ERRORS WHEN USING NONPARAMETRIC
FITTING CRITERIA

B. Yu. Lemeshko   UDC 519.25

It is shown that the mistakes most frequently made when utilizing nonparametric fitting criteria of the Kolmogorov and ω^2 and Ω^2 Mises type are associated with the use of classical results for testing complex hypotheses or with undervaluing the factors influencing the distributions of the statistics of the criteria.
Key words: *nonparametric fitting criteria, testing complex hypotheses.*

In [1] there was noted a number of mistakes most frequently made when utilizing fitting criteria of the χ^2 type. The implementation of recommendations on standardization [2] will promote the correct use of these criteria in applications. At the same time, recommendations on standardization [3] were introduced into force by Gosstandart Rossii (State Standards Committee of Russia) regulating the use of nonparametric fitting criteria of the Kolmogorov, ω^2 Mises (Kramer–Mises–Smirnov), and Ω^2 Mises (Anderson–Darling) types.

Unfortunately, the practice of using nonparametric fitting criteria abounds in many examples of their incorrect use, especially in literature sources of an educational textbook nature. The most typical mistakes involve the use of classical results which are valid when testing simple hypotheses for situations corresponding to the testing of complex hypotheses. The aim of the present work is to indicate to practitioners which factors influence the correctness of statistical conclusions when using nonparametric fitting criteria in applications and what is the degree of their possible influence on the decision made.

When using fitting criteria, we have a simple tested hypothesis of the form H_0: $F(x) = F_0(x, \theta)$ if $F_0(x, \theta)$ is a known probability distribution function with which one is testing the fitting of an observed sample of independent identically distributed quantities $x_1, x_2, ..., x_n$ while θ is the known value of a parameter (scalar or vector). We also have, for example, a complex tested hypothesis of the form H_0: $F(x) \in \{F_0(x, \theta), \theta \in \Theta\}$, if $F_0(x, \theta)$ is a probability distribution function of known form but with an unknown value of the parameter θ which belongs to Θ parameter space. During the testing of the complex hypothesis, we calculate an estimate $\hat{\theta}$ of the parameter for this same sample. It is evident that when the results of the measurements are processed one will frequently encounter the problem of testing complex hypotheses: one first estimates parameters of the model from the sample in order better to adjust it to the observed data and then to test the adequacy of the model.

Nonparametric Criteria When Testing Simple Hypotheses. In criteria of the Kolmogorov type, one employs as the distance between the empirical and theoretical laws the quantity

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

where $F_n(x)$ is the empirical distribution function; $F(x, \theta)$ is the theoretical distribution function; n is the sampling volume. When testing hypotheses, one normally uses statistics of the form [4]

$$S_k = \frac{6nD_n + 1}{6\sqrt{n}},$$

where $D_n = \max(D_n^+, D_n^-)$,

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

n is the sampling volume; $x_1, x_2, ..., x_n$ are the sampling values ordered by size; $F(x, \theta)$ is the function of the distribution law with which the fitting is being tested. The distribution of the quantity S_k for a simple hypothesis in the limit obeys the Kolmogorov law $K(S)$ [4].

In criteria of the ω^2 type, the distance between the hypothetical and empirical distributions is considered in quadratic metric

$$\int_{-\infty}^{\infty} \{E[F_n(x)] - F(x)\}^2 \psi(F(x)) \, dF(x),$$

where $E[\cdot]$ is the mathematical expectation operator.

In criteria of the ω^2 Mises type, when choosing $\psi(t) \equiv 1$, Kramer–Mises–Smirnov statistics is used in the form

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

which for a simple hypothesis obeys the distribution $a1(S)$ [4].

In criteria of the Ω^2 Mises type, when choosing $\psi(t) \equiv 1/t(1-t)$, the Anderson–Darling statistics is of the form

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

In the limit for simple tested hypotheses, this statistics obeys the distribution $a2(S)$ [4].

In the process of testing the fitting using a sample, we calculate the value S^* of the statistics of the criterion used. A decision as to whether to accept or reject a hypothesis H_0 is made on the basis of an arbitrary distribution $G(S | H_0)$ of the statistics S. In the case of the criteria considered and of simple hypotheses this corresponds respectively to $K(S)$, $a1(S)$, and $a2(S)$. If the probability

$$P\{S > S^*\} = \int_{S^*}^{+\infty} g(s | H_0) \, ds$$

is sufficiently large, at least $P\{S > S^*\} > \alpha$, where $g(s | H_0)$ is the arbitrary density and α is the specified significance level (the probability of an error of the first kind, to reject a valid hypothesis H_0), then it is customary to consider that there is no basis for rejecting the hypothesis H_0. In practice, it was customary to compare the calculated value of the statistics S^* with the critical value S_α for a given value of α, the hypothesis H_0 being rejected if $S^* > S_\alpha$. The critical value S_α defined by the equation

$$\alpha = \int_{S_\alpha}^{\infty} g(s | H_0) \, ds$$

is usually taken from the appropriate statistical table. It should be emphasized that making a decision on the basis of testing the inequality $S^* > S_\alpha$ is less preferable, it is less informative.

In the case of simple hypotheses, the limiting distributions of the statistics of the nonparametric criteria considered are independent of the form of the observed distribution law and its parameters. One says that these criteria are "free from the distribution." This advantage has predetermined their widespread use in applications.

Nonparametric Criteria When Testing Complex Hypotheses. When testing complex hypotheses, when the parameters of the observed law $F(x, \theta)$ are being estimated using the same sample, the nonparametric fitting criteria lose their "freedom from the distribution" [5].

The differences between the limiting distributions of the same statistics when testing simple and complex hypotheses are so great that it is absolutely unacceptable to ignore this fact. Warnings about the incorrectness of using classical results when testing complex hypotheses have been made more than once [6–8].

During investigations of the limiting distributions of nonparametric fitting criteria, when testing complex hypotheses, a number of approaches were also adopted to the testing procedure itself. For a sufficiently large sampling volume, the procedure can be divided into two parts, the parameters being estimated using one of them and the fitting being tested using the other [9]. Unfortunately, in practice we are often dealing with samples of quite limited volume and so such an approach rarely proves to be acceptable. The quality of the parameter estimates is considerably inferior and the power of the criteria is reduced, i.e., there is an increase in the probability of errors of the second kind. In certain particular cases, the limiting distributions of the statistics were investigated by analytical methods [10], percentage points of the distributions were constructed by statistical modeling methods [11–14]. For an approximate calculation of "fitting" probabilities of the kind $P(S > S^*)$ (the attainable significance level), formulas were chosen giving quite good approximations for small values of the corresponding probabilities [15–19]. Recommendations [3] were based on the results of investigations [20–28] of distributions of the statistics of nonparametric fitting criteria and on the construction of models of these distributions using a computer procedure for analyzing the laws governing the statistics.

When testing complex hypotheses using an arbitrary distribution law, the statistics $G(S \mid H_0)$ influences the following series of factors determining the "complexity" of the hypothesis [3]: the form of the observed law $F(x, \theta)$ corresponding to the true hypothesis H_0; the type of an estimated parameter and the number of them; in certain situations, the specific value of a parameter (for example, in the case of a gamma distribution); the method used for estimating the parameters [27]. This means that while testing the fitting of an observed sample with the law $F(x, \theta)$, depending on the combination of the above-mentioned factors, we shall be dealing with the testing of different complex hypotheses each of which corresponds to its own (!) limiting distribution of one and the same statistics of the criterion.

Nature of the Dependence on the Form of the Law $F(x, \theta)$. Figure 1 gives the distributions of the statistics of a fitting criterion of the Kolmogorov type when testing a simple hypothesis, a Kolmogorov distribution $K(S)$ and complex hypotheses, when the following laws correspond to the tested hypothesis H_0:

normal law

$$f(x) = \frac{1}{\theta_0 \sqrt{2\pi}} \exp\left[-\frac{(x - \theta_1)^2}{2\theta_0^2} \right];$$

Laplace law

$$f(x) = \frac{1}{2\theta_0} \exp\left(-\left|x - \theta_1\right|/\theta_0\right);$$

Cauchy law

$$f(x) = \frac{\theta_0}{\pi[\theta_0^2 + (x - \theta_1)^2]},$$

and both parameters of the law are estimated using the method of maximum likelihood. The form of the corresponding distributions of the statistics is given in the recommendations [3].
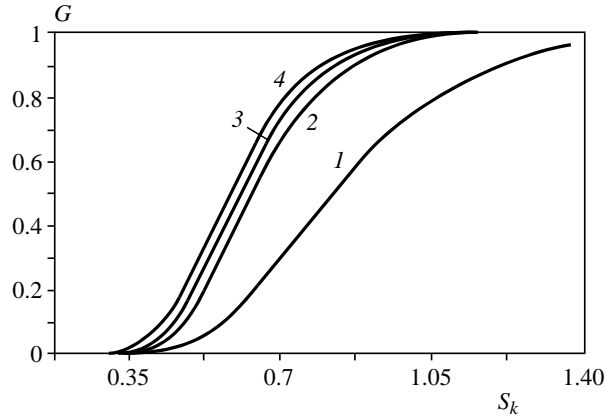
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Fig. 1. Distributions of the statistics of fitting criteria of the Kolmogorov type when testing a simple hypothesis (curve *1*) and complex hypotheses when the tested hypothesis H_0 corresponds to a normal law (curve *3*), a Laplace law (curve *2*), and a Cauchy law (curve *4*), and both parameters of the law are estimated by the method of maximum likelihood.
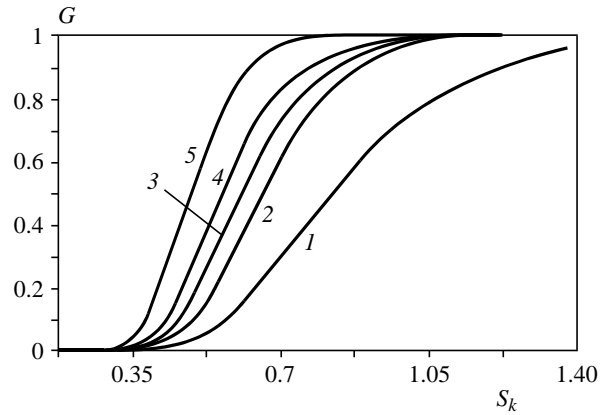

Fig. 2. Distributions of statistics of the Kolmogorov type when testing a simple hypothesis (curve *1*) and complex hypotheses with a Su–Johnson law with the maximum likelihood estimates calculated for one (curve *2*), two (curve *3*), three (curve *4*), and simultaneously all four parameters of the law (curve *5*).

Nature of the Dependence on the Number of Estimated Parameters. The influence of the number of estimated parameters is illustrated in Fig. 2 which shows distributions of statistics of the Kolmogorov type when testing complex hypotheses concerning fitting to a Su–Johnson law

$$f(x) = \frac{\theta_1}{\sqrt{2\pi}\sqrt{(x-\theta_3)^2 + \theta_2^2}} \exp\left\{-\frac{1}{2}\left[\theta_0 + \theta_1 \ln\left\{\frac{x-\theta_3}{\theta_2} + \sqrt{\left(\frac{x-\theta_3}{\theta_2}\right)^2 + 1}\right\}\right]^2\right\}$$

for a number of maximum likelihood estimates of one, two, three, or simultaneously all four parameters of the law. The estimated parameters when testing the corresponding complex hypothesis are indicated in Fig. 2.

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How great is the difference between the distributions of the statistics for the simple and complex hypotheses? Let us assume that when testing the fitting of empirical data to the Su–Johnson distribution the maximum likelihood estimates of all four parameters were calculated and a value of the Kolmogorov statistics of $S_k^* = 0.7$ was obtained. When testing a simple hypothesis, such a value of the statistics would correspond to a probability $P\{S_k > 0.7\} \approx 0.711$ (the hypothesis would have had to be adopted unreservedly) but when testing the given complex hypothesis this same probability scarcely reaches $P\{S_k > 0.7\} \approx 0.032$ (see Fig. 2) and at a significance level of $\alpha = 0.05$ the fitting hypothesis should be rejected.

Nature of the Dependence on the Form of the Estimated Parameter. The distribution of the statistics of nonparametric fitting criteria depends on the form of the estimated parameter. As a rule, the estimation of the displacement parameter when testing a complex hypothesis leads to a more substantial change in the distribution of the statistics, relative to the classical case corresponding to the testing of a simple hypothesis, than does the estimation of the scale parameter or the form parameter of the law. The degree of dependence of the limiting distributions of the statistics on the form of the estimated parameter of the observed law $F(x, \theta)$ is shown in [22].

Nature of the Dependence on the Parameter Values of the Laws. In certain cases when testing complex hypotheses, the distributions of the statistics of nonparametric fitting criteria can depend on the specific parameter value. For example, when testing the hypotheses concerning the gamma distribution

$$f(x) = \frac{1}{\theta_1^{\theta_0} \Gamma(\theta_0)} x^{\theta_0 - 1} \exp(-x/\theta_1),$$

the distributions of the statistics differ considerably for small values of the form parameter θ_0, which must be taken into account, and this practically ceases for $\theta_0 > 5$. Models of the distributions of the statistics of nonparametric criteria when testing complex hypotheses concerning fitting to a gamma distribution and corresponding to different values of θ_0, are given in [3]. However, a gamma distribution is not the only distribution used in applications for which the distributions of the statistics of the criteria depend on the specific parameter values. A similar situation occurs when testing complex hypotheses concerning such laws and distribution families as a Nakagami distribution, beta distribution families of the first and second kind, and an exponential family of distributions. For these cases, the model of the distributions of the statistics of the nonparametric fitting criteria considered have not yet been constructed.

Nature of the Dependence on the Method of Estimating the Parameters. When testing complex hypotheses, the distributions of the statistics of nonparametric fitting criteria are strongly dependent on the estimation method used. By way of an example, Fig. 3 gives distributions of Kolmogorov statistics when testing complex hypotheses concerning the fitting with a normal law when two of its parameters are estimated by the maximum likelihood method and MD estimates obtained by minimizing the Kolmogorov statistics itself are used. As can be seen, the distribution of the statistics is strongly dependent on the form of the estimates used (the estimation method). For example, for an obtained value of the statistics $S_k^* = 0.7$ and a given significance level of $\alpha = 0.05$, in the case when the maximum likelihood estimate is used a normal-law hypothesis should be adopted (see Fig. 3) while it is rejected when using MD estimates of the parameters for the same value of the statistics and the same significance level.

Models of the distributions of the statistics of nonparametric fitting criteria were given in [3] together with tables of percentage points corresponding to the two types of estimate, maximum likelihood and MD estimates. If other methods of estimation are adopted, then it is impossible to use the laws and percentage points of the tables given there. For instance, when calculating estimates using the method of moments the use of the models of the limiting laws corresponding to the use of a maximum likelihood estimate is valid only when the estimates obtained from the method of moments coincide with the maximum likelihood estimate. Such examples are extremely few in number.

Influence of the Accuracy of Estimating Parameters. As was shown above, the method of estimating the parameters (the statistical properties of the estimates) strongly influences the distribution of the statistics of the fitting criteria. Generally speaking, in rare cases estimates of parameters are obtained in the form of certain statistics (functions of samples, prepared formulas). Frequently, estimates are found as a result of implementing a definite iteration process and take the form of certain approximations to the sought solution.
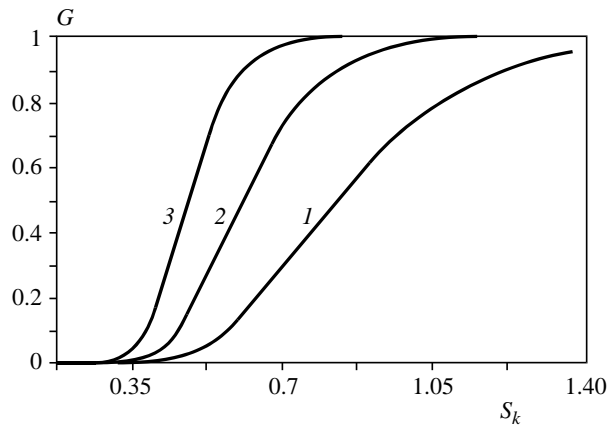
Fig. 3. Distributions of statistics of the Kolmogorov type when testing a simple hypothesis (curve *1*) and complex hypotheses concerning the fitting to a normal law, with the estimation of two of its parameters by the maximum likelihood method (curve *2*) and using MD estimates (curve *3*) obtained by minimizing the statistics itself of the Kolmogorov type.
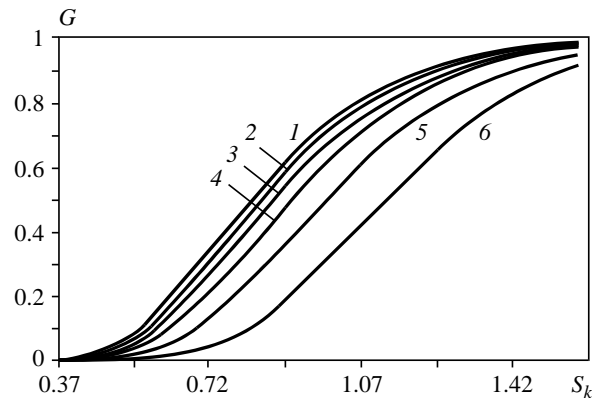

Fig. 4. Distribution function of statistics of the Kolmogorov type for the validity of a simple (curve *1*) tested hypothesis $G(S_k | H_0) = K(S_k)$ and a competing hypothesis $G_n(S_k | H_1)$ for sampling volumes of $n = 100, 300, 500, 1000$, and 2000 observations (respectively curves *2–6*). The hypothesis H_0 corresponds to a normal law, the competing hypothesis H_1 corresponds to a logistical law.

How does the accuracy of calculating the estimates influence the distribution of the statistics of the fitting criterion used? If the asymptotic properties of approximate estimates coincide with those of the accurate estimates, then the distributions of the statistics of the nonparametric fitting criteria will coincide when using both estimates. For instance, so-called single-step estimates [29] which are formed as a first approximation to maximum likelihood estimates calculated using one iteration of the Newton method are quite frequently used in practice. It is shown that such estimates are asymptotically effective and consequently their asymptotic properties coincide with the properties of maximum likelihood estimates. In a case when single-step estimates are used, one can utilize the laws constructed for maximum likelihood estimates [30] as the limiting distributions of the statistics. Thus, whereas the estimating method significantly influences the distribution laws of the fitting criteria statistics, the accuracy of calculating the estimates either fails to reflect on the distributions of the same statistics or reflects on them to a substantially lesser degree.
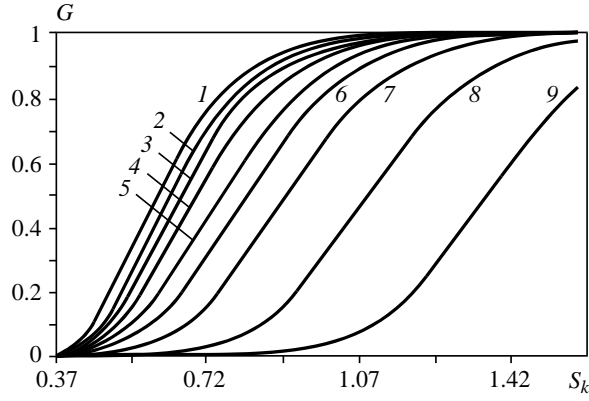
Fig. 5. Distribution function $G(S_k | H_0)$ (curve *1*) and the functions $G_n(S_k | H_1)$ for sampling volumes of $n = 20, 50, 100, 200, 300, 500, 1000$, and 2000 observations (respectively curves *2–9*) when testing a complex hypothesis concerning the fitting to a normal law with the parameters of the law estimated by the maximum likelihood method for the competing hypothesis H_1 corresponding to a logistical law.

Influence of the Sampling Volume on the Distributions of the Statistics. In the majority of sources regarding the use of nonparametric fitting criteria (when testing simple hypotheses), as a rule it is mentioned that the limiting distributions $K(S)$, $a1(S)$, $a2(S)$ for the corresponding criteria can be used for sampling volumes exceeding $n = 50$–100 observations. Generally speaking, when testing both simple and complex hypotheses, the distributions $G(S | H_0)$ of the statistics of the criteria considered are quite close to the limiting distributions (they do not differ greatly) even for sampling volumes of $n = 20$–25 observations [22]. The problems are otherwise.

For small n values, it is difficult to distinguish a pair of close competing hypotheses H_0 and H_1 since their distributions $G(S | H_0)$ and $G(S | H_1)$ turn out to be very close. Any practitioner can remark that for small n values one can equally successfully adopt hypotheses concerning the fitting with a whole series of model laws which differ considerably from each other. The ability of any criteria statistics to distinguish between hypotheses, i.e., their power, increases with an increase in the sampling volume. In the case of testing simple hypotheses, it is problematical to distinguish between two closely similar distribution laws relying on nonparametric fitting criteria. This can be made sufficiently reliable only for large sampling volumes [31]. Figure 4 gives distributions of Kolmogorov statistics when the simple tested hypothesis $G(S_k | H_0) = K(S_k)$ and a competing hypothesis $G_n(S_k | H_1)$ are valid, for sampling volumes of $n = 100, 300, 500, 1000$, and 2000 observations. The tested hypothesis H_0 corresponds to a normal law and the competing hypothesis H_1 corresponds to a logistical law with the density function

$$f(x) = \frac{\pi}{\theta_0 \sqrt{3}} \exp\left\{-\frac{\pi(x - \theta_1)}{\theta_0 \sqrt{3}}\right\} \bigg/ \left[1 + \exp\left\{-\frac{\pi(x - \theta_1)}{\theta_0 \sqrt{3}}\right\}\right]^2 .$$

These two laws are close and, as a rule, are difficult to distinguish using fitting criteria. It follows from Fig. 4 that the specified probability of an error of the first kind (the significance level) is $\alpha = 0.1$, the criterion power $1 - \beta$, where β is the probability of an error of the second kind, is of the order of 0.114 (only!) for $n = 100$, 0.14 for $n = 300$, 0.16 for $n = 500$, 0.235 for $n = 1000$, and 0.38 for $n = 2000$.

Figure 5 shows a similar picture for testing a complex hypothesis concerning the fitting to a normal law with the parameters of the normal law being estimated by the maximum likelihood method for the same competing hypothesis H_1 according to the criterion of the Kolmogorov type. Figure 5 gives the distribution functions $G(S_k | H_0)$ and $G_n(S_k | H_1)$ for sampling volumes of $n = 20, 50, 100, 200, 300, 500, 1000$, and 2000 observations. For the same significance level of $\alpha = 0.1$, the criterion power is found to be considerably larger (by a factor of 2 or 3) and is of the order of 0.134 for

$n = 20$, 0.17 for $n = 50$, 0.23 for $n = 100$, 0.34 for $n = 200$, 0.45 for $n = 300$, 0.64 for $n = 500$, 0.91 for $n = 1000$, and 0.995 for $n = 2000$. This provides evidence that in the case of the testing of complex hypotheses similar hypotheses can differ for moderate sampling volumes.

Characteristic features of the use of fitting criteria when testing complex hypotheses were illustrated using an example of the Kolmogorov type. A similar picture is also characteristic for the distributions of the statistics of other nonparametric criteria [3].

In conclusion, we note that the majority of the errors in using nonparametric fitting criteria which lead to incorrect conclusions are associated with a complete neglect of the fact that when investigators are estimating parameters using sampling they find themselves under the conditions of testing a complex hypothesis. In those rare cases when the investigator is fully aware that one cannot utilize classical results when performing testing of a complex hypothesis, the errors are associated with failing to take into account the variety of the factors which influence the distribution of the statistics of a fitting criterion, and in particular the method of estimation.

When choosing a method of analysis, one should take into account the accuracy of recording the observations. Otherwise this can lead to misunderstandings for the statistical conclusions. When analyzing experimental observations, we are most often dealing with insufficient sampling volumes. However, in certain cases such as for the automated monitoring of various indicators the samples can be of almost any volume but the measurements are then carried out with a limited accuracy. Consequently, in the accumulated sample of observations a limited number of values is taken. The sample is grouped digit-by-digit and the corresponding empirical distribution $F_n(x)$ retains a stepped form for any sampling volume. Because of this, the deviations of $F_n(x)$ from the $F_n(x)$ values used in nonparametric fitting criteria only increase with an increase in the sampling volume, despite the possible agreement between the observed and theoretical laws. In this situation, the testing of a hypothesis as to whether, for instance, a monitored quantity belongs to a normal law inevitably leads to the rejection of the hypothesis being tested. And this is when there can be no pretension to a monitored process. The accuracy of recording the observations should be taken into account when choosing both the method of estimating the parameters and the criterion for testing the hypotheses. In such a situation, it is best to utilize criteria of the χ^2 type.

Thus, by changing the nonparametric fitting criteria of the Kolmogorov, ω^2, and Ω^2 Mises type careful attention should be paid to what hypothesis is being tested, a simple or a complex hypothesis. If it is complex, then factors must be taken into account which influence the "complexity" of the hypothesis (the form of the $F(x, \theta)$ law, the method of estimation, the type of the estimated parameters, the number of them, the significance of the parameter estimate) and one must use the appropriate distribution [3] of the statistics of the criterion used when testing.

The recommendations on standardization [3] embrace by no means a full list of the distribution laws used in applications. In specific problems and applications, specific models of the distribution laws can be used in order to describe the observed random quantities. Naturally, the need arises to test the adequacy of such models. For testing of this kind using fitting criteria, a knowledge is required of the arbitrary statistics distributions $G(S\,|\,H_0)$. It is very problematic to obtain the necessary data analytically (on account of the complexity of solving such problems by analytical methods and of the set of the problems themselves). However, the construction of models of $G(S\,|\,H_0)$ using computer methods of investigation [32] does not raise any fundamental problems. The distributions of statistics and tables of percentage points given in the recommendations of [3] were constructed on the basis of these methods.

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