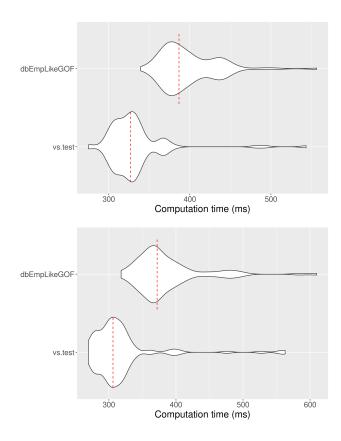


Figure 2: Distributions (violin plots) of computation time of 100 iterations of the functions dbEmpLikeGOF (from package dbEmpLikeGOF) and vs.test for testing normality of a sample of size 50 drawn from the standard normal distribution (top) and for testing uniformity of a sample of size 50 drawn from the uniform distribution on [0,1] (bottom). The p values are estimated by Monte-Carlo simulation, based on 1000 replicates. The red dashed lines are the median computation times.

```
R> library("dbEmpLikeGOF")
R> res.el <- dbEmpLikeGOF(x = samp, testcall = "normal", vrb = FALSE)
R> res.el$teststat
```

[1] 7.975815

Additionally, from a computational view point, some significant differences exist between the functions dbEmpLikeGOF and vs.test. Precisely, the p value returned by dbEmpLikeGOF is computed by default by linear interpolation from a table of pre-computed p values for various sample sizes (from n=10 to 10000) and test statistic values; the p value can be approximated by Monte-Carlo simulation by setting pvl.Table = FALSE. By default, vs.test computes the p value by means of Monte-Carlo simulation or uses the asymptotic distribution (10), depending on the sample size. In both cases, vs.test is nearly twenty percent faster than dbEmpLikeGOF, as illustrated by Figure 2^4 .

 $^{^4}$ Simulations have been performed on a Dell Lattitude E5580 laptop, equipped with an Intel[®] CoreTM i7-7600U CPU at 2.80GHz x 4, with 16GB RAM. R code for generating these figures is available in the file vsgoftest_performances.R, in the directory doc of the package source file.

5. Application to real data

The vs.test package contains environmental data originating from a guidance report edited by the Technology Support Center of the United States Environmental Protection Agency; see Singh, Singh, and Engelhardt (1997). According to Singh et al. (1997), environmental scientists take remediation decisions at suspected sites based on organic and inorganic contaminant concentration measurements. These decisions usually derive from the computation of confidence upper bounds for contaminant concentrations. Testing the goodness-of-fit of specified models hence appears of prior interest. Singh et al. (1997) also points out that contaminant concentration data from sites often appear to follow a skewed probability distribution, making the log-normal family a frequently-used model. The authors illustrate their purpose by applying Shapiro-Wilk test to the log-transformed of the samples aluminium1, manganese, aluminium2 and toluene (stored in the present package)⁵; see the empirical skewness computed in the following code chunk (requires the DescTools package (Signorell 2020) to be installed).

The following code chunks intend to illustrate the use and behavior of the function vs.test for these environmental data. The significant level is fixed to 0.1 as in Singh et al. (1997). Note that warning messages notifying that there are ties in the samples have been dropped out from outputs.

The log-normal hypothesis is not rejected for aluminium1. Similar results are obtained for manganese. Log-normality is rejected for aluminium2.

⁵A succinct description of these data is available by executing the following R command: ?contaminants.

Due to numerous ties in toluene, vs.test can not compute Vasicek entropy estimate unless extend is set to TRUE. Still, vs.test notifies that the constraint (12) is violated for all window sizes, which suggests that data are not likely to be drawn from the log-normal distribution. Turning relax to TRUE yields the following result.

This last result looks spurious because the test statistic is negative – resulting from (12) not being satisfied by setting relax = TRUE. An alternative is to test normality of the log-transformed sample as follows.

```
R> set.seed(1)
R> vs.test(x = log(toluene), densfun = "dnorm", extend = TRUE)

Vasicek-Song GOF test for the normal distribution

data: log(toluene)
Test statistic = 0.6536, Optimal window = 11, p-value = 2e-04
sample estimates:
    Mean St. dev.
4.651002 3.579041
```

The log-normal hypothesis is not rejected for aluminium1 and manganese while it is rejected for aluminium2 and toluene. These results are consistent with those obtained by Singh et al. (1997). Further, the goodness-of-fit to the Pareto distributions is performed for aluminium2 and toluene. Log-normal and Pareto distributions usually compete with closely related generating processes and hard to distinguish tail properties; see for example Malevergne et al. (2011). Goodness-of-fit of Pareto distribution is rejected for aluminium2.

```
R> set.seed(1)
R> vs.test(x = aluminium2, densfun = "dpareto")
```

Vasicek-Song GOF test for the Pareto distribution

Applying vs.test to toluene with default settings yields no result because of numerous ties and the violation of (12). Uniformity of the sample transformed by the cumulative density function of the Pareto distribution can be tested as follows. Goodness-of-fit of the Pareto distribution is not rejected for toluene.

6. Conclusion

Vasicek-Song tests constitute powerful GOF tests for classical parametric families of distributions, relying on an information theoretical framework. They can be easily performed by using the **vsgoftest** package for R. Default and optional settings of the functions provided by the package make the procedure both intuitive and flexible. Its application to real datasets manages to illustrate its practical usage.

The package allows for testing GOF of a significant list of parametric models; this list could be extended in further releases. New entropy-based GOF tests could also be considered by using Rényi entropy and divergence – see Lequesne (2015a), thus extending even more the class of possible distributions, including, e.g., Student distributions.

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