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Applications of bootstrap methods for categorical data analysis

Myoungshic Jhun^{a, *}, Hyeong-Chul Jeong^b

^aDepartment of Statistics, Korea University, 5-1 Anam-dong, Sungbuk-gu, Seoul 136-701, South Korea

^bDepartment of Computer Science and Statistics, Pyongtaek University, Pyongtaek, South Korea

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Abstract

Simultaneous confidence regions for proportions of a single multinomial population, and for a finite number of contrasts from several multinomial populations are proposed. In this paper bootstrap methods are used to construct confidence regions. We compare the performance of bootstrap methods with other methods in terms of average coverage probability by Monte Carlo simulation. Advantages of the bootstrap methods are discussed. © 2000 Elsevier Science B.V. All rights reserved.

Keywords: Simultaneous confidence region; Bootstrap; Average coverage probability

1. Introduction

Construction of simultaneous confidence regions for proportions of a single multinomial population is one of the basic analyses in statistical inference for categorical data. Gold (1963) proposed simultaneous confidence intervals by projecting a confidence ellipsoid based on a chi-square approximation onto proper coordinate axes. Bonferroni confidence intervals, based on the Bonferroni inequality, have also been widely used due to their generality. The second context in which the same type of problem occurs is the construction of simultaneous confidence regions for contrasts among several multinomial populations. Goodman (1964) presented a method

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^{*} Corresponding author.

based on Scheffé's F projection, which is particularly suited to the situation where all contrasts among, say, r multinomial populations may be of interest. However, in practice it is only a finite number of contrasts that are ever examined in application. Bonferroni confidence intervals can also be constructed without too much difficulty. However, these methods are wasteful, in the sense that the family probability error rate is less than the nominal confidence level, instead of being equal to it. Furthermore, for each pivotal statistic, the only distribution theory available is the limiting distribution as the sample size tends to infinity.

In this article, performance of the bootstrap method will be investigated for obtaining confidence regions for multinomial populations, which is the lattice case. Some related theoretical background for the bootstrap methods is as follows. Let T_n be a studentized sum of n i.i.d. random variables with distribution function $F_{\omega}(\cdot)$, and let $H_n(\omega,t) = P_{\omega}[T_n \le t]$, where ω is the parameter for the underlying distribution. If $H_n(\omega,t)$ is regarded as the coverage probability of a confidence set at ω , then $\int_{\Omega} H_n(\omega,t) \xi(\omega) d\omega$ can be regarded as the long run relative frequency of coverage in many independent replications of the experiment, when ω is drawn from the density ξ ; therefore, $\int_{\Omega} H_n(\omega, t) \xi(\omega) d\omega$ can be called the average coverage probability at ξ . In the non-lattice case, Singh (1981) showed that the bootstrap estimator of the sampling distribution of T_n differs from the actual one by an order of magnitude smaller than $1/\sqrt{n}$ with probability one as $n \to \infty$. In the lattice case, Woodroofe and Jhun (1989) showed that in terms of average coverage probability, the bootstrap estimator differs from the very weak expansions by a term of order $1/\sqrt{n}$. However, it was also shown that the coefficient of the term is very small for any ξ with compact support. Agresti and Brent (1998) used average coverage probability, which they called mean coverage probability, to compare several interval estimation methods for binomial proportions.

It will be demonstrated, by using a simulation study, that the bootstrap method has some advantages in constructing confidence regions for multinomial populations. We obtained the results for two densities ξ for the averaging: (1) a uniform distribution, and (2) a variation of a Dirichelet distribution. However, these results can be generalized to any ξ with compact support. In Section 2, bootstrap simultaneous confidence regions for population proportions from a single multinomial population will be introduced. In Section 4, a bootstrap method will be proposed for the construction of simultaneous confidence regions for a finite number of contrasts from several multinomial populations. It also will be shown that the bootstrap method compares favorably with classical methods when only a finite number of linear combinations of cell probabilities are of interest. The comparisons of the procedures are made in terms of the average coverage probability, which is possibly a more relevant description of the performance.

2. Single population

Let us assume that we are sampling from a multinomial population. Let π_i (i = 1, ..., r; $\pi_i > 0$, $\sum_{i=1}^r \pi_i = 1$) be the probability of the *i*th category in the population.

For a sample of n individuals or items from the population, let N_i be the number which fall in category $i(n = \sum_{i=1}^r N_i)$. The maximum likelihood estimator of the probability π_i is $p_i = N_i/n$.

Now, we are interested in constructing a simultaneous confidence region for $(\pi_1, \pi_2, ..., \pi_r)$. We may consider a quantity $\chi^2 = n \sum_{i=1}^r (p_i - \pi_i)^2 / p_i$, which asymptotically follows a chi-squared distribution with (r-1) degrees of freedom. Based on the quantity χ^2 , the simultaneous confidence region for $(\pi_1, \pi_2, ..., \pi_r)$ is obtained as

$$\left[(\pi_1, \pi_2, \dots, \pi_r) : n \sum_{i=1}^r \frac{(p_i - \pi_i)^2}{p_i} \le \chi_{r-1}^2 (1 - \alpha) \right], \tag{2.1}$$

where $\chi_{r-1}^2(1-\alpha)$ is the upper $100(1-\alpha)$ th percentile of the chi-squared distribution with r-1 degrees of freedom.

Instead of using the chi-squared distribution in (2.1), we can use the bootstrap estimator of the sampling distribution of χ^2 . Given $(p_1, p_2, ..., p_r)$, let $\chi^{2*} = n \sum_{i=1}^r (p_i^* - p_i)^2/p_i^*$ where p_i^* (i=1,...,r) denotes the maximum likelihood estimator for a parametric bootstrap sample. Then, a $100(1-\alpha)\%$ bootstrap simultaneous confidence region for $(\pi_1, \pi_2, ..., \pi_r)$ is

$$\left[(\pi_1, \pi_2, \dots, \pi_r) : n \sum_{i=1}^r \frac{(p_i - \pi_i)^2}{p_i} \le Q(1 - \alpha) \right], \tag{2.2}$$

where $Q(1-\alpha)$ is the $100(1-\alpha)$ th percentile of the bootstrap distribution of χ^{2*} . To construct a simultaneous confidence region for $(\pi_1, \pi_2, ..., \pi_r)$, we may also consider a quantity

$$T_{(r)} = \max_{1 \le i \le r} [|T_i| = |\sqrt{n}(p_i - \pi_i)|/\sqrt{p_i(1 - p_i)}]. \tag{2.3}$$

Note that the T_i 's are correlated, and a closed form of the sampling distribution of $T_{(r)}$ is fairly complicated. However, we may obtain a bootstrap estimator of the sampling distribution without too much difficulty. Now, consider the bootstrap distribution of the conditional quantity

$$T_{(r)}^* = \max_{1 \le i \le r} [|T_i^*| = |\sqrt{n}(p_i^* - p_i)|/\sqrt{p_i^*(1 - p_i^*)}]. \tag{2.4}$$

Using the bootstrap estimator of the sampling distribution of $T_{(r)}$, let $t^*(1-\alpha)$ be the $100(1-\alpha)$ th percentile of the bootstrap distribution of $T_{(r)}^*$. Then, a $100(1-\alpha)\%$ simultaneous confidence region for $(\pi_1, \pi_2, ..., \pi_r)$ is obtained as

$$\left[\pi_i \in p_i \pm t^*(1-\alpha)\sqrt{\frac{p_i(1-p_i)}{n}} \text{ for all } i=1,\ldots,r\right]. \tag{2.5}$$

Asymptotic justification of the bootstrap confidence regions (2.2) and (2.5) can be obtained by using the results of Singh (1981). On the other hand, Bonferroni's inequality plays an important role in the construction of simultaneous confidence intervals for the multinomial proportions $(\pi_1, \pi_2, ..., \pi_r)$. Let r denote the number for cells, then $100(1-\alpha)\%$ Bonferroni simultaneous confidence intervals are

$$\left[\pi_i \in p_i \pm t \left(\frac{\alpha}{2r}, n-1\right) \sqrt{\frac{p_i(1-p_i)}{n}} + \frac{1}{2n} \text{ for all } i = 1, \dots, r\right], \tag{2.6}$$

where $t(\alpha/2r, n-1)$ is the $100(1-\alpha/2r)$ th percentile of the t distribution with n-1 degrees of freedom. In fact, there are several versions of the Bonferroni intervals including a standard normal distribution instead of a t distribution. However, to clarify the point of this paper, we use a t distribution with a continuity correction. See Agresti and Brent (1998) for the comparison of interval estimation methods for binomial proportions.

3. Simulation study

To study the performance of the procedures introduced, a Monte Carlo investigation was done. By using the average coverage probability, performance of the simultaneous confidence regions based on the bootstrap methods are compared with other competing ones. There may be other methods, but this study is limited to the simultaneous confidence regions explained in (2.1), (2.2), (2.5), and (2.6). Shapes of the confidence regions by using (2.1) and (2.2) are elliptical, while rectangular by using (2.5) or (2.6).

Samples were drawn from a multinomial distribution with parameters $(\pi_1, \pi_2, ..., \pi_r)$ and, for $\alpha = 0.05$ and 0.10, the confidence regions were constructed from 1000 bootstrap replications. The confidence regions were checked if they contained $(\pi_1, \pi_2, ..., \pi_r)$. For each sample, a random vector $(\pi_1, \pi_2, ..., \pi_r)$ was generated from a probability density function ξ . We obtained the results for two densities ξ for the averaging: (1) a uniform distribution over a simplex defined by $(\pi_1, \pi_2, ..., \pi_r)$; (2) a variation of a Dirichelet distribution concentrated around the center of the simplex. This was repeated 1000 times independently in order to get an estimate of the average coverage probability. Programming was done in Fortran PowerStation 4.0 compiled by an IBM PC. Random numbers from the required distributions were generated by using an IMSL subroutine. The results of this simulation are shown in Table 1.

Confidence region (2.1) based on a chi-squared distribution is poor for small sample sizes, but gets better as sample size increases. However, the bootstrap simultaneous confidence regions, (2.2) and (2.5), perform very well for even relatively small sample sizes. It is interesting to observe that there is no apparent difference between the two bootstrap confidence regions (2.2) and (2.5). Since each Bonferroni interval underestimates the coverage probability, average coverage probability of the simultaneous confidence for the Bonferroni method is fairly close to the nominal one in some cases. Similar phenomena was discovered by Agresti and Brent (1998) in

Table 1 Estimated average coverage probabilities for the simultaneous confidence intervals for $(\pi_1, \pi_2, ..., \pi_r)$. χ^2 , Boot1, Boot2 and Bonf refer to (2.1), (2.1), (2.5) and (2.6), respectively

				ζ: un	iform		ξ : variation of Dirichelet					
r	n	$(1-\alpha)$	χ^2	Boot1	Boot2	Bonf	χ^2	Boot1	Boot2	Bonf		
3	30	0.90	0.867	0.891	0.886	0.938	0.870	0.914	0.911	0.935		
		0.95	0.913	0.939	0.935	0.958	0.918	0.950	0.950	0.958		
	50	0.90	0.886	0.909	0.911	0.937	0.875	0.917	0.910	0.929		
		0.95	0.933	0.955	0.957	0.964	0.931	0.960	0.962	0.959		
	70	0.90	0.873	0.893	0.894	0.922	0.858	0.888	0.896	0.919		
		0.95	0.926	0.946	0.947	0.959	0.927	0.957	0.958	0.960		
	100	0.90	0.885	0.903	0.906	0.930	0.878	0.899	0.896	0.916		
		0.95	0.937	0.949	0.952	0.961	0.931	0.948	0.945	0.954		
	200	0.90	0.888	0.897	0.901	0.922	0.886	0.894	0.900	0.933		
		0.95	0.932	0.942	0.947	0.958	0.943	0.952	0.948	0.962		
4	30	0.90	0.839	0.870	0.871	0.915	0.818	0.884	0.884	0.902		
		0.95	0.886	0.918	0.925	0.937	0.870	0.928	0.930	0.935		
	50	0.90	0.866	0.901	0.902	0.922	0.845	0.910	0.906	0.903		
		0.95	0.912	0.948	0.942	0.956	0.905	0.960	0.956	0.943		
	70	0.90	0.865	0.907	0.898	0.913	0.851	0.903	0.899	0.907		
		0.95	0.914	0.944	0.945	0.950	0.906	0.949	0.950	0.942		
	100	0.90	0.859	0.898	0.891	0.911	0.858	0.895	0.892	0.902		
		0.95	0.916	0.945	0.942	0.948	0.915	0.945	0.946	0.942		
	200	0.90	0.884	0.908	0.904	0.921	0.881	0.896	0.896	0.920		
		0.95	0.942	0.953	0.955	0.958	0.927	0.944	0.951	0.953		
5	30	0.90	0.811	0.878	0.883	0.905	0.780	0.876	0.875	0.884		
		0.95	0.872	0.935	0.936	0.933	0.838	0.925	0.933	0.921		
	50	0.90	0.846	0.904	0.904	0.902	0.817	0.901	0.901	0.880		
		0.95	0.899	0.946	0.953	0.933	0.870	0.944	0.948	0.923		
	70	0.90	0.842	0.889	0.892	0.906	0.827	0.898	0.896	0.884		
		0.95	0.896	0.944	0.940	0.930	0.886	0.957	0.947	0.923		
	100	0.90	0.851	0.895	0.896	0.903	0.861	0.901	0.901	0.898		
		0.95	0.907	0.944	0.943	0.940	0.905	0.955	0.953	0.929		
	200	0.90	0.858	0.894	0.896	0.906	0.872	0.895	0.901	0.911		
		0.95	0.914	0.945	0.948	0.943	0.927	0.954	0.952	0.951		

the binomial case. But, Bonferroni intervals (2.6) overestimate the average coverage probability, especially for 90% confidence levels, even for large sample sizes. Overall, bootstrap confidence regions tend to outperform the classical ones in terms of having average coverage probabilities close to the nominal confidence levels.

4. Several populations

Let us assume that we are sampling from r independent multinomial populations. Let π_{ij} $(i=1,\ldots,r;\ j=1,\ldots,c;\ \pi_{ij}>0,\ \sum_{j=1}^{c}\pi_{ij}=1$ for all i) be the probability of

the *j*th category in the *i*th population. For a sample of n_i individuals or items from the *i*th population, let N_{ij} be the number of responses falling in the *j*th category for the *i*th population. The maximum likelihood estimators of the probabilities π_{ij} are $p_{ij} = N_{ij}/n_i$.

Suppose that we are interested in constructing simultaneous confidence intervals for all linear functions $\theta = \sum_{i=1}^r \sum_{j=1}^c b_{ij} \pi_{ij}$ where $\sum_{i=1}^r b_{ij} = 0$ for j = 1, ..., c. Now, θ is estimated by $\hat{\theta} = \sum_{i=1}^r \sum_{j=1}^c b_{ij} p_{ij}$ and we have $100(1 - \alpha)\%$ simultaneous confidence intervals of the form

$$\hat{\theta} - (\chi_{(r-1)(c-1)}^2(\alpha))^{1/2} s \le \theta \le \hat{\theta} + (\chi_{(r-1)(c-1)}^2(\alpha))^{1/2} s, \tag{3.1}$$

where $s^2 = \sum_{i=1}^{r} (1/n_i)(\sum_{j=1}^{c} b_{ij}^2 p_{ij} - (\sum_{j=1}^{c} b_{ij} p_{ij})^2).$

Confidence intervals of form (3.1) were obtained by Goodman (1964) based on Scheffé's F projection. However, the probability is $1 - \alpha$ that *all* contrasts will be included in their respective intervals. If we are interested in a specific set of, say K contrasts $\theta_1, \theta_2, \ldots, \theta_K$, then $100(1-\alpha)\%$ Bonferroni simultaneous confidence intervals can be obtained as

$$\hat{\theta}_k - s(\hat{\theta}_k) z_k \le \theta_k \le \hat{\theta}_k + s(\hat{\theta}_k) z_k \quad \text{for } k = 1, \dots, K,$$
(3.2)

where z_k is the $100(1 - \beta_k)$ th percentile of the standard normal distribution and $\sum_{k=1}^K \beta_k = \alpha/2$. However, Bonferroni intervals are rather conservative, and when K is large they are unnecessarily long. Goodman's confidence intervals of form (3.1) can be more powerful than the Bonferroni intervals, if the number of comparisons is large enough. It is well-known that Scheffé's F projection method is comparable with other multiple comparison tests as it considers all linear combinations. But, it is only a finite number of contrasts that are examined in any practical applications. Therefore, these procedures are wasteful, in the sense that the probability error rate is less than α , instead of being equal to it.

5. Bootstrap simultaneous confidence intervals

We apply the bootstrap method to construct simultaneous confidence intervals for the finite collection of linear combinations $\theta_1, \theta_2, \dots, \theta_K$. Consider a quantity

$$B_{(K)} = \max_{1 \le i \le K} \left[\frac{|\hat{\theta}_1 - \theta_1|}{s(\hat{\theta}_1)}, \frac{|\hat{\theta}_2 - \theta_2|}{s(\hat{\theta}_2)}, \dots, \frac{|\hat{\theta}_K - \theta_K|}{s(\hat{\theta}_K)} \right]$$

and as an estimator of the sampling distribution of $B_{(K)}$, use the bootstrap distribution of

$$B_{(K)}^* = \max_{1 \le i \le K} \left[\frac{|\hat{\theta}_1^* - \hat{\theta}_1|}{s(\hat{\theta}_1^*)}, \frac{|\hat{\theta}_2^* - \hat{\theta}_2|}{s(\hat{\theta}_2^*)}, \dots, \frac{|\hat{\theta}_K^* - \hat{\theta}_K|}{s(\hat{\theta}_K^*)} \right],$$

where $\hat{\theta}_k^* = \sum_{i=1}^r \sum_{j=1}^c b_{ij}^k p_{ij}^*$ and $s^{2*} = \sum_i^r (1/n_i)(\sum_j^c b_{ij}^2 p_{ij}^* - (\sum_j^c b_{ij} p_{ij}^*)^2)$ with p_{ij}^* the maximum likelihood estimator for the bootstrap sample.

Beran (1988) showed that the bootstrap approaches can handle the asymptotics for a finite number of linear combinations. Given a sample from multinomial populations, $100(1-\alpha)\%$ bootstrap simultaneous confidence intervals for $\theta_1, \theta_2, \dots, \theta_K$ are

$$\hat{\theta}_k - s(\hat{\theta}_k)Q(1-\alpha) \le \theta_k \le \hat{\theta}_k + s(\hat{\theta}_k)Q(1-\alpha) \quad \text{for } k = 1, \dots, K,$$
(3.3)

where $Q(1-\alpha)$ is the $100(1-\alpha)$ th percentile of the bootstrap distribution of $B_{(K)}^*$. Note that only the finite number of contrasts of interest were considered in constructing the bootstrap simultaneous confidence intervals, and there is no loss that happened in either Scheffé's projection or the Bonferroni inequality. Thus there is no waste in coverage probability for the bootstrap method, which is a clear advantage over the others.

6. Simulation study

As in Section 2, a Monte Carlo investigation was done to compare the procedures introduced. By using the average probability, performance of the bootstrap simultaneous confidence regions are compared with that of the other competing ones. There may be other methods, but this study is limited to the simultaneous confidence regions explained in (3.1)–(3.3).

Samples were drawn from a multinomial distribution with parameters π_{ij} (i = 1, ..., r; j = 1, ..., c; $\pi_{ij} > 0$, $\sum_{j=1}^{c} \pi_{ij} = 1$ for all i) and, for $\alpha = 0.05$ and 0.10, the confidence intervals were constructed from 1000 bootstrap replications. The confidence intervals were checked if they contained $\theta_1, \theta_2, ..., \theta_K$. For the finite number of linear combinations, the following two cases were considered.

Case	1:	r = 3,	c = 3,	K = 3,	with	b_{ij}	of	the	type
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		b^1_{ij}			b_{ij}^2			b_{ij}^3			
	1	2	3	1	2	3	1	2	3		
1	1	2	3	1	2	3	0	0	0		
2	-1	-2	-3	0	0	0	1	2	3		
3	0	0	3	-1	-2	-3	-1	-2	-3		

Case 2: r = 3, c = 4, K = 5, with b_{ij} of the type

b^1_{ij}				b	2 i <i>j</i>			b_{ij}^3		b_{ij}^4				b_{ij}^5						
	1	2	3	4	1	2	3	4	1	2	3	4	1	2	3	4	1	2	3	4
1	1	2	3	4	1	2	3	4	0	0	0	0	1	2	3	4	2	4	6	8
2 -	-1	−2 ·	-3	-4	0	0	0	0	1	2	3	4	-2	-4	-6	-8	-1	-2	-3	-4
3	0	0	0	0	-1	-2	-3	-4	-1	-2	-3	-4	1	2	3	4	-1	-2	-3	<u>-4</u>

Table 2 Estimated average coverage probabilities for the simultaneous confidence intervals for $\theta_1, \theta_2, \dots, \theta_K$. Goodman, Bonferroni and Bootstrap refer to (3.1), (3.2) and (3.3), respectively

			ξ : Uniform		ξ : Variation of Dirichelet					
n_i	$1-\alpha$	Goodman	Bonferroni	Bootstrap	Goodman	Bonferroni	Bootstrap			
Case 1										
30	0.900	0.979	0.886	0.885	0.982	0.899	0.900			
	0.950	0.991	0.939	0.947	0.992	0.935	0.942			
50	0.900	0.977	0.911	0.905	0.977	0.890	0.887			
	0.950	0.992	0.950	0.952	0.991	0.940	0.942			
70	0.900	0.989	0.902	0.890	0.977	0.918	0.908			
	0.950	0.997	0.953	0.951	0.990	0.954	0.956			
100	0.900	0.983	0.918	0.904	0.975	0.922	0.914			
	0.950	0.989	0.954	0.950	0.988	0.952	0.950			
Case 2										
30	0.900	0.992	0.924	0.901	0.988	0.933	0.889			
	0.950	0.999	0.953	0.944	0.995	0.970	0.951			
50	0.900	0.996	0.921	0.885	0.994	0.936	0.908			
	0.950	0.997	0.951	0.940	0.997	0.961	0.946			
70	0.900	0.992	0.932	0.901	0.995	0.937	0.896			
	0.950	0.996	0.962	0.943	0.998	0.968	0.951			
100	0.900	0.996	0.928	0.883	0.995	0.933	0.886			
	0.950	0.998	0.968	0.948	0.998	0.973	0.946			

For each sample, a random vector $\{\pi_{ij}: j=1,\ldots,c\}$ was generated from a probability density function ξ . We obtained the results for two densities ξ for the averaging: (1) a uniform distribution over a simplex defined by $(\pi_{i1},\pi_{i2},\ldots,\pi_{ic})$ for each i; (2) a variation of a Dirichelet distribution concentrated around the center of the simplex, as in Section 2. This was repeated 1000 times independently in order to get an estimate of the average coverage probability. Table 2 shows the estimated average coverage probabilities at various sample sizes. Fig. 1 illustrates the simulation results for two densities ξ as a function of sample size.

Goodman's simultaneous intervals (3.1) have greater estimated coverage probability than the nominal one as expected, because it considers all possible linear combinations. Bonferroni intervals also have greater estimated average coverage than the nominal one, and as the number of linear combinations increases the difference becomes larger. Increasing sample size does not help the overestimation problem. By contrast, estimated average coverage probability of the bootstrap method is close to the nominal confidence level even for small sample sizes in both cases.

In conclusion, the proposed bootstrap method is more accurate, at least in terms of average coverage probability, and is not wasteful since it considers only a finite number of contrasts of interest.

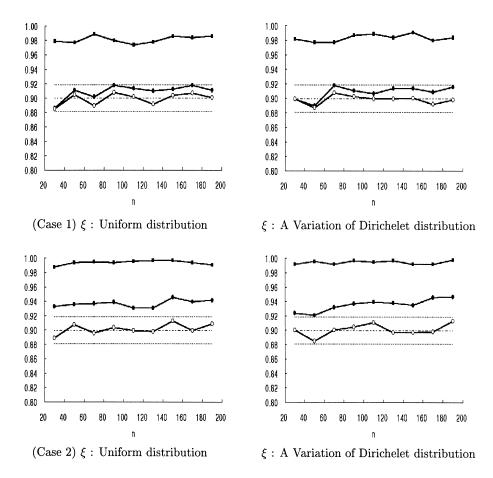


Fig. 1. Estimated average coverage probabilities as a function of sample size n for $1 - \alpha = 0.9$. Goodman (\blacksquare Line), Bonferroni (\bullet Line) and Bootstrap (\circ Line) are computed from (3.1), (3.2) and (3.3), respectively. The dotted lines gives the 95% upper and lower limit of nominal coverage probability 0.9.

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