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APPLICATION OF NONPARAMETRIC GOODNESS-OF-FIT TESTS: PROBLEMS AND SOLUTION*

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In this paper, the problems of application of nonparametric goodness-of-fit tests in the case of composite hypotheses have been considered. The factors influencing test statistic distributions have been discussed. A manual on application of nonparametric tests have been prepared. The proposed recommendations would reduce errors in statistical inference when using considered tests in practice.

Keywords: Composite hypotheses of goodness-of-fit; Anderson-Darling test, Cramer-von Mises-Smirnov test, Kolmogorov test, Kuiper test, Watson test, Zhang tests.

1. Introduction

In applications of statistical data analysis, there are a lot of examples of incorrect usage of nonparametric goodness-of-fit tests (Kolmogorov, Cramer-von Mises Smirnov, Anderson-Darling, Kuiper, Watson, Zhang tests). The most common errors in testing composite hypotheses are associated with using classical results obtained for simple hypotheses.

There are simple and composite goodness-of-fit hypotheses. A simple hypothesis tested has the following form $H_0: F(x) = F(x,\theta)$, where $F(x,\theta)$ is the distribution function, which is tested for goodness-of-fit with observed sample, and θ is an known value of parameter (scalar or vector). A composite hypotheses tested has the form $H_0: F(x) \in \{F(x,\theta), \theta \in \Theta\}$, where Θ is the definition domain of parameter θ. If estimate $\hat{\theta}$ of scalar or vector parameter of tested distribution was not found by using the sample, for which goodness-of-fit hypothesis is tested, then the application of goodness-of-fit test for composite hypothesis is similar to the application of test in the case of simple hypothesis.

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The problems arise in testing composite hypothesis, when estimate $\hat{\theta}$ of the distribution parameter was found by using the same sample on which goodness-of-fit hypothesis is tested.

2. Goodness-of-fit tests for simple hypotheses

In the case of simple hypotheses, nonparametric tests are "free from distribution", i.e. the limiting distribution of statistics of classical nonparametric goodness-of-fit tests do not depend on a tested distribution and its parameters.

The Kolmogorov test (which is usually called the Kolmogorov–Smirnov test) is based on statistic

$$D_n = \sup_{|x|<\infty} \left| F_n(x) - F(x,\theta) \right|, \tag{1}$$

where $F_n(x)$ is the empirical distribution function; $F(x,\theta)$ is the hypothetical distribution function; n is the sample size. The limiting statistic distribution for testing simple hypothesis has been obtained by Kolmogorov in Ref. [6]. The distribution function of $\sqrt{n}\cdot D_n$ uniformly converges to the Kolmogorov distribution function $K(S)$ as $n \to \infty$, see Ref. [3, 11].

The Kolmogorov test is recommended to be used with Bolshev's correction, see Ref. [3, 11]:

$$S_K = \sqrt{n} D_n + \frac{1}{6\sqrt{n}} = \frac{6nD_n + 1}{6\sqrt{n}}, \tag{2}$$

where

$$D_n = \max\left(D_n^+, D_n^-\right),\ D_n^+ = \max_{1\le i\le n}\left\{\frac{i}{n} - F(x_i,\theta)\right\},\ D_n^- = \max_{1\le i\le n}\left\{F(x_i,\theta) - \frac{i-1}{n}\right\},$$

$x_1 \le x_2 \le \ldots \le x_n$ is the variational series (the sample sorted in increasing order).

The Cramer-von Mises Smirnov test is based on statistic

$$S_\omega = n\omega_n^2 = \frac{1}{12n} + \sum_{i=1}^{n}\left\{F(x_i,\theta) - \frac{2i-1}{2n}\right\}^2, \tag{3}$$

which has distribution $a1(s)$, when a simple hypothesis is tested, see Ref. [3, 11].

Statistic of the **Anderson-Darling test** has the form (Ref. [1, 2])

$$S_\Omega = -n - 2\sum_{i=1}^{n}\left\{\frac{2i-1}{2n}\ln F(x_i,\theta) + \left(1 - \frac{2i-1}{2n}\right)\ln(1 - F(x_i,\theta))\right\} \tag{4}$$

and has distribution $a2(s)$ for simple hypotheses, see Ref. [3, 11].

The Kuiper test is based on statistic $V_n = D_n^+ + D_n^-$ (Ref. [7]). It is preferred to use it in the form (Ref. [25])

$$V = V_n\left(\sqrt{n} + 0.155 + \frac{0.24}{\sqrt{n}}\right), \tag{5}$$

or in the form (Ref. [8])

$$V_n^{mod} = \sqrt{n}(D_n^+ + D_n^-) + \frac{1}{3\sqrt{n}}. \tag{6}$$

This statistic has distribution $Ku(s) = 1 - \sum_{m=1}^{\infty} 2(4m^2s^2 - 1)e^{-2m^2s^2}$, see Ref. [7].

The statistic of **Watson test** has the form (Refs. [26, 27])

$$U_n^2 = \sum_{i=1}^{n}\left(F(x_i,\theta) - \frac{i - \frac{1}{2}}{n}\right)^2 - n\left(\frac{1}{n}\sum_{i=1}^{n}F(x_i,\theta) - \frac{1}{2}\right)^2 + \frac{1}{12n} \tag{7}$$

and has distribution $W(s) = 1 - 2\sum_{m=1}^{\infty}(-1)^{m-1}e^{-2m^2\pi^2 s}$ for simple hypotheses tested.

The statistics of **Zhang test** can be written as (Refs. [8])

$$Z_A = -\sum_{i=1}^{n}\left[\frac{\log\{F(x_i,\theta)\}}{n - i + \frac{1}{2}} + \frac{\log\{1 - F(x_i,\theta)\}}{i - \frac{1}{2}}\right], \tag{8}$$

$$Z_C = \sum_{i=1}^{n}\left[\log\left\{\frac{[F(x_i,\theta)]^{-1} - 1}{(n - \frac{1}{2})/(i - \frac{3}{4}) - 1}\right\}\right]^2, \tag{9}$$

$$Z_K = \max_{1\le i\le n}\left(\left(i - \frac{1}{2}\right)\log\left\{\frac{i - \frac{1}{2}}{nF(x_i,\theta)}\right\} + \left(n - i + \frac{1}{2}\right)\log\left[\frac{n - i + \frac{1}{2}}{n\{1 - F(x_i,\theta)\}}\right]\right). \tag{10}$$

The tests based on statistics Z_A and Z_C have higher power in comparison with the Kolmogorov, Cramer-von Mises-Smirnov and Anderson-Darling tests. However, the application of these powerful tests is complicated because of the dependence of statistic distributions on the sample size.

3. Problems of application of tests for composite hypotheses

In the case of testing composite hypotheses, all nonparametric goodness-of-fit tests lose their property of being distribution free, if parameters estimation is based on the same sample, on which the hypothesis is tested. Statistic distributions $G(S|H_0)$ of these tests depend on:

- distribution $F(x,\theta)$ corresponding to tested hypothesis H_0 (see Fig. 1);
- the type and the number of parameters estimated;
- the estimation method used (see Fig. 2);
- in some cases, a particular value of parameter (for example, in the case of gamma-distribution).

The statistic distributions for simple hypotheses and the distributions of the same statistics for composite hypotheses are quite different. Therefore, it is unacceptable to disregard this difference.

On Fig. 1, empirical distributions $G(S_n|H_0)$ of Cramer-von Mises-Smirnov statistic S_ω are presented for the case of testing composite hypothesis H_0, when the maximum likelihood method is used for estimation of two parameters.

The dependence of the test statistic distribution on estimation method used is shown on Fig. 2. There are density functions $g(S_n|H_0)$ of Kolmogorov test statistic S_K with the following methods for estimating parameters of the normal distribution: the methods based on minimizing statistics S_K, S_ω, S_Ω (*MD*-estimates) and the maximum likelihood method.

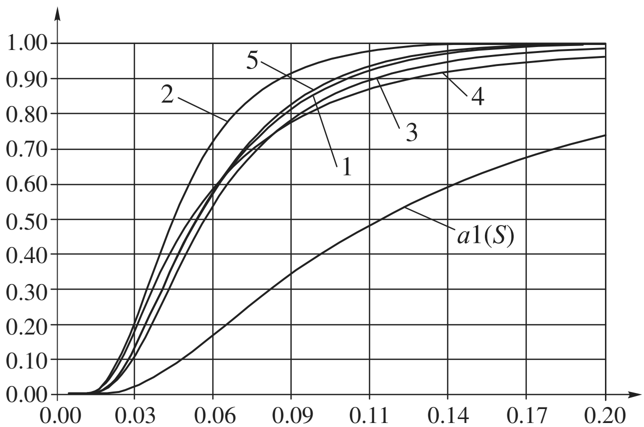

Fig. 1. Distributions $G(S_n|H_0)$ of Cramer-von Mises-Smirnov test statistic S_ω in the case of estimation of two parameters of the distribution corresponding to H_0 (*1* – normal, *2* – logistic, *3* – Laplace, *4* – extreme-value (minimum), *5* – Cauchy), maximum likelihood method is used, $a1(s)$ is the distribution function for simple hypotheses tested.

Moreover, the greatest problem consists in the dependence of test statistic distributions on specific value of the distribution shape parameter. For example, in the case of generalized normal distribution with density

$$f(x) = \frac{\theta_2}{2\theta_1 \Gamma(1/\theta_2)} \exp\left\{ -\left(\frac{|x-\theta_0|}{\theta_1} \right)^{\theta_2} \right\}, \tag{11}$$

the value of shape parameter θ_2 influences the statistic distributions of nonparametric goodness-of-fit tests. Such influence is illustrated on Fig. 3 in the case of estimating three parameters of (11) by the maximum likelihood method.

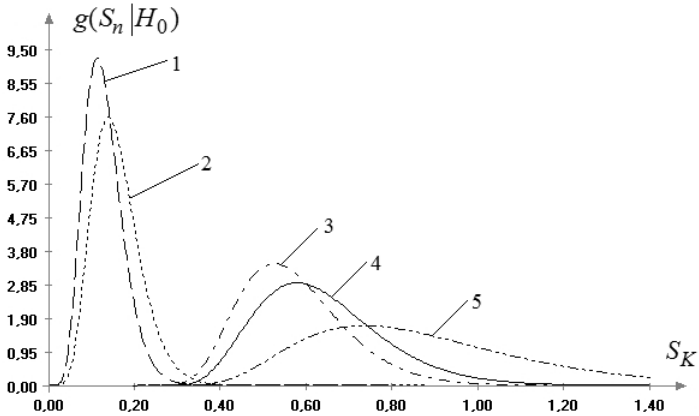

Fig. 2. Distribution densities $g(S_n|H_0)$ of statistic S_K in the case of testing composite hypothesis (H_0 – normal distribution, two parameters estimated: *1 – MD*-estimates S_K; *2 – MD*-estimates S_ω; *3 – MD*-estimates S_Ω; *4* – maximum likelihood method; $k(s)$ –density of Kolmogorov distribution).

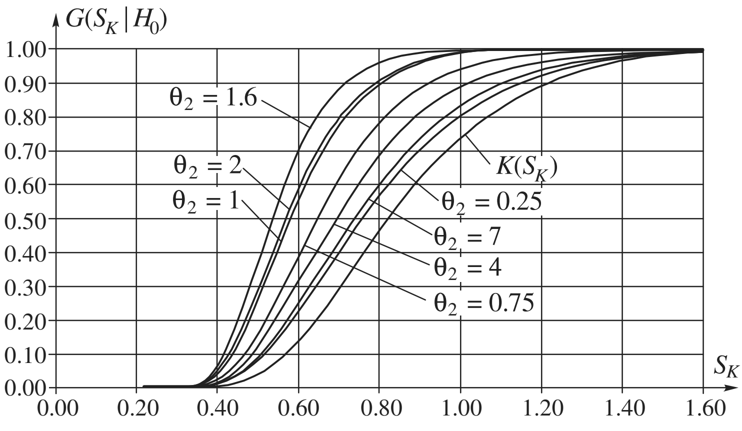

Fig. 3. The dependence of statistic distribution of the Kolmogorov test on the value of shape parameter θ_2, when three distribution parameters of the generalized normal distribution are estimated.

4. Application of tests for composite hypotheses: solution of problems

The investigation of limiting statistic distributions of nonparametric goodness-of-fit tests for composite hypotheses was initiated in Ref. [5].

Various approaches have been used for solving problems in this area: the limiting statistic distributions have been studied by analytical and numerical methods. In particular cases, the tables of percentage points for the limiting statistic distributions of nonparametric tests have been obtained by using statistical simulation methods.

Apparently, the first papers, in which the Monte-Carlo method and computer simulation appeared to be an efficient method for the development of applied mathematical statistic, were Refs. [22, 23]. In these papers, the percentage points for the Kolmogorov test statistic (without Bolshev's correction) were obtained for testing composite hypotheses relative to normal distribution law.

In a number of our papers, the analytically simple models, approximating the limiting statistic distributions of nonparametric tests in the case of testing composite hypotheses, when unknown parameters are estimated with the maximum likelihood method, have been constructed by using computer simulate-on of statistic distributions relative to various distributions corresponding to hypothesis H_0. The recommendations for standardization R 50.1.037-2002 have been published on the basis of these studies (Ref. [24]). Later, results presented in Ref. [24] have been made more precise and extended in Refs. [8-16]. At present, the manual (Ref. [17]) based on obtained results has been prepared and intended to replace recommendations in Ref. [24].

The manual Ref. [17] includes the tables of percentage points and the models of limiting statistic distributions of nonparametric tests (altogether 63 tables), which can be used for testing various composite hypotheses (on the following distributions: exponential, seminormal, Rayleigh, Maxwell, Laplace, normal, log-normal, Cauchy, logistic, extreme-value (minimum and maximum), *Sb*-Johnson, *Sl*-Johnson, *Su*-Johnson, Weibull, generalized Weibull, family of gamma-distribution, family of beta-distribution, generalized normal, inverse Gaussian distribution). Moreover, the manual includes the description of computer simulation techniques for research of probabilistic regularities, which can be used for investigation of test statistic distributions.

The tables of percentage points and the models of test statistics distributions were based on simulated samples of the statistics with size $N = 10^6$. The difference between actual distribution $G(S|H_0)$ and empirical distribution $G_N(S|H_0)$ does not exceed 10^{-3} for such N. The values of the test statistic were calculated using samples of pseudorandom values simulated for the observed distribution $F(x,\theta)$ with the size $n=10^3$. In such a case, distribution $G(S_n|H_0)$ practically equal to the limiting one $G(S|H_0)$. The given models can be used for statistical analysis if the sample sizes $n>25$.

Unfortunately, the dependence of the nonparametric goodness-of-fit tests statistics distributions for testing composite hypotheses on the values of the shape parameter (or parameters) (see Fig. 3) appears to be for many parametric distributions implemented in the most interesting applications, particularly in problems of survival analysis and reliability. This is true for families of gamma-, beta-distributions of the 1st, 2nd and 3rd kind, generalized normal, generalized Weibull, inverse Gaussian distributions, and many others.

5. An interactive method to study distributions of statistics

In the cases, when statistic distributions of nonparametric tests depend on a specific values of shape parameter(s) of tested distribution, the statistic distribution cannot be found in advance (before computing corresponding estimates). In such situations, it is recommended to find the test statistic distribution by using interactive mode in statistical analysis process, see Ref. [18], and then, to use this distribution for testing composite hypothesis.

The dependence of the test statistics distributions on the values of the shape parameter or parameters is the most serious difficulty that is faced while applying nonparametric goodness-of-fit criteria to test composite hypotheses in different applications.

Since estimates of the parameters are only known during the analysis, so the statistic distribution required to test the hypothesis could not be obtained in advance. For the criteria with statistics (8) - (10), the problem is harder to be solved as statistics distributions depend on the samples sizes. Therefore, the statistics distributions of applied test should be obtained interactively during statistical analysis (see Ref. [19, 20]), and then should be used to make conclusions about composite hypothesis under test.

The implementation of such an interactive mode requires a developed software that allows parallelizing the simulation process and taking available computing resources. The usage of parallel computing enables to decrease the time of simulation of the required test statistic distribution $G_N(S_n|H_0)$ (with the required accuracy), which is used to calculate the achieved significance level $P\{S_n \geq S^*\}$, where S^* is the value of the statistic calculated using an original sample.

In the software system (see Ref. [4]), the interactive method for the research of statistics distributions is implemented for the following nonparametric goodness-of-fit tests: Kolmogorov, Cramer-von Mises-Smirnov, Anderson-Darling, Kuiper, Watson and three Zhang tests. Moreover, the different methods of parameter estimation can be used there.

The following example demonstrates the accuracy of calculating the achieved significance level depending on sample size N of simulated interactively empirical statistics distributions (Software system, Ref. [4]).

Example. It is necessary to check a composite hypothesis on goodness-of-fit of the inverse Gaussian distribution with the density function

$$f(x)=\frac{1}{\theta_2}\left(\frac{\theta_0}{2\pi\left(\frac{x-\theta_3}{\theta_2}\right)^3}\right)^{1/2}\exp\left(-\frac{\theta_0\left(\left(\frac{x-\theta_3}{\theta_2}\right)-\theta_1\right)^2}{2\theta_1^2\left(\frac{x-\theta_3}{\theta_2}\right)}\right)$$

on the basis of the following sample of the size $n=100$:

0.945	1.040	0.239	0.382	0.398	0.946	1.248	1.437	0.286	0.987
2.009	0.319	0.498	0.694	0.340	1.289	0.316	1.839	0.432	0.705
0.371	0.668	0.421	1.267	0.466	0.311	0.466	0.967	1.031	0.477
0.322	1.656	1.745	0.786	0.253	1.260	0.145	3.032	0.329	0.645
0.374	0.236	2.081	1.198	0.692	0.599	0.811	0.274	1.311	0.534
1.048	1.411	1.052	1.051	4.682	0.111	1.201	0.375	0.373	3.694
0.426	0.675	3.150	0.424	1.422	3.058	1.579	0.436	1.167	0.445
0.463	0.759	1.598	2.270	0.884	0.448	0.858	0.310	0.431	0.919
0.796	0.415	0.143	0.805	0.827	0.161	8.028	0.149	2.396	2.514
1.027	0.775	0.240	2.745	0.885	0.672	0.810	0.144	0.125	1.621

The shift parameter θ_3 is assumed to be known and equal to 0.

The shape parameters θ_0, θ_1, and the scale parameter θ_2 are estimated using the sample. The maximum likelihood estimates (MLEs) calculated using the sample above are the following $\hat{\theta}_0=0.7481$, $\hat{\theta}_1=0.7808$, $\hat{\theta}_2=1.3202$. The statistics distributions of nonparametric goodness-of-fit tests depend on the values of the shape parameters θ_0 and θ_1 (see Ref. [21]), does not depend on the value of the scale parameter θ_2 and have to be calculated using values $\theta_0=0.7481$, $\theta_1=0.7808$.

The calculated values of the statistics S_i^* for Kuiper, Watson, Zhang, Kolmogorov, Cramer-von Mises-Smirnov, Anderson-Darling tests and achieved significance levels for these values $P\{S\geq S_i^*\,|H_0\}$ (p-values), obtained with different accuracy of simulation (with different sizes N of simulated samples of statistics) are given in Table 1.

The similar results for testing goodness-of-fit of the Γ-distribution with the density:

$$f(x)=\frac{\theta_1}{\theta_2\Gamma(\theta_0)}\left(\frac{x-\theta_3}{\theta_2}\right)^{\theta_1\theta_0-1}e^{-\left(\frac{x-\theta_3}{\theta_2}\right)^{\theta_1}}$$

on the given sample, are given in Table 2. The MLEs of the parameters are $\hat{\theta}_0=2.4933$, $\hat{\theta}_1=0.6065$, $\hat{\theta}_2=0.1697$, $\hat{\theta}_4=0.10308$. In this case, the distribution of test statistic depends on the values of the shape parameters θ_0 and θ_1.

Table 1. The achieved significance levels for different sizes N when testing goodness-of-fit of the inverse Gaussian distribution

The values of tests statistics	$N=10^3$	$N=10^4$	$N=10^5$	$N=10^6$
$V_n^{mod}=1.1113$	0.479	0.492	0.493	0.492
$U_n^2=0.05200$	0.467	0.479	0.483	0.482
$Z_A=3.3043$	0.661	0.681	0.679	0.678
$Z_C=4.7975$	0.751	0.776	0.777	0.776
$Z_K=1.4164$	0.263	0.278	0.272	0.270
$S_K=0.5919$	0.643	0.659	0.662	0.662
$S_\omega=0.05387$	0.540	0.557	0.560	0.561
$S_\Omega=0.3514$	0.529	0.549	0.548	0.547

Table 2. The achieved significance levels for different sizes N when testing goodness-of-fit of the Γ-distribution

The values of tests statistics	$N=10^3$	$N=10^4$	$N=10^5$	$N=10^6$
$V_n^{mod}=1.14855$	0.321	0.321	0.323	0.322
$U_n^2=0.057777$	0.271	0.265	0.267	0.269
$Z_A=3.30999$	0.235	0.245	0.240	0.240
$Z_C=4.26688$	0.512	0.557	0.559	0.559
$Z_K=1.01942$	0.336	0.347	0.345	0.344
$S_K=0.60265$	0.425	0.423	0.423	0.424
$S_\omega=0.05831$	0.278	0.272	0.276	0.277
$S_\Omega=0.39234$	0.234	0.238	0.238	0.237

Fig. 4 presents the empirical distribution and two theoretical ones (IG-distribution and Γ-distribution), obtained by the sample above while testing composite hypotheses.

The results presented in Table 1 and Table 2 show that estimates of p-value obtained for IG-distribution higher than estimates of p-value for the Γ-distribution, i.e. the IG-distribution fits the sample given above better than the Γ-distribution. Moreover, it is obvious that the number of simulated samples of statistics $N = 10^4$ is sufficient to obtain the estimates of p-value with desired accuracy in practice, and this fact does not lead to the noticeable increase of time of statistical analysis.

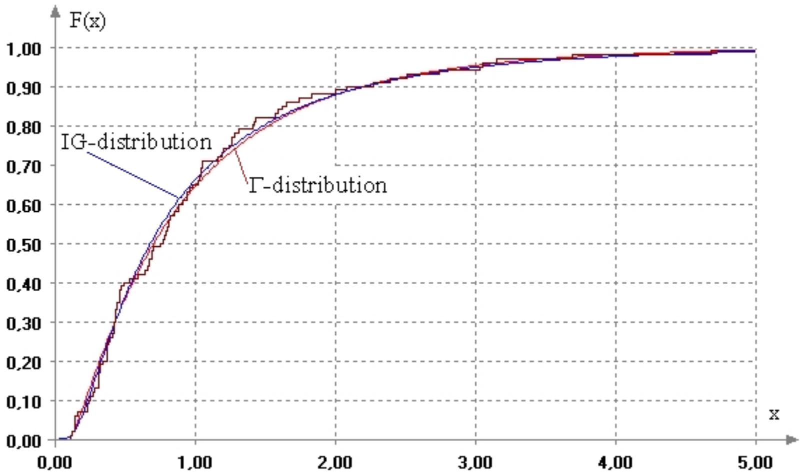

Fig. 4. Empirical and theoretical distributions (IG-distribution and Γ-distribution), calculated using given sample

6. Conclusion

The prepared manual for application of nonparametric goodness-of-fit tests (Ref. [17]) and the technique of interactive simulation of tests statistic distributions provide the correctness of statistical inferences when testing composite and simple hypotheses.

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