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ON GOODNESS-OF-FIT TESTING UNDER SMALL SAMPLE SIZE

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Dedicated to Lubomír Kubáček on the occasion of his 70th birthday

ABSTRACT. The paper presents an alternative goodness-of-fit test for discrete distributions based on a sample from multinomial distribution. The given computational procedure is useful for deriving the critical region and the size of the test for small samples from the multinomial distribution. In the special case of testing for binomial distribution we compute the size of the (asymptotic) χ^2 goodness-of-fit test and compare the critical regions for the same significance level of those two tests. Finally, the properties of the empirical distribution function of the χ^2 goodness-of-fit test statistic are investigated for small samples.

1. Introduction

Goodness-of-fit testing concerning the sample distribution resulting from observations and a corresponding hypothesized theoretical distribution arises in almost all scientific, technical, economical, and other investigations, see, e.g., Cramér (1946), Cressie and Read (1984), Kocherlatoka and Kocherlatoka (1986), Zelterman (1987), and Pederson and Johnson (1990). The χ^2 goodness-of-fit test introduced by Pearson (1900) is one of the most commonly used statistical tools for testing fit of distributions.

In this paper we give an alternative goodness-of-fit test for discrete distributions based on a sample from multinomial distribution. The given computational procedure is useful for deriving the critical region and the size of the test for small samples from the multinomial distribution. Then, in the special case of testing for binomial distribution, we compute the size of the traditional χ^2 goodness-of-fit test and compare the critical regions of these tests. Finally, the properties

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of the empirical distribution function of the χ^2 goodness-of-fit test statistic are investigated for small samples.

Consider the following situation. Let $y_1, y_2, \dots, y_N$ be the observed values. Suppose that they form a random sample from a discrete nonnegative integer valued variable Y. Partition its range into a finite number of mutually disjoint sets $S_1, \dots, S_k$, i.e., $\bigcup_{i=1}^{k} S_i = \mathbb{N}_0$, $\mathbb{N}_0 = \{0, 1, 2, \dots\}$ and $S_i \cap S_j = \emptyset$ for all $i \neq j$. Let X_i, $i = 1, \dots, k$, denote the random variable defined as the number of observed values in S_i. Then, based on the sample $y_1, y_2, \dots, y_N$, we get the vector $(n_1, n_2, \dots, n_k)$, that is the realization of the random vector $X = (X_1, \dots, X_k)$. The joint distribution of X is multinomial with parameters $\pi_1, \dots, \pi_k$ and N, i.e.,

$$P\{X_1 = n_1, \dots, X_k = n_k\} = \frac{N!}{n_1! \dots n_k!} \pi_1^{n_1} \pi_2^{n_2} \dots \pi_k^{n_k}, \tag{1}$$

where $n_i \in \{0, 1, \dots, N\}$, $i = 1, \dots, k$, and $n_1 + n_2 + \dots + n_k = N$. The parameters $\pi_1, \dots, \pi_k$ are the theoretical probabilities

$$\pi_i = P\{Y \in S_i\}, \qquad i = 1, \dots, k, \tag{2}$$

which are assumed to be positive. The problem to be solved can be formulated as follows: to decide if the obtained sample is a sample from a population determined by a given probability mass function (pmf) $\{P_0^*(\theta), P_1^*(\theta), \dots\}$ which depends on unknown parameters $\theta = (\theta_1, \dots, \theta_m) \in \Theta$, where Θ denotes the corresponding parameter space, i.e., whether the pmf of Y is $\{P_0^*(\theta), P_1^*(\theta), \dots\}$, $\theta \in \Theta$. If we denote $P_i(\theta) = \sum_{j \in S_i} P_j^*(\theta)$, then the null hypothesis to be tested is that there exists a parameter $\theta \in \Theta$ such that

$$H_0: \pi_i = P_i(\theta), \qquad i = 1, \dots, k. \tag{3}$$

The well-known standard solution to the test of H_0 is based on the fact that for the ML estimator $\hat{\theta}(X_1, \dots, X_k)$ of θ under regularity assumptions on $P_i(\theta)$ the χ^2-statistic

$$\chi^2 = \sum_{i=1}^{k} \frac{\left(X_i - NP_i(\hat{\theta})\right)^2}{NP_i(\hat{\theta})} \tag{4}$$

has asymptotically central χ^2_{k-m-1} distribution, m is the number of estimated parameters, see, e.g., Cramér (1946).

In case of small samples, to determine the actual distribution of the proposed test statistic may be a serious problem. The natural questions arise: "When is the asymptotic distribution (practically) achieved?"; "What to do with sparse S_i?"; "What is the size of the test for finite sample size N?". For more details see, e.g., Altmann (1994), where the above mentioned problems are met in linguistics.

In this paper we address the following problems:

(1) To suggest an alternative method for testing H_0 given in 3 that is based on exact probability statements valid for small samples.

(2) To compare the properties of the χ^2 goodness-of-fit test and the proposed test mentioned in (i).

(3) To investigate the empirical cumulative distribution function (cdf) of the test statistic (4) and compare it with the cdf of the χ^2_{k-m-1} distribution.

We shall demonstrate mainly (ii) and (iii), the particular case of testing for binomial distribution, in situations with very small sample sizes.

2. An alternative test

If the null hypothesis (3) is true then $X = (X_1, \dots, X_k)$ follows multinomial distribution with parameters $P_1(\theta), \dots, P_k(\theta)$ and N.

Let

$$X = (X_1, \dots, X_k) \tag{5}$$

be the test statistic. For given significance level α, the approximate critical region $W_{\alpha,N}$ for testing H_0 is constructed in the following way:

(1) For every vector $x = (x_1, \dots, x_k)$ of nonnegative integers with $\sum_{i=1}^{k} x_i = N$, compute the value

$$P_{\mathrm{ML}} = \sup_{\theta \in \Theta} \frac{N!}{x_1! \dots x_k!} P_1^{x_1}(\theta) \dots P_k^{x_k}(\theta) \,. \tag{6}$$

(2) Sort the points with respect to their increasing P_{ML} value. Hence, we obtain the sequence of points

$$R_N = \left\{ \left(x_1^{(1)}, \dots, x_k^{(1)}\right), \dots, \left(x_1^{(t)}, \dots, x_k^{(t)}\right) \right\}, \tag{7}$$

where t denotes the total number of different points.

(3) The (approximate) α-critical region $W_{\alpha,N}$ for testing H_0 (for given $\alpha \in (0,1)$) is

$$W_{\alpha,N} = \bigcup_{i=1}^{i_\alpha} \left\{ \left(x_1^{(i)}, \dots, x_k^{(i)}\right) : i = 1, \dots, i_\alpha \right\}, \tag{8}$$

where the critical index $i_\alpha \in \{1,2,\dots,t\}$ is chosen in such a way that

$$\alpha^* = \sup_{\theta\in\Theta} \sum_{s=1}^{i_\alpha} \frac{N!}{x_1^{(s)}!\dots x_k^{(s)}!}\, P_1^{x_1^{(s)}}(\theta)\dots P_k^{x_k^{(s)}}(\theta) \le \alpha$$
$$< \sup_{\theta\in\Theta} \sum_{s=1}^{i_\alpha+1} \frac{N!}{x_1^{(s)}!\dots x_k^{(s)}!}\, P_1^{x_1^{(s)}}(\theta)\dots P_k^{x_k^{(s)}}(\theta)\,. \tag{9}$$

Remark 1. It is easy to see that the size of the test α^* is an approximation of the chosen significance level α, and $\alpha^* \le \alpha$.

Remark 2. For given hypothetical discrete probability distribution (like Poisson, Binomial, Geometric, or other distribution), i.e., for a given class of pmf's $P_\theta = \{P_0^*(\theta),\ P_1^*(\theta), \dots\}$, $\theta\in\Theta$, given N and k, and $S_1,\dots,S_k$, we can according to (c) compute the α-critical region $W_{\alpha,N}$. If the realization $(n_1,\dots,n_k)$ obtained from observed values $(y_1,\dots,y_N)$ belongs to $W_{\alpha,N}$, we reject H_0, i.e., we reject the agreement between the distribution of a set of sample values and the given hypothetical distribution, at the significance level α. The size of the suggested test is α^*.

EXAMPLE 1. Let $y_1,\dots,y_N$ be the observed values, $y_i\in\{0,1,2\}$. Consider the null hypothesis H_0: *The sample comes from binomial distribution $Binom(2,\theta)$.* Thus $P_\theta = \{P_0^*(\theta),\ P_1^*(\theta),\ P_2^*(\theta)\}$, $\Theta=(0,1)$, $k=3$, $S_i=\{i+1\}$, $i=0,1,2$, and

$$P_i(\theta) = \binom{2}{i-1}\theta^{i-1}(1-\theta)^{3-i}, \qquad i=1,2,3\,. \tag{10}$$

For every triple $x=(x_1,x_2,x_3)$ of integers with $x_1+x_2+x_3=N$, $x_i\ge 0$, $i=1,2,3$ compute

$$P_{\mathrm{ML}} = \sup_{0\le\theta\le1} \frac{N!}{x_1!\,x_2!\,x_3!}\, P_1^{x_1}(\theta)P_2^{x_2}(\theta)P_3^{x_3}(\theta) \tag{11}$$

and sort all these points according to their increasing values (6). Further, for every $i\in\{1,2,\dots,t\}$ calculate

$$P_{\mathrm{cum}}(i) = \sup_{0\le\theta\le1} \sum_{s=1}^{i} \frac{N!}{x_1^{(s)}!\,x_2^{(s)}!\,x_3^{(s)}!}\, P_1^{x_1^{(s)}}(\theta)P_2^{x_2^{(s)}}(\theta)P_3^{x_3^{(s)}}(\theta)\,. \tag{12}$$

If $N=10$ then t, the number of all possible points x, equals to 66. The results for $N=10$ are summarized in the Table 1.

According to (c), for $N=10$ and $\alpha=0.1$, we obtain

$$P_{\mathrm{cum}}(24) = \sup_{0\le\theta\le1} \sum_{s=1}^{24} \frac{10!}{x_1^{(s)}!\,x_2^{(s)}!\,x_3^{(s)}!}\, P_1^{x_1^{(s)}}(\theta)P_2^{x_2^{(s)}}(\theta)P_3^{x_3^{(s)}}(\theta) = 0.0963\,,$$

$$P_{\mathrm{cum}}(25) = \sup_{0\le\theta\le1} \sum_{s=1}^{25} \frac{10!}{x_1^{(s)}!\,x_2^{(s)}!\,x_3^{(s)}!}\, P_1^{x_1^{(s)}}(\theta)P_2^{x_2^{(s)}}(\theta)P_3^{x_3^{(s)}}(\theta) = 0.1011\,.$$

i	$x^{(i)}$	P_{ML}	P_{cum}	i	$x^{(i)}$	P_{ML}	P_{cum}
1	$(5,0,5)$	0.0002	0.0002	34	$(5,3,2)$	0.0480	0.2381
2	$(4,0,6)$	0.0003	0.0004	35	$(1,7,2)$	0.0486	0.2820
3	$(6,0,4)$	0.0003	0.0006	36	$(2,7,1)$	0.0486	0.3260
4	$(3,0,7)$	0.0006	0.0008	37	$(3,4,3)$	0.0641	0.3901
5	$(7,0,3)$	0.0006	0.0009	38	$(1,2,7)$	0.0649	0.3914
6	$(0,10,0)$	0.0010	0.0018	39	$(7,2,1)$	0.0649	0.3928
7	$(2,0,8)$	0.0020	0.0019	40	$(0,6,4)$	0.0665	0.4056
8	$(8,0,2)$	0.0020	0.0019	41	$(4,6,0)$	0.0665	0.4184
9	$(4,1,5)$	0.0027	0.0043	42	$(2,4,4)$	0.0719	0.4665
10	$(5,1,4)$	0.0027	0.0067	43	$(4,4,2)$	0.0719	0.5146
11	$(3,1,6)$	0.0040	0.0083	44	$(1,6,3)$	0.0767	0.5658
12	$(6,1,3)$	0.0040	0.0099	45	$(3,6,1)$	0.0767	0.6171
13	$(0,9,1)$	0.0054	0.0148	46	$(2,6,2)$	0.0769	0.6940
14	$(1,9,0)$	0.0054	0.0197	47	$(2,5,3)$	0.0850	0.7709
15	$(2,1,7)$	0.0094	0.0204	48	$(3,5,2)$	0.0850	0.8478
16	$(7,1,2)$	0.0094	0.0211	49	$(1,3,6)$	0.0877	0.8542
17	$(4,2,4)$	0.0120	0.0331	50	$(6,3,1)$	0.0877	0.8606
18	$(3,2,5)$	0.0144	0.0427	51	$(1,5,4)$	0.0959	0.8991
19	$(5,2,3)$	0.0144	0.0523	52	$(4,5,1)$	0.0959	0.9375
20	$(1,0,9)$	0.0150	0.0523	53	$(1,4,5)$	0.0997	0.9568
21	$(9,0,1)$	0.0150	0.0523	54	$(5,4,1)$	0.0997	0.9760
22	$(0,8,2)$	0.0164	0.0633	55	$(0,5,5)$	0.1052	0.9837
23	$(2,8,0)$	0.0164	0.0743	56	$(5,5,0)$	0.1052	0.9914
24	$(1,8,1)$	0.0220	0.0963	57	$(0,4,6)$	0.1513	0.9946
25	$(2,2,6)$	0.0249	0.1011	58	$(6,4,0)$	0.1513	0.9978
26	$(6,2,2)$	0.0249	0.1059	59	$(0,3,7)$	0.2045	0.9987
27	$(3,3,4)$	0.0354	0.1379	60	$(7,3,0)$	0.2045	0.9996
28	$(4,3,3)$	0.0354	0.1700	61	$(0,2,8)$	0.2702	0.9998
29	$(0,7,3)$	0.0365	0.1846	62	$(8,2,0)$	0.2702	1.0000
30	$(3,7,0)$	0.0365	0.1993	63	$(0,1,9)$	0.3774	1.0000
31	$(1,1,8)$	0.0383	0.1995	64	$(9,1,0)$	0.3774	1.0000
32	$(8,1,1)$	0.0383	0.1996	65	$(0,0,10)$	1.0000	1.0000
33	$(2,3,5)$	0.0480	0.2189	66	$(10,0,0)$	1.0000	1.0000

TABLE 1

The α-critical region, $\alpha = 0.1$, is $W_{0.1,10} = \bigcup_{s=1}^{24} \left(x_1^{(s)}, x_2^{(s)}, x_3^{(s)}\right)$ and the size of the test is $\alpha^* = 0.0963$.

3. The size of the χ^2 goodness-of-fit test

Under the standard χ^2 goodness-of-fit testing procedure for testing H_0 we reject the null hypothesis at given significance level α if the observed χ^2-statistic (4), with ML estimate of θ

$$\hat{\theta}(x_1,\dots,x_k) = \operatorname*{argmax}_{\theta\in\Theta} \prod_{i=1}^{k} P_i^{x_i}(\theta) \tag{13}$$

is greater than the critical value $\chi^2_{k-m-1}(\alpha)$ of the (asymptotically derived) central χ^2 distribution with $k-m-1$ degrees of freedom. For given $\alpha \in (0,1)$ the critical region generated by the χ^2-statistic (4) is given as

$$W_{\alpha,N}^{\chi^2} = \left\{x = (x_1,\dots,x_k)\colon \chi^2 > \chi^2_{k-m-1}(\alpha)\right\}. \tag{14}$$

Compute the size of the test based on critical region $W_{\alpha,N}^{\chi^2}$ as

$$\alpha^* = \sup_{\theta\in\Theta} \sum_{x\in W_{\alpha,N}^{\chi^2}} \frac{N!}{x_1!\dots x_k!} P_1^{x_1}(\theta)\dots P_k^{x_k}(\theta). \tag{15}$$

In fact, α^* is the size of the χ^2 goodness-of-fit test (4).

EXAMPLE 1 (continued). To get the critical region $W_{0.1,10}^{\chi^2}$, for each $x^{(i)}$ from Table 1 we have computed the ML estimate $\hat{\theta}(x^{(i)})$ according to (13), and the value of the χ^2-statistic (4). The results are given in Table 2.

The asymptotic distribution of χ^2-statistic (4) is χ^2_1, so the $\alpha = 0.1$ critical value is 2.7055. $W_{0.1,10}^{\chi^2}$ consists of the points $x^{(i)}$ for which $\chi^2(x^{(i)}) > 2.7055$. In Table 2, these points are labeled with a star. The size of the χ^2 goodness-of-fit test based on the critical region $W_{0.1,10}^{\chi^2}$ is, according to (15), $\alpha^* = 0.1355$.

It is of some interest to compare the critical regions $W_{\alpha,N}$ and $W_{\alpha,N}^{\chi^2}$ obtained according to (8) and (14), respectively. For given $\alpha = 0.1$ and $N = 10$ the two critical regions are depicted in the Figure 1. The visual inspection of the picture suggest that the two methods generate very close critical regions.

4. Empirical distribution of χ^2-statistic for small sample sizes

Another look at the χ^2-statistic for small sample sizes can be obtained by investigating its empirical cdf.

i	$x^{(i)}$	$\hat{\theta}$	χ^2	i	$x^{(i)}$	$\hat{\theta}$	χ^2
1	$(5,0,5)^*$	0.5000	10.000	34	$(5,3,2)$	0.3500	1.1605
2	$(4,0,6)^*$	0.6000	10.000	35	$(1,7,2)$	0.5500	1.7151
3	$(6,0,4)^*$	0.4000	10.000	36	$(2,7,1)$	0.4500	1.7151
4	$(3,0,7)^*$	0.7000	10.000	37	$(3,4,3)$	0.5000	0.4000
5	$(7,0,3)^*$	0.3000	10.000	38	$(1,2,7)$	0.8000	1.4063
6	$(0,10,0)^*$	0.5000	10.000	39	$(7,2,1)$	0.2000	1.4062
7	$(2,0,8)^*$	0.8000	10.000	40	$(0,6,4)$	0.7000	1.8367
8	$(8,0,2)^*$	0.2000	10.000	41	$(4,6,0)$	0.3000	1.8367
9	$(4,1,5)^*$	0.5500	6.3677	42	$(2,4,4)$	0.6000	0.2778
10	$(5,1,4)^*$	0.4500	6.3677	43	$(4,4,2)$	0.4000	0.2778
11	$(3,1,6)^*$	0.6500	6.0874	44	$(1,6,3)$	0.6000	0.6250
12	$(6,1,3)^*$	0.3500	6.0874	45	$(3,6,1)$	0.4000	0.6250
13	$(0,9,1)^*$	0.5500	6.6942	46	$(2,6,2)$	0.5000	0.4000
14	$(1,9,0)^*$	0.4500	6.6942	47	$(2,5,3)$	0.5500	0.0010
15	$(2,1,7)^*$	0.7500	5.3778	48	$(3,5,2)$	0.4500	0.0010
16	$(7,1,2)^*$	0.2500	5.3778	49	$(1,3,6)$	0.7500	0.4000
17	$(4,2,4)^*$	0.5000	3.6000	50	$(6,3,1)$	0.2500	0.4000
18	$(3,2,5)^*$	0.6000	3.4028	51	$(1,5,4)$	0.6500	0.0978
19	$(5,2,3)^*$	0.4000	3.4028	52	$(4,5,1)$	0.3500	0.0978
20	$(1,0,9)^*$	0.9000	10.000	53	$(1,4,5)$	0.7000	0.0227
21	$(9,0,1)^*$	0.1000	10.000	54	$(5,4,1)$	0.3000	0.0227
22	$(0,8,2)^*$	0.6000	4.4444	55	$(0,5,5)$	0.7500	1.1111
23	$(2,8,0)^*$	0.4000	4.4444	56	$(5,5,0)$	0.2500	1.1111
24	$(1,8,1)^*$	0.5000	3.6000	57	$(0,4,6)$	0.8000	0.6250
25	$(2,2,6)^*$	0.7000	2.7438	58	$(6,4,0)$	0.2000	0.6250
26	$(6,2,2)^*$	0.3000	2.7438	59	$(0,3,7)$	0.8500	0.3114
27	$(3,3,4)$	0.5500	1.5519	60	$(7,3,0)$	0.1500	0.3114
28	$(4,3,3)$	0.4500	1.5519	61	$(0,2,8)$	0.9000	0.1235
29	$(0,7,3)^*$	0.6500	2.8994	62	$(8,2,0)$	0.1000	0.1235
30	$(3,7,0)^*$	0.3500	2.8994	63	$(0,1,9)$	0.9500	0.0277
31	$(1,1,8)^*$	0.8500	3.6947	64	$(9,1,0)$	0.0500	0.0277
32	$(8,1,1)^*$	0.1500	3.6947	65	$(0,0,10)$	1.0000	0.0000
33	$(2,3,5)$	0.6500	1.1605	66	$(10,0,0)$	0.0000	0.0000

TABLE 2

In what follows we show the empirical distribution of the χ^2-statistic (4) under H_0: *The sample comes from binomial distribution* $Binom(k-1,\theta)$, $\theta \in (0,1)$ in different situations. In particular, we consider $N = 10, 20, 30$ and 50, and $k = 3, 7$. We have simulated random samples from binomial distribution

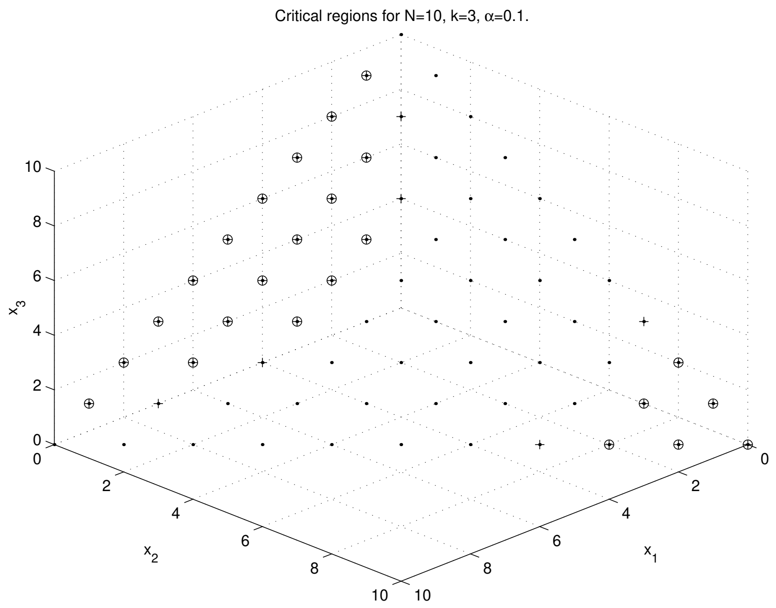

FIGURE 1. The $\alpha = 0.1$ critical regions for testing the hypothesis on binomial distribution with $N = 10$ and $k = 3$. The points from $W^{\chi^2}_{0.1,10}$ are denoted by $+$ and the points from $W_{0.1,10}$ are denoted by $\circ$.

under various prior assumptions on the parameter $\theta \in \Theta = (0,1)$. We have generated two types of empirical distributions. The first type was generated for fixed parameter value $\theta = 0.5$ and $\theta = 0.1,\ 0.3,\ 0.7,\ 0.9$. The second type of empirical distribution was generated for randomly (uniformly) chosen parameter $\theta \in (0,1)$ for each realization of the χ^2-statistic. The number of simulated realizations in each case was fixed to 10000. The results are plotted in Figures 2–4.

5. Discussion

(1) In Section 2 we have suggested an alternative method of construction of the goodness-of-fit test for small samples which could be applied under quite reasonable conditions, which ensure the existence and computability of the maximum likelihood estimates of the parameters.

(2) This method allows also to calculate the size of the standard χ^2 goodness-of-fit test for small samples (under the above mentioned conditions).

(3) It was shown in Example 1 that the size of the χ^2 goodness-of-fit test is 0.1355. So, it is greater than the theoretical (asymptotic) significance

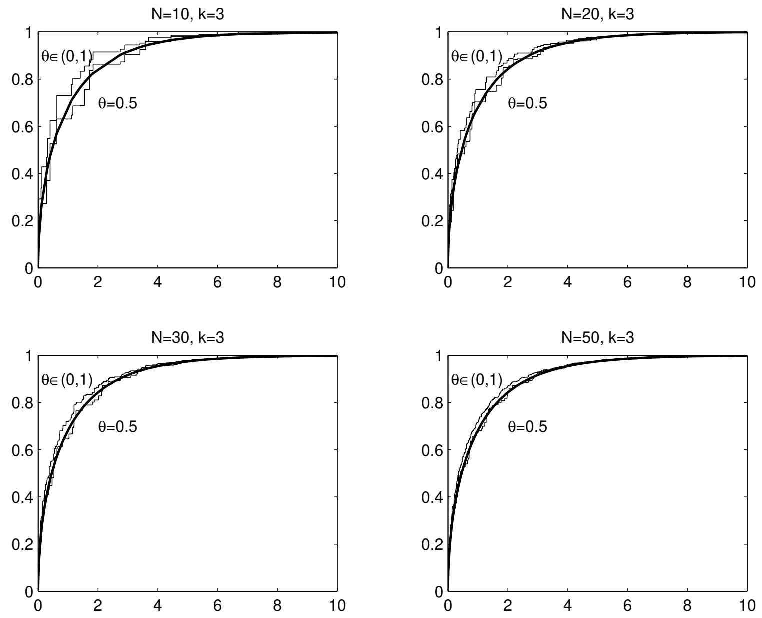

FIGURE 2. The empirical cdf's of the χ^2-statistic (4) under H_0 compared with the asymptotic cdf of χ_1^2 (bold line).

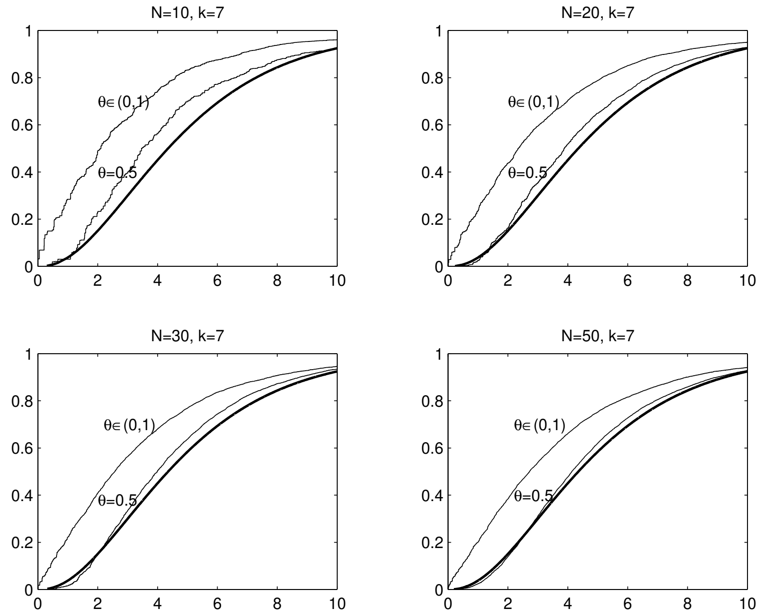

FIGURE 3. The empirical cdf's of the χ^2-statistic (4) under H_0 compared with the asymptotic cdf of χ_5^2 (bold line).

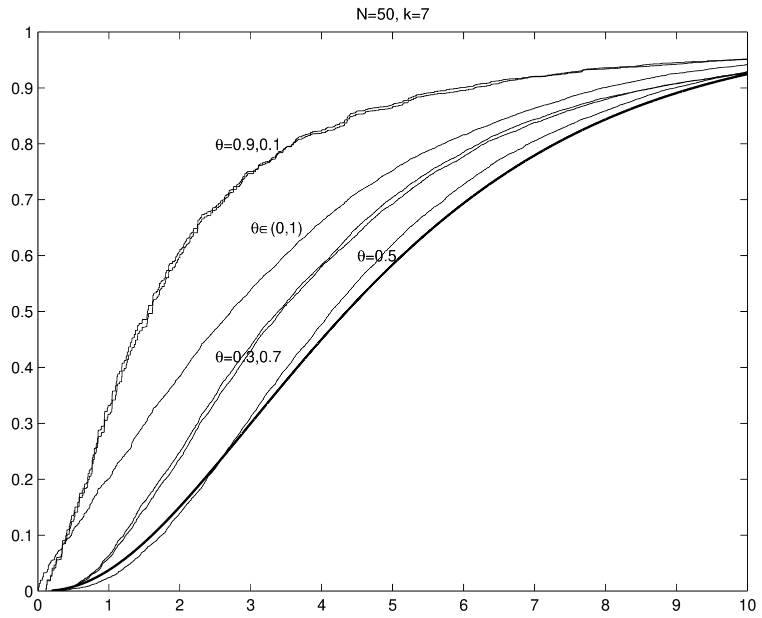

FIGURE 4. The empirical cdf's of the χ^2-statistic (4) under H_0 generated for $\theta = 0.1, 0.3, 0.5, 0.7, 0.9$, and random $\theta \in (0,1)$ compared with the asymptotic cdf of χ^2_5 (bold line).

level $\alpha = 0.1$. However, according to other our investigations this result is not general.

(4) Our simulation study showed that the standard χ^2 goodness-of-fit test has quite good properties even for small sample sizes. Generally, in all studied cases, under the null hypothesis (for different prior choices of $\theta \in \Theta$) the empirical cdf's of the χ^2-statistic were shifted left from the asymptotic (theoretical) cdf. Example 1 illustrates the opposite situation, which was observed only for very small values of k (the number of classes). These observations indicate that the standard χ^2 goodness-of-fit test tends to be a conservative test, i.e., the size of the test is smaller then the required significance level.

(5) We have observed that for testing hypothesis on binomial distribution the theoretical (asymptotic) distribution of the χ^2 test statistic best corresponds to the empirical distribution of (4) generated under H_0 with prior choice of the parameter $\theta = 0.5$. This observation gives immediate remedy for calculation of the size of the (small sample) test based on simulations in this particular case.

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