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Malte Bismarck; Christel Deutschmann; Dana Králová
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SIMULATION STUDIES ON MODEL SEARCH IN 3-DIMENSIONAL CONTINGENCY TABLES. PRELIMINARY RESULTS

MALTE BISMARCK, CHRISTEL DEUTSCHMANN, DANA KRÁLOVÁ

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Summary. In model search procedures for multidimensional contingency tables many different measures are used for decision for the goodness of model search, for instance α , AIC or R^2 . Simulation studies should give us an insight into the behaviour of the measures with respect to the data, the sample size, the number of degrees of freedom and the probability given distribution. To this end different log-linear models for 3-dimensional contingency tables were given and then 1,000 contingency tables were simulated for each model and for several sample sizes and the various decision measures were computed. Summarizing the results we count empirical frequencies of the choice of the true model under various circumstances. This leads to our concluding discussion of properties of the model acceptance criteria under consideration.

Keywords: Contingency Table; Model Search; Measures for Decision; Log-linear Model; Simulation Study.

I. INTRODUCTION

There are many approaches to the search for an appropriate association structure for a multidimensional contingency table, the earliest having been given by Victor [8] and Goodman [5], [7]. Model search for contingency tables is considered to be the decision for the "best" estimate of the unknown true multinomial distribution under various model assumptions. Here we take as a reference set the set of graphical models as a subset (of the set) of all hierarchical log-linear models. The model search procedures differ mainly with regard to the set of permitted models, to the strategy of search and to the measure used, which defines what means the "best" approximation within a set of constructed models. Different strategies and decision criteria may lead to various results. It is to research which decision measure is the most appropriate one for model search in multidimensional contingency table analysis.

II. THE MOST FREQUENTLY APPLIED MEASURES FOR MODEL SELECTION

The most frequently applied measures for estimating which model is the best are the following:

1. The probability of rejecting a model M_0 in the sense of a significance test:

$$\alpha(M_0) = {}^a P(\chi^2(df_0) > Y^2(M_0))$$

(Y^2) denotes the log-likelihood-ratio test statistic, df_0 the degrees of freedom of M_0 , $=^a$ the asymptotic equivalence given by the relation $Y^2(M_0) = {}^a \chi^2(df_0)$.) In this case the problem is the interpretation of α . Though α is defined as the probability of rejecting a hypothesis, this model measure can be considered a measure of plausibility only in an exploratory sense.

2. The R^2 -measure proposed by Goodman [6] in analogy to the coefficient of determination in multiple regression analysis:

$$R^2(M_0) = \frac{Y^2(M_1) - Y^2(M_0)}{Y^2(M_1)}$$

The R^2 -value reflects the percent improvement in formal goodness of fit of M_0 over M_1 . M_1 is the completely restricted model which contains only the parameters of the first order.

3. Because the results of model selection should be both the most parsimonious and the best fitting models, the standardized fit measure R^2 is modified to a non-standardized fit index Δ ([9]) so that it reflects goodness of fit as well as parsimony. Δ is defined as

$$\Delta(M_0) = \frac{Y^2(M_1)/df_1 - Y^2(M_0)/df_0}{Y^2(M_1)/df_1}$$

In contrast to R^2 , Δ can decrease in value if restrictions are cancelled from the model, i.e., if the improvement in goodness of fit is not commensurable with the loss of freedom.

4. Recently a measure of Akaike and Sakamoto [3] $AIC(M_0) = Y^2(M_0) - 2df_0$ has often been used. This follows from the AIC-information measure which is defined as

$$AIC(\hat{\theta}^k) = (-2) \ln g(x/\hat{\theta}^k) + 2k$$

([1], [2]), where k is the number of parameters within the model which are adjusted to attain the maximum of the likelihood function g . $AIC(\hat{\theta}^k)$ is an asymptotically unbiased estimate of the expected entropy. The entropy can be interpreted as the logarithm of the probability of getting the true distribution by sampling from the assumed distribution. In terms of these four measures we can define the following criteria for model selection:

Select the model with

- A. the maximum α , or
- B. the minimum AIC, or

- C. $R^2(M_0) \geq 0.8$ and the minimum of degrees of freedom (in the following denoted by $\text{mod } R^2(M_0)$) or
 D. the maximum Δ .

III. EVALUATING DECISION CRITERIA BY SIMULATION STUDIES

Simulation studies for 3-dimensional contingency tables should give us a first insight into the behaviour of the usual decision criteria dependent on random variations in the data, on the sample size, on the degrees of freedom, and on the probability distribution. A set of unsaturated hierarchical log-linear models with their corresponding multinomial distributions was defined. Then 1·000 contingency tables were simulated for each given distribution, the several measures were calculated, and the frequencies of choice of the true model with respect to the several decision criteria were counted. For the contingency table simulation the computer program SCET¹⁾ with the pseudorandom generator SERAPH²⁾ was used. The decision measures for the models were calculated by a module of the contingency table analysis program KONTAN³⁾.

4.1. Simulation Results for $2 \times 2 \times 2$ -Tables

4.1.1. Choice of the Model A/B/C. The simulation studies show that if model A/B/C with approximately equally weighted cell probabilities (model I in Fig. 1) was given, the AIC-criterion found the true model at 60 per cent independently of the sample size. With $\max \alpha$ the true choice is done only between 18–20 per cent and with $\max \Delta$ between 12–15 per cent (Fig. 1). The frequency of choice of the remaining unrestricted hierarchical models is approximately the same when using $\max \alpha$, whereas when using $\text{mod } R^2$ or $\max \Delta$ the models AB/AC/BC (~ 25 per cent) and AB/AC, AB/BC, AC/BC are more frequently chosen in comparison with the models A/BC, B/AC and C/AB. Models having only one parameter of the second order equal to zero are chosen by AIC only at 6–7 per cent independently of the sample size n . With the given model A/B/C but very unequally weighted cell probabilities (model II in the figure) the simulation results differ from the ones shown in Fig. 1. The frequency of choice of the true model by $\max \alpha$ and $\max \Delta$ more heavily depends on the sample size. It is interesting that the true decisions are tripling for $n \geq 500$ in comparison with $n = 100$. Moreover, the model AB/AC/BC is clearly favoured for $n < 100$. For the models both with homogeneous and unhomogeneous

¹⁾ SCET has been written by D. Králová, Psychiatric Research Institute, Prague.

²⁾ SERAPH is a program from the program library MABIF by VEB Kombinat ROBOTRON, Dresden.

³⁾ KONTAN has been written by A. Angelus, Martin-Luther-University Halle, Computer Centre.

cell probabilities and $n \geq 500$ the R^2 -measure is less than 0.8 at 50 per cent of the simulated tables (Fig. 3).

4.1.2. Choice of the Model A/BC. If the model A/BC is given, the simulations of various probability distributions for this model show that for small sample sizes all our criteria also find the true model only at 5 – maximum 20 per cent. For sample size $n = 100$ the frequency of true decisions increases to about 10–30 per cent if $\max \alpha$, $\max \Delta$ or $\text{mod } R^2$ is used, and to 16–50 per cent for AIC. For $n \geq 500$ this frequency increases to about 70 per cent for AIC and to 60–100 percent for $\text{mod } R^2$, whereas it is constant for $\max \alpha$ and $\max \Delta$ (Fig. 2). The frequency of choice of models which are more restricted (A/B/C) decreases with the increasing sample size to almost zero for AIC (Fig. 5). Figure 6 shows the frequencies of the choice of models having more parameters than the correct model (AC/BC, AB/BC, AB/AC/BC). It is shown that neither the models with a probability distribution near to the model A/B/C (model II in the figures) nor the models the distributions of which are more different from A/B/C (model I in the figures) can be identified. This effect could also be observed with the frequency of choice of “false” models, that is these models and the true model are not nested (Fig. 4).

4.1.3. Choice of the Model AC/BC. If the model AC/BC is given the frequency of the choice of the true model again depends on the distance between the given distribution and the other hierarchical log-linear models. Considering a distribution which clearly differs from a model with less parameters (model I in the figures) the frequency of the choice of the correct model is about 15–40 per cent for all measures and $n < 100$. For $n \geq 100$ the frequency increases especially if the criteria AIC and $\text{mod } R^2$ are used (up to 85 per cent and 100 per cent; see fig. 7). More restricted models are most frequently chosen if the criterion AIC is applied (about 60 per cent if n is small). But this frequency decreases to zero with increasing sample size regardless of which measure is used (Fig. 9). Figure 10 shows the frequency of choice of the model AB/AC/BC. This frequency is independent of n when applying $\max \alpha$ and $\max \Delta$ and decreases to zero with increasing sample size if $\text{mod } R^2$ is used. Only if we use AIC we select the model AB/AC/BC more frequently to a greater than with a smaller n . For $n \geq 500$ the relative frequency of the choice of the false model is near zero and independent with the criterion used (Fig. 8). If the distribution of the given model is near of those of the other more restricted to models (model II in the figure) $\text{mod } R^2$ responds most sensitively. The frequency of choice of the true model does not increase as the sample size increases. The number of falsely selected models decreases more slowly with increasing n when applying the other criteria.

4.2. Simulation Results for $a \times b \times c$ – Tables ($a, b, c \geq 2$). In order to see if the results of model search change with the increasing number of categories of the

variables with respect to the criteria considered, we simulated $4 \times 4 \times 4$ -, $2 \times 5 \times 5$ - and $2 \times 2 \times 2$ -tables for the given models.

The sample sizes were restricted to $n = 100, 600, 6000$ because the computing time was very long for simulations of such tables. For the given model A/B/C we can observe that the frequency of true selections increases when using AIC with an increasing number of cells whereas it is approximately the same for $\max \alpha$ or $\max \Delta$. The sample size is unimportant (Fig. 11). The greater the number of cells, the higher is the portion of the tables with $R^2 < 0.8$ (for $4 \times 4 \times 4$ -tables more than 90 per cent). If the models A/BC and C/AB are given the frequency of true decisions gets also higher with an increasing number of cells when using the AIC-acceptance criterion. The criteria $\max \alpha$, $\max \Delta$ and $\text{mod } R^2$ decide similarly as in the $2 \times 2 \times 2$ -case (Figs. 12, 13). Also in these examples, the better the given distribution approximates another model, the more depend the results of the model selection on the sample size. This is most clear if we apply $\text{mod } R^2$ or \min AIC and if the given model approximates a more restricted model. Models with $R^2 < 0.8$ occur more frequently, more restricted models were more frequently selected when using AIC for $n = 100$ (see model II in Fig. 12). For the table in Fig. 12 the selection of the true model is more frequent than in the case of the table $2 \times 2 \times 2$. This holds for all criteria except AIC (model I in Fig. 12, model C/AB in Fig. 13).

With the given models AC/BC and AB/AC the frequency of choice of the true model is greater than in the case of a $2 \times 2 \times 2$ -table for a small n provided we use $\max \alpha$ or $\max \Delta$. We obtained the same results using AIC except for the case that the given distribution is close to a model with fewer parameters (model II in Fig. 15). The frequency of choice of the true model with respect to $\text{mod } R^2$ is largely varying with regard to numbers of cells of the tables and to sample sizes. Both cases in Fig. 7 for $2 \times 2 \times 2$ -tables can be also found in Figs. 14 and 15 (model II in Fig. 15 and model I in Fig. 14). The number of true selections increases more slowly with the increasing sample size when considering model I in Fig. 12 in contrast to model I in Fig. 7, while it is greater for model II in Fig. 15 than for model II in Fig. 7 with $n \leq 600$. For large sample sizes the number of true selections is approximately the same as for $2 \times 2 \times 2$ -tables when using $\max \alpha$ or $\max \Delta$, whereas when applying AIC it is also greater for this given model. Similar situation occur already for small n and especially when $\max \alpha$, $\max \Delta$ are used, but also $\text{mod } R^2$ models with a too large number of parameters were more frequently chosen. It is interesting that for almost all criteria the frequencies of true decisions for $n = 600$ differ slightly from the frequencies for $n = 6,000$.

5. Conclusions. The simulation studies indicate that the AIC-criterion is the most appropriate one among all the considered criteria for model search in exploratory data analyses. Especially for sufficiently large sample sizes ($n > 100$) and for $a \times b \times c$ -tables with $a, b, c \geq 2$, AIC is the most stable criterion. Moreover, it tends to the selection of models with fewer parameters in contrast to the criteria

$\max \alpha$ and $\max \Delta$ which significantly more frequently select models including more parameters even for a small n . The frequency of choice of the true model when using \min AIC is greater than those which apply $\max \alpha$ or $\max \Delta$. It is not surprising that the results produced by the α -criterion are not so good. In model search procedures we are actually interested in accepting a more restricted model and not in rejecting the other one. But the α -measure estimates the probability of falsely rejecting a more restricted model in favour of the alternative model, which is totally unrestricted. It is amazing that model selections applying $\max \Delta$ yield no better results in comparison with the other criteria, but on the contrary the number of true decisions is frequently lower than that using $\max \alpha$. Besides, we have demonstrated that the decision for the true model directly or indirectly depends on the sample size and on the magnitude of the cell probabilities underlying the simulated contingency tables regardless of which criterion is used. Theoretically, $\max \Delta$ and $\text{mod } R^2$ are independent of the sample size n . But the various selection results for several n could be interpreted in the way that the magnitude of the random variations of the simulated frequencies in the tables depends on the given sample size provided that for a small size the discreteness of the simulated frequency distribution has a greater effect. For this reason there is a relationship between the sample size, the given probability distribution and nearness and distance. The more the given cell probabilities and the corresponding estimated expected cell frequencies approximate the other multiplicative conditions (models), the smaller is the chance to find the true model, the more frequently a false model is chosen, the greater the necessary sample size must be. This situation is reflected most by the $\text{mod } R^2$ -criterion, which measures the lack of fit with respect to the model of global independence. It responds extremely to the distance of the given distribution to a model which is more restricted. $\text{Mod } R^2$ very frequently yields true decisions only in such cases when the distance is large enough (especially for large n). Otherwise the more restricted model is almost always chosen or the R^2 values are smaller than 0.8, which become greater than 0.8 at models which are less restricted. A very small value of R^2 corresponds to a model having a lot of parameters equal to zero. It was clearly demonstrated that exploratory analyses, too, need an adequate sample size. For a very small n ($n \leq 100$ for $2 \times 2 \times 2$ -tables and $n < 600$ for $4 \times 4 \times 4$ -tables) true models were more seldom chosen for all criteria used, most rarely for $\max \alpha$ or $\max \Delta$. When using AIC the disadvantage of a small sample size is partly neutralized by the number of cells, i.e., the number of degrees of freedom. Though also $\max \Delta$ considers the degrees of freedom this effect evidently has not such consequences at model selection as when applying \min AIC. Indeed, for no given distribution the frequency of choice of the true model was close to 100 per cent when using AIC, even for $n = 5\,000$, $6\,000$. The frequencies were about the same for $n \geq 500$ and $n \geq 600$, except for a few cases. For model selection one should take into consideration the results of $\text{mod } R^2$ and the R^2 -measures in addition to the AIC-criterion, if $\text{mod } R^2$ decides in favour of a model with fewer parameters or if the R^2 -measure is very small for

a sufficiently large n , for instance. In further simulation studies we want to explore additional criteria, for instance, the criterion used in Goodman's stepwise procedure or the R^2 -measure with reference to other models than A/B/C. Further we want to study the behaviour of acceptance criteria with regard to the model AB/AC/BC and estimate the risk of decision for several measures.

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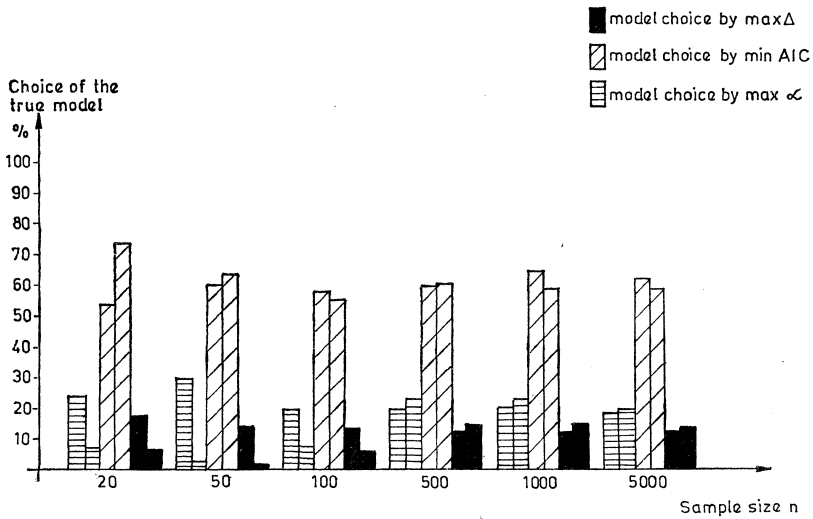


Fig. 1. Frequencies of Choice of the True Model A/B/C for a $2 \times 2 \times 2$ -Table. Model I (First Column): $p_{\cdot,1} = 0.5$; $p_{\cdot,2} = 0.5$; $p_{1,\cdot} = 0.4$; $p_{2,\cdot} = 0.6$; $p_{1..} = 0.3$; $p_{2..} = 0.7$; Model II (Second Column): $p_{\cdot,1} = 0.1$; $p_{\cdot,2} = 0.9$; $p_{1,\cdot} = 0.05$; $p_{2,\cdot} = 0.95$; $p_{1..} = 0.2$; $p_{2..} = 0.8$.

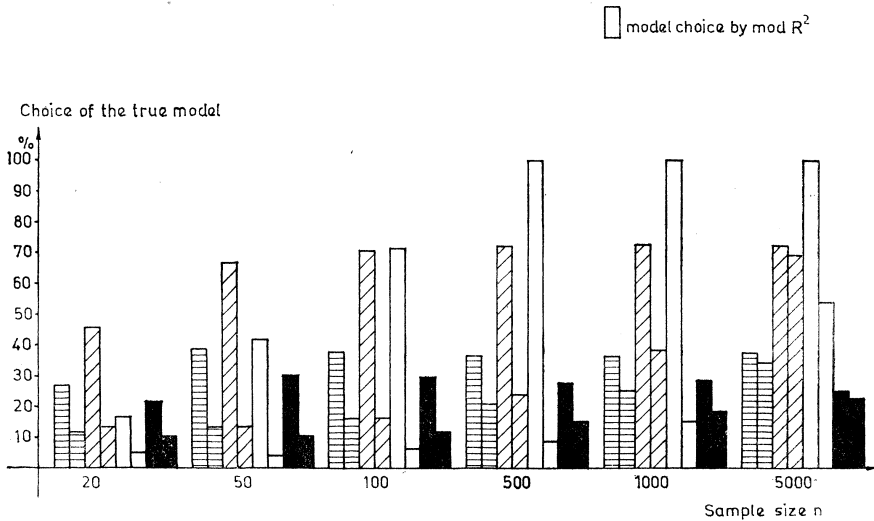


Fig. 2. Frequencies of Choice of the True Model A/BC for a $2 \times 2 \times 2$ -Table. Model I (First Column): $p_{1..} = 0.5$; $p_{2..} = 0.5$; $p_{11} = 0.3$; $p_{21} = 0.1$; $p_{12} = 0.2$; $p_{22} = 0.4$. Model II (Second Column): $p_{1..} = 0.5$; $p_{2..} = 0.5$; $p_{11} = 0.1$; $p_{21} = 0.2$; $p_{12} = 0.2$; $p_{22} = 0.5$.

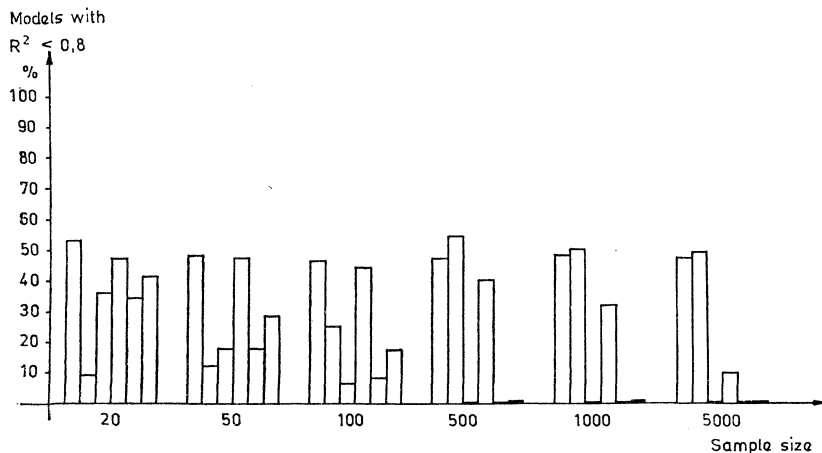


Fig. 3. Frequencies of Models with $R^2 < 0.8$. Column 1: Model A/B/C (I); Column 2: Model A/B/C (II); Column 3: Model A/BC (I); Column 4: Model A/BC (II); Column 5: Model AC/BC (I); Column 6: Model AC/BC (II).

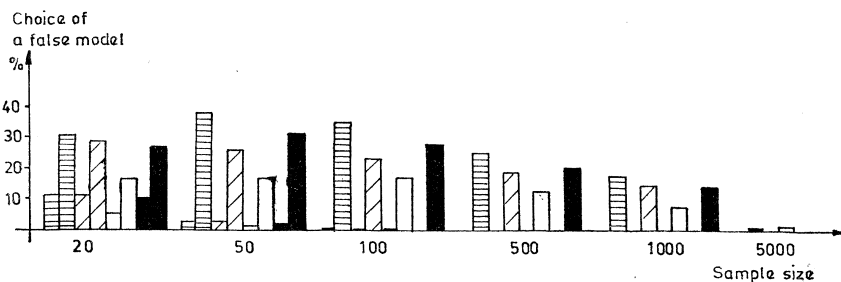


Fig. 4. Frequencies of Choice of a False Model if Model A/BC is Given for a $2 \times 2 \times 2$ -Table.

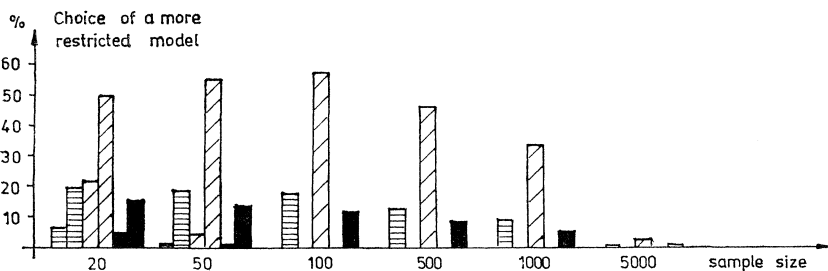


Fig. 5. Frequencies of Choice of a More Restricted Model if Model A/BC is Given for a $2 \times 2 \times 2$ -Table.

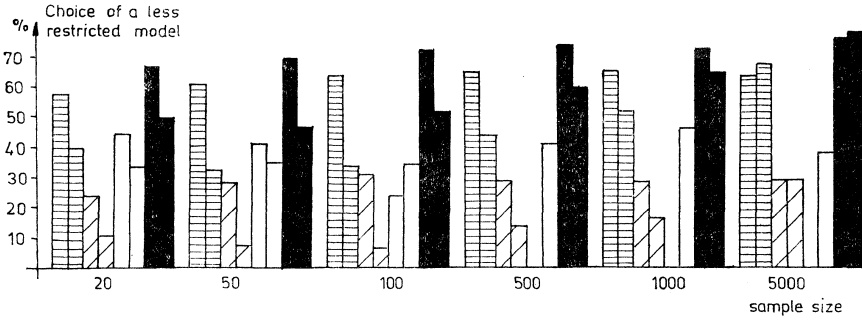


Fig. 6. Frequencies of Choice of a Less Restricted Model if Model A/BC is Given for a $2 \times 2 \times 2$ -Table.

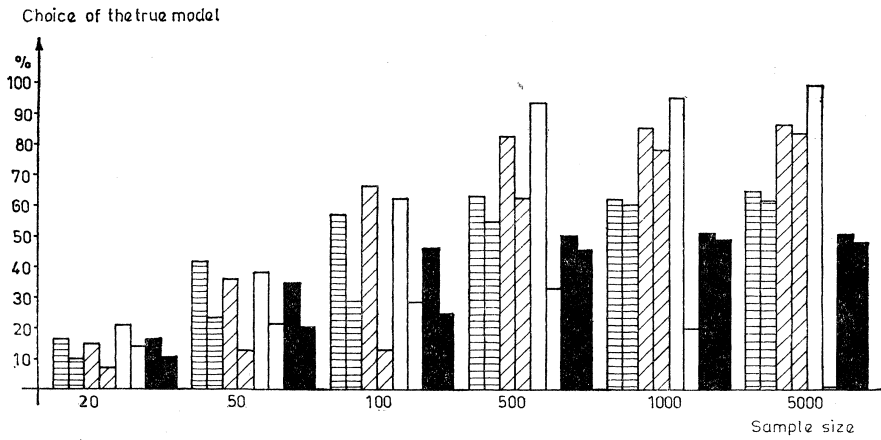


Fig. 7. Frequencies of Choice of the True Model AC/BC for $r \times 2 \times 2$ -Table. Model I (First Column): $p_{.1} = 0.5$; $p_{.2} = 0.5$; $p_{1.1} = 0.1$; $p_{1.2} = 0.2$; $p_{2.1} = 0.4$; $p_{2.2} = 0.3$; $p_{11} = 0.1$; $p_{12} = 0.25$; $p_{21} = 0.4$; $p_{22} = 0.25$. Model II (Second Column): $p_{.1} = 0.6$; $p_{.2} = 0.4$; $p_{1.1} = 0.2$; $p_{1.2} = 0.1$; $p_{2.1} = 0.4$; $p_{2.2} = 0.3$; $p_{11} = 0.45$; $p_{12} = 0.2$; $p_{21} = 0.15$; $p_{22} = 0.2$.

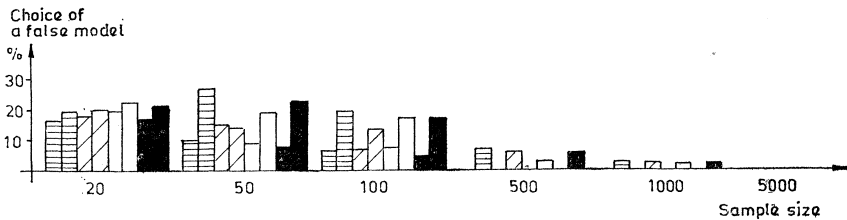


Fig. 8. Frequencies of Choice of a False Model if Model AC/BC is Given for a $2 \times 2 \times 2$ -Table.

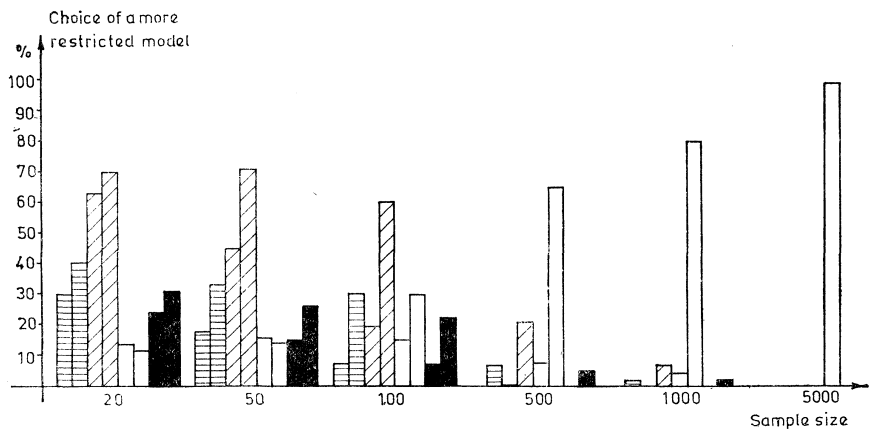


Fig. 9. Frequencies of Choice of a More Restricted Model if Model AC/BC is Given for a $2 \times 2 \times 2$ -Table.

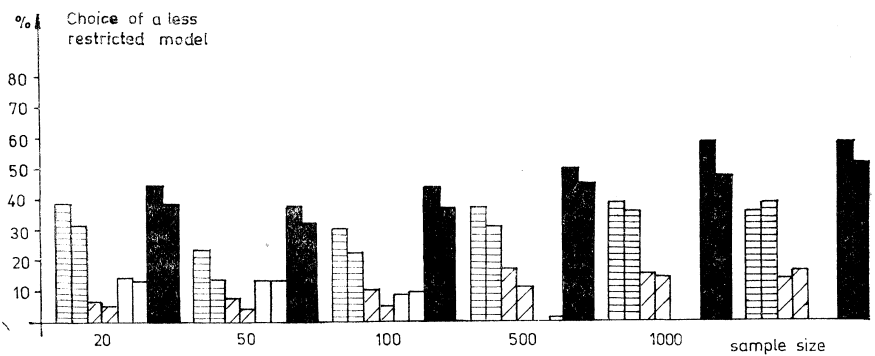


Fig. 10. Frequencies of Choice of a Less Restricted Model if Model AC/BC is Given for a $2 \times 2 \times 2$ -Table.

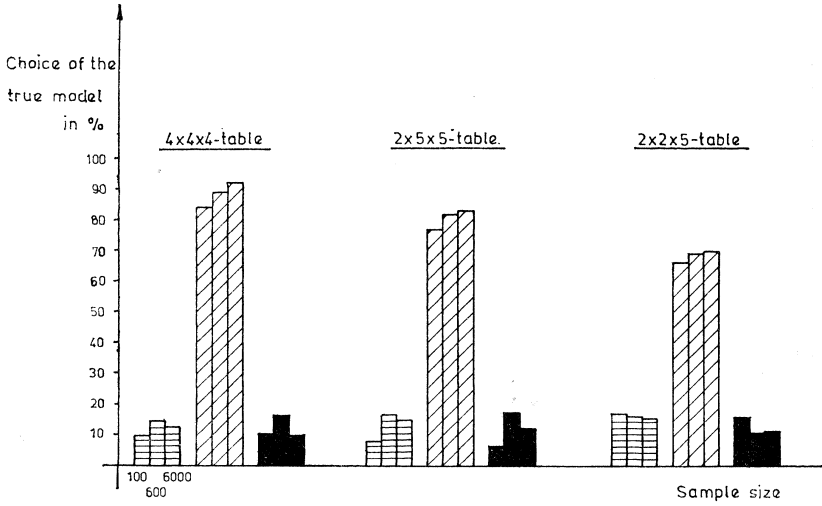
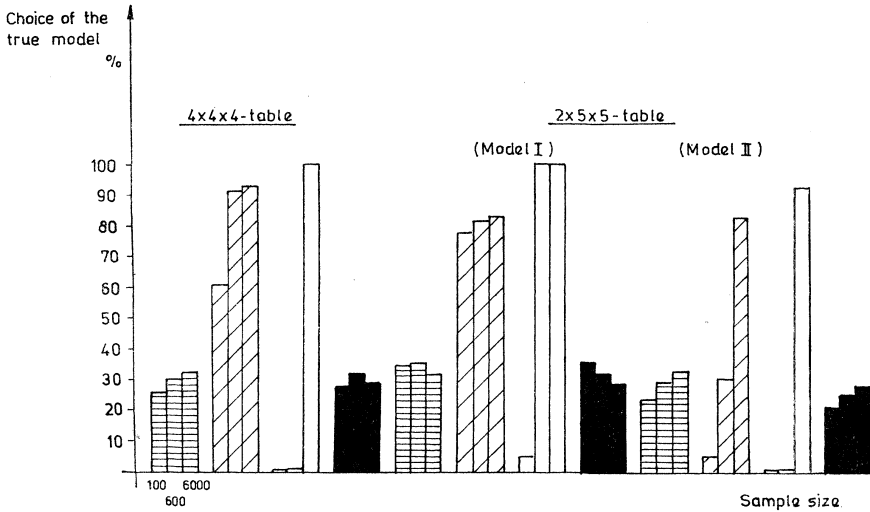


Fig. 11. Frequencies of Choice of the True Model A/B/C for $a \times b \times c$ -Tables. ($4 \times 4 \times 4$ -Table: $p_{i..} = 0.1$; $i = 1, 2, 3$; $p_{4..} = 0.7$; $p_{.j.} = 0.25$; $j = 1, 2, 3, 4$; $p_{..k} = 0.25$; $k = 1, 2, 3, 4$, $2 \times 5 \times 5$ -Table: $p_{i..} = 0.5$; $i = 1, 2$; $p_{.j.} = 0.1$; $j = 1, 2, 3, 4$; $p_{.5.} = 0.6$; $p_{..k} = 0.1$; $k = 1, 2, 3, 4$; $p_{..5} = 0.6$, $2 \times 2 \times 5$ -Table: $p_{1..} = 0.5$; $p_{2..} = 0.5$; $p_{.2.} = 0.5$; $p_{.1.} = 0.6$; $p_{..k} = 0.1$; $k = 1, 2, 3, 4$; $p_{.5} = 0.6$;))



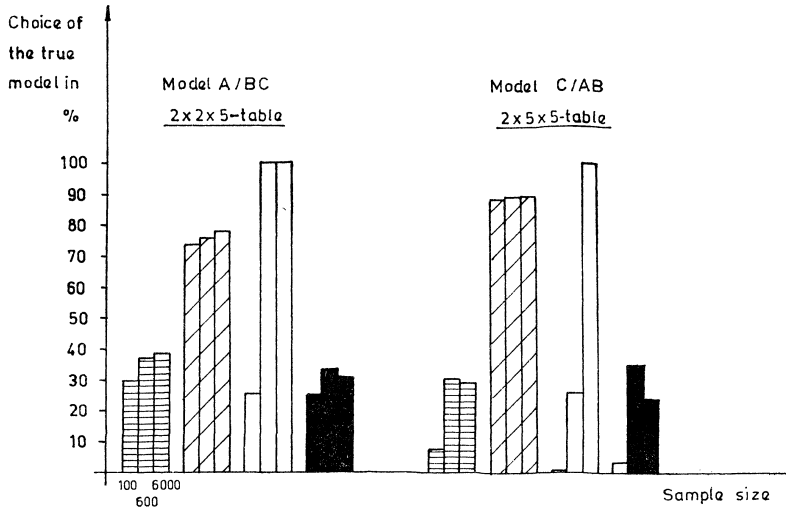


Fig. 13. Frequencies of Choice of the True Model for $a \times b \times c$ -Tables $2 \times 2 \times 5$ -Table: $p_{1..} = 0.1$; $p_{2..} = 0.9$; $p_{.1k} = 0.05$; $k = 1, \dots, 4$; $p_{.15} = 0.5$; $p_{.2k} = 0.06$; $k = 1, \dots, 5$; $2 \times 5 \times 5$ -Table: $p_{..k} = 0.05$; $k = 1, \dots, 4$; $p_{..5} = 0.8$; $p_{11.} = 0.55$; $p_{ij.} = 0.05$; $i = 1$; $j = 2, \dots, 5$; $p_{ij.} = 0.05$; $i = 2$; $j = 1, \dots, 5$;

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Fig. 12. Frequencies of Choice of the True Model A/BC for $a \times b \times c$ -Tables. $4 \times 4 \times 4$ -Table: $p_{i..} = 0.25$; $i = 1, \dots, 4$; $p_{.11} = 0.3$; $p_{.21} = 0.2$; $p_{kj.} = 0.05$; $j = 3, 4$; $k = 1$; $p_{.jk} = 0.05$; $j = 1, \dots, 4$; $k = 2$; $p_{.jk} = 0.025$; $j = 1, \dots, 4$; $k = 3, 4$; $2 \times 5 \times 5$ -Table: Model I: $p_{i..} = 0.5$; $i = 1, 2$; $p_{.jk} = 0.02$; $j = 1, \dots, 5$; $k = 1, \dots, 4$; $p_{.j5} = 0.025$; $j = 1, \dots, 4$; $p_{.55} = 0.5$; Model II: $p_{i..} = 0.5$; $i = 1, 2$; $p_{.jk} = 0.02$; $j = 1, \dots, 5$; $k = 1, \dots, 4$; $p_{.j5} = 0.1$; $j = 1, \dots, 4$; $p_{.55} = 0.2$.

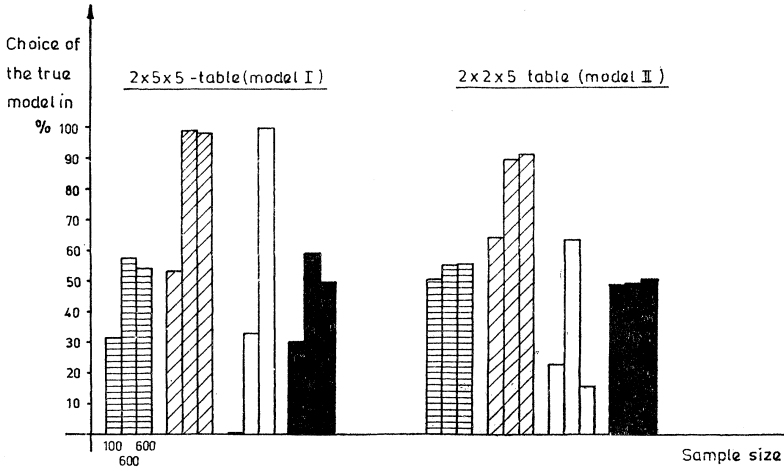


Fig. 14. Frequencies of Choice of the True Model AB/AC for $a \times b \times c$ -Tables Model I: $p_{1..} = 0.2$; $p_{2..} = 0.8$; $p_{1.k} = 0.04$; $k = 1, \dots, 5$; $p_{2.k} = 0.1$; $k = 1, \dots, 4$; $p_{2.5} = 0.4$; $p_{1j.} = 0.02$; $j = 1, \dots, 4$; $p_{2j.} = 0.16$; $j = 1, \dots, 5$; $p_{15.} = 0.12$; Model II: $p_{1..} = 0.2$; $p_{2..} = 0.8$; $p_{1.k} = 0.04$; $k = 1, \dots, 5$; $p_{2.k} = 0.05$; $k = 1, \dots, 4$; $p_{2.5} = 0.6$; $p_{ij.} = 0.1$; $i = 1$; $j = 1, 2$; $p_{21.} = 0.2$; $p_{22.} = 0.6$;

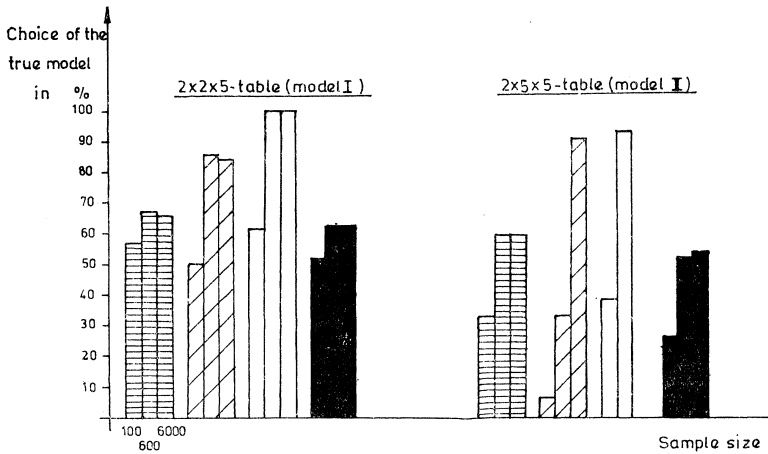


Fig. 15. Frequencies of Choice of the True Model AC/BC for $a \times b \times c$ -Tables. Model I: $p_{.k} = 0.1$; $k = 1, \dots, 4$; $p_{..5} = 0.6$; $p_{1.k} = 0.05$; $k = 1, \dots, 4$; $p_{1.5} = 0.1$; $p_{2.k} = 0.05$; $k = 1, \dots, 4$; $p_{2.5} = 0.5$; $p_{jk} = 0.05$; $j = 1, 2$; $k = 1, 2, 3$; $p_{14} = 0.01$; $p_{24} = 0.09$; $p_{15} = 0.3$; $p_{25} = 0.3$; Model II: $p_{.k} = 0.1$; $k = 1, \dots, 4$; $p_{..5} = 0.6$; $p_{1.k} = 0.01$; $k = 1, \dots, 4$; $p_{1.5} = 0.3$; $p_{2.k} = 0.09$; $k = 1, \dots, 4$; $p_{2.5} = 0.3$; $p_{jk} = 0.02$; $j = 1, \dots, 5$; $k = 1, \dots, 4$; $p_{j5} = 0.1$; $j = 1, \dots, 4$; $p_{55} = 0.2$;

Souhrn

SIMULAČNÍ STUDIE PRO MODELY V TROJROZMĚRNÝCH KONTINGENČNÍCH TABULKÁCH. PŘEDBĚŽNÉ VÝSLEDKY

MALTE BISMARCK, CHRISTEL DEUTSMANN, DANA KRÁLOVÁ

Při hledání modelu multidimensionální tabulky kontingence jsou používány různé míry pro test dobré shody např. α , AIC nebo R^2 . Simulační studie nám mohou přinést hlubší pochopení chování těchto měř vzhladem k velikosti výběru, stupňům volnosti a volbě rozložení pravděpodobnosti. V práci jsou studovány různé logaritmicko-lineární modely tří-dimenzionální kontingence. Pro každý model je generováno 1000 kontingenčních tabulek s možností volby rozsahu výběru a statistiky pro test dobré shody. V simulačních experimentech jsou zjišťovány empirické četnosti správnosti výběru modelu za různých předpokladů. Je provedena diskuse vlastností statistik testů pro přijetí resp. zamítnutí daného modelu.

Author' address: Dipl. Math. *Malte Bismarck*, Dr. *Christel Deutschmann*, Institute of Biostatistics and Med. Informatics, MLU Halle, Krausenstrasse 14, Halle, 4020; RNDr *Dana Králová*, Výzkumný ústav psychiatrický, Ústavní 91, 181 03 Praha 8.