Modeling the Goodness-of-Fit Test Based on the Interval Estimation of the Probability Distribution Function

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Abstract. The paper presents a new goodness-of-fit test on the basis of the interval estimate of the probability distribution function. The comparative analysis is carried out for the proposed test and for the Kolmogorov test. The results of the numerical modeling show that the proposed test has greater performance than the Kolmogorov test in specific cases. The analysis of correlation properties of the normalized empirical cumulative distribution function is carried out. As a result, we obtain the equation for calculating the significance level of the proposed goodness-of-fit test.

Keywords: goodness-of-fit, statistical hypothesis, interval estimate, correlation function

1 Introduction

Statistical analysis of experimental data often reduces to testing the hypothesis of the agreement of the empirical probability distribution function with the predicted theoretical one [1–4]. Solutions for this problem usually involve goodness-of-fit (GoF) tests such as Kolmogorov, Cramer-von Mises or χ^2-test. This approach has the following negative features that complicate its implementation 1). There is no a valid algorithm for choosing the type I error probability (significance level or the probability of rejecting the true hypothesis) 2). The probability of the type II error is not considered (the probability of accepting the false hypothesis) 3). Selection of the statistic of a GoF test is determined by the solely technical condition. That is computability of the conditional probability distribution law of this statistic in cases when the evaluated hypothesis is valid. Therefore, the GoF test constructed does not represent the optimal solution for the examined problem 4). Conventional GoF tests represent the difference between the empirical and the theoretical distribution function as just a single number. This sometimes appears to be a too rough estimate of the agreement of two real-valued functions.

The features mentioned can decrease the quality of the decision procedure. For that reason the problem of development of new GoF tests of higher quality remains important and this topic is debated in literature [1–5].

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Papers [6, 7] present a new GoF test on the basis of the interval estimate of the cumulative distribution function (CDF). The proposed method uses a more accurate measure of the difference of the empirical and theoretical distribution functions compared to a single number.

In the current paper we examined the performance of the interval estimate test with a computational experiment. The results show that the proposed method is more efficient than the Kolmogorov test in case when the true distribution has greater variance then the estimated one. In the opposite case both methods show nearly equal efficiency. Correlation properties of the normalized empirical CDF were examined. It is shown that this function can be considered with a good accuracy as a Markov process. On this basis we construct an algorithm for computing the significance level of the proposed GoF test. Analytical solutions are in good agreement with the results of the numerical modeling.

2 The Interval Estimate Goodness-of-Fit Test

Let $F(x) = P(\xi \leq x)$, $-\infty < x < \infty$ be the true CDF of the examined random variable ξ, where $P(\xi \leq x)$ is the probability of $\xi \leq x$. We represent the measurements of ξ by a sample $x_1, \ldots, x_n$ of the size n. The empirical CDF of a sample (the point estimate of the function F) is defined as $\hat{F}(x) = \nu(x_i \leq x)/n$, where $\nu(x_i \leq x)$ is the number of elements x_i such as $x_i \leq x$. The random variable $\nu(x_i \leq x)$ has the binomial probability distribution: $P(\nu = k) = C_n^k p^k q^{n-k}$, $k = 0, 1, \ldots, n$, where C_n^k is the number of k-combinations from a set of size n, $p = P(\xi \leq x) = F(x)$ and $q = 1-p$. Let $\mathbf{M}$, $\mathbf{D}$ be the operators of mathematical expectation and dispersion, respectively. Thus, $\mathbf{M}\nu = np$, $\mathbf{D}\nu = npq$, $\mathbf{M}\hat{F}(x) = F(x)$ and $\mathbf{D}\hat{F}(x) = F(x)[1 - F(x)]/n$. If the probability p is constant and $0 < p < 1$ then, according to the local Moivre-Laplace theorem, the binomial distribution converges to the normal distribution as $n \to \infty$. Therefore, we may assume that for $n \gg 1$ the value

$$\eta(x) = \frac{\left[\hat{F}(x) - F(x)\right]\sqrt{n}}{\sqrt{F(x)\left[1 - F(x)\right]}} \tag{1}$$

is normally distributed with zero expected value and unit variance.

In the paper [6] the Moivre-Laplace asymptotic is used to construct an interval estimate of the function $F(x)$ as a confidence interval $[z_1, z_2]$ with a given confidence factor $1-\alpha$ (we also use the α symbol to denote the significance level of the Kolmogorov test). The boundaries $[z_1, z_2]$ of the confidence interval are defined by the condition: $P(|\eta| \leq \varepsilon) = 1-\alpha$, where ε is the solution to the equation $\Phi(\varepsilon) = 1-\alpha/2$ and $\Phi(\varepsilon)$ is the probability density function (PDF) of the normally distributed random variable with zero mathematical expectation and unit variance. The boundaries $[z_1, z_2]$ are obtained as the solutions for the equation $\eta^2 = \varepsilon^2$ for $F(x)$ and represented as follows:

$$z_{2,1} = \frac{2\hat{F}n + \varepsilon^2}{2(n + \varepsilon^2)} \pm \frac{\sqrt{4n\varepsilon^2(1 - \hat{F})\hat{F} + \varepsilon^4}}{2(n + \varepsilon^2)}. \tag{2}$$

Testing a statistical hypothesis H_0 that a function $F_0(x)$ is the true CDF of a random variable ξ reduces to checking the condition $F_0(x) \in [z_1(x), z_2(x)]$. If the condition is true for each $x \in [x_{min}, x_{max}]$ then the hypothesis H_0 is accepted, otherwise it is refused. x_{min} and x_{max} here represent the lowest and the highest values in the sample. The suggested procedure was implemented as an algorithm with 3 inputs: a dataset $(x_1, \ldots, x_n)$, a significance level α and an estimated CDF $F_0(x)$. The functions $\hat{F}$ and $F_0(x)$ are evaluated in N points with the step of Δx over the argument x not grater than $(x_{max} - x_{min})/5n$.

3 The Computational Experiment

Modeling the hypothesis H_0 testing procedure involves the following steps. First, a sample $(x_1 \ldots x_n)$ of the random variable ξ distributed as $F(x)$ is generated. Then the empirical CDF $\widehat{F}(x)$ is calculated and the hypothesis H_0 is tested using the Kolmogorov test and the interval estimate test. This procedure was repeated for m independent samples of the variable ξ and two values were obtained: the frequency of the event "H_0 is accepted" according to the Kolmogorov test – $\nu_1(H_0)$ and according to the interval estimate test – $\nu_2(H_0)$. The frequency ν here means the ratio of the number of occurrences of H_0 to the number of samples m.

The computational experiment was conducted for the following series of values of the confidence factor α: 0.0002, 0.0006, 0.001, 0.002, 0.006, 0.02, 0.06, 0.2, 0.4 and for six hypotheses H_L, H_0, H_1, H_2, H_3, H_4, one of which is valid. The hypotheses $H_0, \ldots, H_4$ correspond to the following values of the argument β: 1, 1.5, 2, 2.5, 3 of a family of distributions [2] with the PDF:

$$f(x) = c \cdot \exp\left[-\left(\frac{|x|}{\gamma}\right)^{\beta}\right], \tag{3}$$

where the arguments γ and c are determined by the condition of the equivalence of the variance to 1 and by the normalization condition.

Two instances of true hypothesis were examined: H_L – ξ is distributed by the Laplace law with zero expectation, variance equals to 1.65 and $H_G - \xi$ has the normal distribution (corresponds to $\beta = 2$ for the distribution (2)). The variance of the Laplace distribution is obtained as the minimum of the value $\int_{-\infty}^{\infty} |f_L(x) - f_G(x)|\, dx$, where f_L is the PDF of the Laplace distribution and f_G is the PDF of the normally distributed random variable. The size n of each sample and the number of samples m were set to 100. The results of the computing of $\nu_1(H_i)$ and $\nu_2(H_i)$ are represented in the table 1-A for the correct hypothesis H_L and in the table 1-B for the correct hypothesis H_G.

A GoF test performance can be evaluated by the following variable: $\Delta = \sum_{i=0}^{4} |\nu(H) - \nu(H_i)|/5$, where H is the correct hypothesis. As we can see from the table 1-A, the maximum value of Δ for the interval estimate test is equals to 0.728 with the significance level $\alpha = 0.0006$. For the Kolmogorov test the maximum is $\Delta = 0.226$ with $\alpha = 0.4$. Therefore, in this case interval estimate test provides more reliable results compared to the Kolmogorov test. In the table 1-B we need to exclude the frequency $\nu(H_2)$ for calculating Δ correctly, because the hypothesis H_2 is equivalent to

Table 1. The frequencies ν_1 and ν_2 for the correct hypothesis H_L (Laplace distribution) – A and H_G (Gaussian distribution) – B

A

α	H_L	H_0	H_1	H_2	H_3	H_4
Kolmogorov test						
0.0002	1	1	1	1	1	1
0.0006	1	0.99	1	1	1	1
0.001	1	0.99	1	0.99	0.99	1
0.002	1	1	0.99	1	1	0.97
0.006	0.99	0.96	0.98	0.99	1	0.98
0.02	0.97	0.94	1	0.97	0.98	0.98
0.06	0.95	0.91	0.94	0.94	0.93	0.9
0.2	0.84	0.56	0.76	0.7	0.67	0.59
0.4	0.63	0.33	0.53	0.55	0.33	0.28
Interval estimate test						
0.0002	0.75	0.29	0.04	0.03	0	0
0.0006	0.78	0.15	0.07	0.04	0	0
0.001	0.75	0.18	0.05	0.03	0.01	0
0.002	0.77	0.19	0.09	0.02	0	0.01
0.006	0.66	0.14	0.02	0.01	0	0.01
0.02	0.49	0.05	0.02	0	0	0
0.06	0.2	0.01	0.01	0	0	0
0.2	0	0	0	0	0	0
0.4	0	0	0	0	0	0

B

α	H_G	H_0	H_1	H_2	H_3	H_4
Kolmogorov test						
0.0002	1	1	1	1	1	1
0.0006	1	1	1	1	1	1
0.001	1	0.99	1	1	1	1
0.002	0.99	0.99	0.99	1	1	1
0.006	0.99	0.96	1	1	0.99	1
0.02	0.99	0.78	0.98	0.96	0.99	0.97
0.06	0.96	0.71	0.93	0.97	0.93	0.94
0.2	0.8	0.41	0.85	0.84	0.82	0.78
0.4	0.64	0.13	0.54	0.71	0.57	0.5
Interval estimate test						
0.0002	0.81	0.74	0.96	0.86	0.59	0.38
0.0006	0.83	0.77	0.91	0.79	0.67	0.54
0.001	0.86	0.7	0.95	0.8	0.57	0.41
0.002	0.72	0.55	0.83	0.76	0.46	0.31
0.006	0.68	0.38	0.72	0.56	0.41	0.31
0.02	0.48	0.27	0.54	0.37	0.26	0.16
0.06	0.12	0.03	0.24	0.26	0.12	0.07
0.2	0.02	0	0	0.02	0	0
0.4	0	0	0	0	0	0

the true hypothesis H_G. Here for the Kolmogorov test the maximum $\Delta = 0.205$ with $\alpha = 0.4$ and the interval estimate test shows the maximum $\Delta = 0.247$ with $\alpha = 0.001$. Thus, we may assume that if the true hypothesis is H_G, both algorithms are nearly equal in performance. It should also be mentioned that the proposed method has better performance only on small sampling sizes, because with the increase of a sampling size the error of any conventional GoF test asymptotically converges to zero.

4 Covariance of the Empirical Distribution Function

A random function of a real argument is called a random process in literature. According to this $\hat{F}(x)$, $\eta(x)$ are random processes. To calculate the significance level α_0 of the GoF test constructed on the basis of the interval estimate, we define the covariance of the empirical CDF:

$$K(x, x+u) = \mathbf{M}\left[\hat{F}(x) - F(x)\right]\left[\hat{F}(x+u) - F(x+u)\right] =$$
$$= \mathbf{M}\hat{F}(x)\hat{F}(x+u) - F(x)F(x+u). \quad (4)$$

If $u \geq 0$, then we can assume

$$r(x, x+u) = \mathbf{M}\hat{F}(x)\hat{F}(x+u) = \mathbf{M}\hat{F}(x)\left\{\hat{F}(x) + \left[\hat{F}(x+u) - \hat{F}(x)\right]\right\}. \quad (5)$$

We consider that $\hat{F}(x)$ and $\hat{F}(x+u)-\hat{F}(x)$ are independent random variables. This statement holds true if the value of the argument x is sufficiently small, such as $F(x) \leq 0.25$. Here $\hat{F}(x)$ is defined with a relatively small number $\nu(x_i \leq x)$ of sample elements such that $x_i \in (-\infty, x]$. Significant uncertainty remains in regard to the number of sample elements $\nu(x < x_i \leq x+u)$ which define the value $\hat{F}(x+u)-\hat{F}(x)$ and have to fit into the interval $(x, x+u]$. With the increase of x, e.g. if $F(x) > 0.5$, this uncertainty decreases and random values $\hat{F}(x)$ and $\hat{F}(x+u)-\hat{F}(x)$ become significantly correlated.

Let us show that for small arguments x and $x+u$, $u > 0$, the random variables under study can be assumed independent. Let the event $A = \{\nu(x_i \leq x) = n_1\}$, $B = \{\nu(x < x_i \leq x+u) = n_2\}$ and $C = \{\nu(x_i > x+u) = n_3\}$. The sample size is $n = n_1 + n_2 + n_3$. We denote the probabilities $p_1 = P(\xi \leq x)$, $p_2 = P(x < \xi \leq x+u)$ and $p_3 = P(\xi > x+u)$. The probability $P(B)$ of the event B is described by the binomial distribution:

$$P(B) = C_n^{n_2} p_2^{n_2} (1-p_2)^{n-n_2},\ n_2 = 0, 1, \ldots, n. \tag{6}$$

Similarly the conditional probability $P(B/A)$ of the event B given that A has occurred:

$$P(B/A) = C_{n-n_1}^{n_2} p_2^{n_2} (1-p_2)^{n-n_1-n_2},\ n_2 = 0, 1, \ldots, n-n_1, \tag{7}$$

From the equations (6), (7) we obtain:

$$V = \frac{P(B)}{P(B/A)} = \frac{n!(n-n_1-n_2)!}{(n-n_2)!(n-n_1)!}(1-p_2)^{n_1} \tag{8}$$

Small values of x and $x+u$ correspond to the conditions $n_1 << n$, $n_2 << n$, $n_1 + n_2 << n$ and the factorial asymptotic can be approximated with a good accuracy by $n! \approx \sqrt{2\pi n} n^n e^{-n}$. Thus, we can substitute the factorials in (8) with the approximate expressions and calculate $\ln V$. In the expression obtained we expand the function $ln(1+y)$ in a series about the parameter y to order y^2. Here we consider that the ratios n_1/n, n_2/n, $(n_1+n_2)/n$ and the value p_2 are small parameters. After rather simple transformations we obtain

$$\ln V \approx n_1 \left(\frac{n_2}{n} - p_2 \right). \tag{9}$$

The value n_2/n converges in probability to p_2 as $n \to \infty$. Therefore, if n is finite and n_1, n_2 are small, the value $\ln V \approx 0$ compared to n. Hence, $P(B) \approx P(B/A)$ and the events A and B can be considered independent.

Assuming the variables independence in (5) we obtain

$$r(x, x+u) = \mathbf{M}\hat{F}^2(x) + F(x)\left[F(x+u) - F\right],\ u \geq 0. \tag{10}$$

Considering that $\mathbf{M}\hat{F}(x) = \mathbf{D}\hat{F} + F^2(x)$, thus

$$r(x, x+u) = \mathbf{D}\hat{F}(x) + F(x)F(x+u),\ u \geq 0. \tag{11}$$

Similarly for $u < 0$ we find

$$r(x, x+u) = \mathbf{D}\hat{F}(x+u) + F(x+u)F(x),\ u < 0. \tag{12}$$

We use equations (11, 12) to substitute terms in (4):

$$K(x,x+u) = \begin{cases} \mathbf{D}\hat{F}(x), & u \geq 0, \\ \mathbf{D}\hat{F}(x+u), & u < 0. \end{cases} \tag{13}$$

Hence, covariance function of the process $\eta(x)$ is equal to

$$\rho(x,x+u) = \mathbf{M}\eta(x)\eta(x+u) = \begin{cases} \sqrt{\dfrac{F(x)\,[1-F(x)]}{F(x+u)\,[1-F(x+u)]}}, & u \geq 0, \\ \sqrt{\dfrac{F(x+u)\,[1-F(x+u)]}{F(x)\,[1-F(x)]}}, & u < 0. \end{cases} \tag{14}$$

Function ρ simplifies if we substitute x for $y = x + u/2$. Therefore, for any u

$$\rho\left(y - \frac{u}{2}, y + \frac{u}{2}\right) = \sqrt{\frac{F\left(y - \frac{|u|}{2}\right)\left[1 - F\left(y - \frac{|u|}{2}\right)\right]}{F\left(y + \frac{|u|}{2}\right)\left[1 - F\left(y + \frac{|u|}{2}\right)\right]}}. \tag{15}$$

Let u be a small parameter and there is a PDF $f(y) = \partial F(y)/\partial y$. We expand the function F in a series:

$$F\left(y + \frac{|u|}{2})\right) = F(y) + f(y)\frac{|u|}{2} + \ldots \tag{16}$$

and substitute the function in (15) for (16):

$$\rho\left(y - \frac{u}{2}, y + \frac{u}{2}\right) = \sqrt{\frac{1 - a|u|}{1 + a|u|} \cdot \frac{1 + b|u|}{1 - b|u|}} \approx (1 - a|u|)(1 + b|u|) \approx e^{-(a-b)|u|}, \tag{17}$$

where $a = f(y)/2F(y)$, $b = f(y)/2[1 - F(y)]$.

Function (17) represents the covariance function of a random process only when $a - b > 0$ i.e. for such values of y that $F(y) < 0.5$. This statement is in good agreement with the assumption of independence of the random variables $\nu(x_i \leq x)$ and $\nu(x < x_i \leq x + u)$ for relatively small x and u. It should be mentioned that we may obtain the result similar to the formulas (15, 17) for relatively large arguments y such as $F(y) > 0.75$.

To test the obtained relations function ρ is calculated using the equation (15) for the normal distribution ($F = F_G$) and for the Laplace distribution ($F = F_L$). The results obtained can be approximated with a good accuracy by the exponential equation (17) for any values of the parameter y in the set $\{y : F(y) < 0.4\}$ and $|u| < y$.

Equations (15, 17) define the covariance function of the process $\eta(x)$ for relatively a small values of the parameter y. We simulate the estimates of the correlation function of the process $\eta(x)$ to obtain the complete representation of its correlation properties. Therefore, we examine two hypotheses: $\eta(x)$ is a second-order stationary process and $\eta(x)$ is a non-stationary process. For each sample $x_1, \ldots, x_n$ we calculate the trajectory of the process $\eta(x)$ for $x \in [-5, 5]$ according to the equation (1). Then we define the sequence $\eta_1, \ldots, \eta_N$ by the sampling of the argument x with the step Δx to calculate the covariance estimate

$$B(k) = \frac{1}{N} \sum_{i=1}^{N-k} \eta_i \eta_{i+k},\ k = 0, 1, \ldots, N/2. \tag{18}$$

To improve the accuracy we find the average covariance estimation $B_0(k)$ for m samples. Minimization with respect to the parameter λ:

$$\sum_{k=0}^{N/2} \left[B_0(k) - e^{-\lambda k}\right]^2 \to \min_{\lambda} \tag{19}$$

defines an optimal value of λ for the approximation of the estimate $B_0(k)$ by the function $e^{-\lambda k}$. These results allow us to assume that the covariance function of the random process $\eta(x)$ has a form of an exponent. For example if $n = 50$ and $m = 10^3$, then the average deviation $\left|B_0(k) - e^{-\lambda k}\right|$ equals to 0.007. In this case the optimal value of the parameter $\lambda \approx 0.8\Delta x$.

Assuming that the process $\eta(x)$ is non-stationary we define its covariance estimate as:

$$B(i, k) = \frac{1}{m} \sum_{l=1}^{m} \eta_i^{(l)} \eta_{i+k}^{(l)},\ i = 1, \ldots, N - k, \tag{20}$$

where $\eta_1^{(l)}, \ldots, \eta_N^{(l)}$ is the array of values of the process $\eta(x)$ and l is the index of the corresponding sample. If $\eta(x)$ is a stationary process, then for the given k the function $B(i, k)$ is a constant value within the error limits for all $i = 1, \ldots, N - k$. To check this property we evaluate function $B(i, k)$ for given value $k\Delta x$. This value equals to 0, 0.01, 0.1, 0.2 and 0.5 times the length of the interval $[-5, 5]$, which is the domain of $\eta(x)$. The process $\eta(x)$ has a zero mathematical expectation and a unit variance. Therefore, as it is expected, $B(i, k)$ remains a constant for small values of $k\Delta x$ (i.e. 0 and 0.01) and for the value of 0.5, which is relatively large. For $k\Delta x = 0.1$ we observe the maximum deviation of $B(i, k)$ from a constant approximately by 0.1 near the middle value $i = (N - k)/2$. Hence, as a first approximation, the random process $\eta(x)$ can be considered a second-order stationary process with an exponential correlation function.

5 Significance Level of the Goodness-of-Fit Test

If a random process $\eta(x)$ with a zero mathematical expectation and a unit variance is Markov, normal and stationary, its correlation function has the following form $\rho(u) = e^{-\lambda|u|}$. This result is known in literature as the Doob's theorem. It is not difficult to derive, by analyzing the proof of that theorem, that if a random process $\eta(x)$ is normal, stationary and have a correlation function of the form $\rho(u) = e^{-\lambda|u|}$, then this process is Markov. Thus, the significance level evaluation problem for the proposed GoF test reduces to calculating the probability of hitting the boundaries of the interval $[-\varepsilon, \varepsilon]$

of the normal stationary Markov process $\eta(x)$. Let p_0 be the probability of accepting the true hypothesis. Thus,

$$p_0 = P\left[\bigcap_{i=1}^{N}(|\eta_i| \le \varepsilon)\right] = \int_{-\varepsilon}^{\varepsilon} \ldots \int_{-\varepsilon}^{\varepsilon} f_N(y_1, \ldots, y_N) dy_1, \ldots, dy_N, \tag{21}$$

where $\bigcap$ is the set intersection operation, f_N is the joint PDF of the normal random variables $\eta_1, \ldots, \eta_N$.

Numerical evaluation of the equation (21) is not possible due to the high integral multiplicity. If we consider all random variables $\eta_1, \ldots, \eta_N$ mutually independent, then it follows from (21) that $p_0 = (1 - \alpha)^N$. The numerical simulation results show that an error of approximately 10% occurs for values near the optimal $\alpha \approx 0.001$.

Considering the statistical correlation between the elements of the Markov chain $\eta_1, \ldots, \eta_N$ allows us to reduce the calculation error. For this purpose we examine the joint PDF of variables η_i and η_{i+1}:

$$f_2(v_1, v_2) = \frac{1}{2\pi\sqrt{1-\rho^2}} \exp\left[-\frac{v_1^2 + v_2^2 - 2\rho v_1 v_2}{2(1-\rho^2)}\right], \tag{22}$$

and calculate the probability

$$Q = P(|\eta_i| \le \varepsilon \bigcap |\eta_{i+1}| \le \varepsilon) = \int_{-\varepsilon}^{\varepsilon}\int_{-\varepsilon}^{\varepsilon} f_2(v_1, v_2) dv_1 dv_2. \tag{23}$$

Random events $|\eta_i| \le \varepsilon \bigcap |\eta_{i+1}| \le \varepsilon$ for $i = 1, 4, 7, \ldots$ are statistically independent as $\eta(x)$ is a Markov process. Therefore, approximately $p_0 = Q^{N/3}$. Using this formula for calculation reduces the error to the order of 4-5%. Thus, the significance level of the GoF test based on the interval estimate is defined by the equation $\alpha_0 = 1 - Q^{N/3}$.

Conclusion

The results obtained show that GoF test on the basis of the interval estimate is significantly more efficient then Kolmogorov test if the true distribution function has grater variance than the hypothetical one. Otherwise the advantage of the proposed test is insignificant. It is shown that normalized empirical CDF is similar to a Markov process on the statistical properties. We yield an equation for approximate calculation of the significance level of the proposed GoF test.

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