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Balanced Simultaneous Confidence Intervals in Logistic Regression Models

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ABSTRACT

Simultaneous confidence intervals for the parameters in the logistic regression models with random regressors are considered. A method based on the bootstrap and its stochastic approximation will be developed. A key idea in using the bootstrap method to construct simultaneous confidence intervals is the concept of prepivoting which uses the transformation of a root by its estimated cumulative distribution function. Repeated use of prepivoting makes the overall coverage probability asymptotically correct and the coverage probabilities of the individual confidence statements asymptotically equal. This method is compared with ordinary asymptotic methods based on Scheffe's and Bonferroni's through Monte Carlo simulation.

1. INTRODUCTION

Simultaneous confidence intervals for the linear combinations $u^t\beta$ are constructed, where u is a p-dimensional vector of parameters in the logistic regression model. The model will be described briefly in the next section. A resampling approach described in this paper generates simultaneous confidence intervals which possess the following two properties:

(i) the overall coverage probability is asymptotically correct;

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(ii) the coverage probabilities of the individual confidence statements which define the simultaneous confidence intervals are asymptotically equal.

Property (ii) is termed asymptotic balance. It means that the simultaneous confidence intervals treat each constituent confidence statement fairly. An example of balanced simultaneous confidence intervals is Scheffe's method for the parameters in the context of normal linear models, see for example, Miller(1981). For the present paper, notations and theorems from Beran(1988) will be used. The index set $\mathcal{U}$ in our case contains a finite number of elements, which includes the important cases such as individual components of the vector β, Scheffe's simultaneous confidence intervals for linear contrasts, and Tukey's simultaneous confidence intervals for pairwise contrasts.

In section 2, the model to be discussed is described and some asymptotic properties of the maximum likelihood estimator for the parameter β are summarized. In section 3, a method of constructing balanced simultaneous confidence intervals will be explained briefly, then in the last section a Monte Carlo study is provided to compare this method with some other classical approaches.

2. MODEL AND MLE

Suppose we have n independent and identically distributed random vectors $(Y_i, X_i{}^t)$ for $i = 1, 2, \cdots, n$ such that the covariates X_is are p-variate random vectors with unknown distribution function $G(x)$. Assume that the third moment of X_i exists. Given $X = x$, the random response Y takes value 1 with probability $p = 1/[1 + \exp(-x^t\beta)]$, and take value 0 with probability $1 - p$.

In the sequel, β_0 denotes the true but unknown parameter of the probability model which is supposed to generate our sample, and β is any parameter in the p-dimensional Euclidean space $\mathcal{B}$ such that $X^t\beta$ lies in the real line with probability 1. The following gives a summary of the probability model to be considered and the estimators to be used in this paper. For a more detailed account of the binary response models including the logistic regression models, see McCullagh and Nelder(1990).

Log-likelihood for a single observation is given by

$$l(\beta, G; y, x) = yx^t - \log[1 + \exp(x^t\beta)] + \text{constants.} \tag{2.1}$$

Easily, using the chain rule, it can be shown that the first derivative and the second derivative of l with respect to β are given by

$$\nabla l = x(y-p), \text{ and} \tag{2.2}$$

$$\nabla^2 l = -xx^t p(1-p), \text{ respectively.} \tag{2.3}$$

So the information matrix with respect to β is given by

$$I(\beta) = E[XX^t p(1-p)], \tag{2.4}$$

which can be consistently estimated by

$$\hat{I} = \frac{1}{n}\sum_{i=1}^{n} X_i X_i{}^t \hat{p}_i(1-\hat{p}_i), \tag{2.5}$$

where $\hat{p}_i = 1/[1+\exp(-X_i\hat{\beta}_n)]$, and $\hat{\beta}_n$ is the maximum likelihoood estimator of β_0.

We have the usual asymptotic results such as strong consistency, and asymptotic normality of the maximum likelihood estimator of β_0. McCullagh and Nelder(1983) gives an iterative algorithm to obtain such a solution. For a more detailed account of asymptotic results in more general set up, see Fahrmeir and Kaufmann (1985). Section 2 of Lee(1990) gives a more detailed account of the probability model, the resampling algorithm and the asymptotic validity of bootstrap approximation.

3. CONSTRUCTION OF BALANCED SIMULTANEOUS CONFIDENCE INTERVALS

Let $\mathcal{T}_n$ be the set of all possible values of $u^t\beta$ as β ranges over the parameter set $\mathcal{B}$. Approximate confidence intervals for $u^t\beta$ may be obtained by referring a function of $u^t\beta$ and of the sample to an estimated quantile of that function's sampling distribution. This function is called the root of the confidence intervals, and will be denoted by $R_{n,u}$. Either asymptotic theory or bootstrap methods can be used to estimate the quantile. Beran(1987) suggests that studentizing reduces level error in general. He also suggests that, when the asymptotic distribution of the roots $\{R_{n,u}\}$ are identical; and when the asymptotic distribution of $\sup_u R_{n,u}$ is continuous and does not depend on the unknown parameter, say θ, asymptotically, the simultaneous confidence intervals are balanced and has overall coverage probability $1-\alpha$. Therefore as a root

$$R_{n,u} = |n^{1/2}u^t(\hat{\beta}_n - \beta)|/(u^t\hat{I}^{-1}u)^{1/2} \tag{3.1}$$

will be used for confidence intervals of the form;

$$u^t\hat{\beta}_n \pm d_{n,u}\hat{\sigma}_{n,u}/n^{1/2}, \tag{3.2}$$

where $\hat{\sigma}_{n,u} = (u^t\hat{I}^{-1}u)^{1/2}$, and $d_{n,u}$ is the critical value determined from the sample.

The following triangular array argument will be needed in the construction of the balanced simultaneous confidence intervals based on bootstrap. Refer to Lee(1990) for the sketch of the proof.

Triangular Array Convergence

Let ρ denote Prohorov metric on $\mathcal{G}$, the space of the cumulative distribution function of the covariates $G(\cdot)$. Huber(1981, chapter 2) gives a detailed account of various metrics which metrize probability measures. Define the following distance on $\Theta = \mathcal{B} \times \mathcal{G}$; if $\theta_1 = (\beta_1, G_1), \theta_2 = (\beta_2, G_2)$, where β_1, β_2 belong to $\mathcal{B}$, and G_1, G_2 belong to $\mathcal{G}$, then for some metric $\|\cdot\|$ on the space of positive definite matrices,

$$d(\theta_1, \theta_2) = \rho(G_1, G_2) + |\beta_1 - \beta_2| + \|I(\beta_1) - I(\beta_2)\|.$$

Let $\theta_n = (\beta_n, G_n)$ be a sequence of parameters such that the distance $d(\theta_n, \theta)$ tends to 0 as n tends to ∞. Throughout, $\mathcal{L}(\cdot|P)$ denotes the probability law of a random variable under probability measure P. P_n denotes the probability measure when the parameters in our model are given by $\theta_n = (\beta_n, G_n)$. Then

$$\mathcal{L}(R_{n,u}|P_n) \rightarrow |\ Z\ | \text{ in distribution }, \tag{TAC}$$

where Z is a standard normal random variable.

By simultaneously asserting the above confidence intervals, we obtain simultaneous confidence intervals for the family of parametric functions of the form, $\{u^t\beta; u \in \mathcal{U}\}$. More fully, let $\mathcal{T}$ denote the set of all possible values of $\{u^t\beta; u \in \mathcal{U}\}$ as β ranges over $\mathcal{B}$. Every point in this range can be written in a component form $\{u^t\beta; u \in \mathcal{U}\}$, where $u^t\beta \in \mathcal{T}_u$. In this notation, the simultaneous confidence intervals described above can be written as

$$u^t\beta_n \pm d_{n,u}\sigma_{n,u}/n^{1/2} \text{ for all } u \in \mathcal{U}. \tag{3.3}$$

The critical value $d_{n,u}$ is determined from the sample in a manner to be specified below.

Remark. Potentially we are interested in the construction of a confidence band for the probability of success, $E(Y|x)$, which is given by $1/[1+\exp(-x^t\beta)]$. This can be done by a delta method, and will not be explored in the present paper.

Construction of Balanced Simultaneous Confidence Intervals

The following describes an algorithm to construct balanced simultaneous confidence intervals based on bootstrap method.

(i) Let $H_{n,u}(\,\cdot\,,\theta)$ be the left continuous cumulative distribution function of the root $R_{n,u}$, and $H_n(\,\cdot\,,\theta)$ be the left continuous cumulative distribution function of the transformed root $\sup_u\{H_{n,u}(R_{n,u},\theta)\}$.

(ii) Natural, plug-in estimates of $H_{n,u}$ and H_n are, respectively,

$$\hat{H}_{n,u}=H_{n,u}(\,\cdot\,,\hat{\theta}),\ \text{and}\ \hat{H}_n=H_n(\,\cdot\,,\hat{\theta}),\ \text{where}\ \hat{\theta}_n=(\hat{\beta}_n,\hat{G}_n), \tag{3.4}$$

a consistent estimator of θ. The maximum likelihood estimator and the empirical cumulative distribution function from the covariates will be used, that is, the above estimators are bootstrap versions of $H_{n,u}$ and H_n, respectively.

(iii) Find the largest t-th quantiles of $H_{n,u}$ and H_n. That is, let

$$\hat{H}_{n,u}^{-1}(t)=\sup\{x:\hat{H}_{n,u}(x) \tag{3.5}$$

$$\hat{H}_n^{-1}(t)=\sup\{x:\hat{H}_n(x)\le t\}. \tag{3.6}$$

(iv) Then a bootstrap version of the simultaneous confidence intervals is given by

$$u^t\hat{\beta}_n\pm d_{n,u}\hat{\sigma}_{n,u}/n^{1/2}\ \text{for all}\ u\in\mathcal{U}, \tag{3.7}$$

where $d_{n,u}=\hat{H}_{n,u}^{-1}[\hat{H}_n^{-1}(1-\alpha)]$.

Remark. It should be pointed out here that (3.4) implies the bootstrap samples are drawn from the Bernoulli distribution in a parametric way as described in section 2 of Lee(1990). If you draw the pairs with replacement, then you are dealing with a different probability model as explained in section 3 of Lee(1990).

The calculation of $d_{n,u}$ involves two steps;

(a) Find the largest $(1-\alpha)$-th quantile of $\hat{H}_n$ and call it c_n.

(b) Find the largest c_n-th quantile of $\hat{H}_{n,u}$ for all $u \in \mathcal{U}$.

This is the critical value in (3.7). For a motivation of such a critical value, see Beran(1990). The above simultaneous confidence intervals can be rewritten as follows;

$$\{\,\cdot\,; \hat{H}_n[\sup_u \hat{H}_{n,u}\{R_{n,u}(\,\cdot\,)\}] \le 1-\alpha\}. \tag{3.8}$$

The key idea visible in the above representation is the concept of prepivoting, first introduced in Beran(1987), which means the transformation of a root by its estimated cumulative distribution function. Prepivoting takes $R_{n,u}$ into $\hat{H}_{n,u}\{R_{n,u}(\,\cdot\,)\}$, whose asymptotic distribution is usually uniform on the interval (0, 1) for every choice of u. This property ensures the asymptotic balance of the simultaneous confidence intervals given above. Prepivoting also takes $\sup_u \hat{H}_{n,u}\{R_{n,u}(\,\cdot\,)\}$ into $\hat{H}_n[\sup_u H_{n,u}\{R_{n,u}(\,\cdot\,)\}]$, whose asymptotic distribution is again typically uniform on the interval (0, 1). This property ensures that the asymptotic coverage probability of the simultaneous confidence intervals described above is $1-\alpha$.

The following is an easy consequence of Theorem 4.1 in Beran(1988). We just have to check the *Assumptions 1 ~ 4* therein, so the details will be omitted.

Theorem 3.1. Suppose $\alpha \in (0,1)$, and $\lim_{n\to\infty}\theta_n = \theta$. Then

$$\lim_{n\to\infty} P_n(u^t\beta_n \in u^t\hat{\beta}_n \pm d_{n,u}\hat{\sigma}_{n,u}/n^{1/2} \text{ for all } u \in \mathcal{U}) = 1-\alpha \tag{3.9}$$

and

$$\lim_{n\to\infty} \sup_u |P_n(u^t\beta_n \in u^t\hat{\beta}_n \pm d_{n,u}\hat{\sigma}_{n,u}/n^{1/2}) - H^{-1}(1-\alpha)| = 0, \tag{3.10}$$

where $H^{-1}(1-\alpha)$ is the $(1-\alpha)$-th quantile of the cumulative distribution function of a random variable $\sup_u \Psi(|u^tW|/(u^tI^{-1}(\beta_0)u)^{1/2})$ with W distributed according to a p-variate normal distribution having 0-mean vector and $I^{-1}(\beta_0)$ as its covariance matrix, and $\Psi(\,\cdot\,)$ is the folded standard normal distribution function, i.e., the distribution function of $|\,Z\,|$ when Z is a standard normal random variable. Moreover, $\hat{H}_n^{-1}(1-\alpha)$ tends in P_n probability to $H^{-1}(1-\alpha)$.

For example, when $\mathcal{U}$ is a subspace of dimension q, the second statement of the theorem reduces to

$$\lim_{n\to\infty} \sup_u |P_n(u^t\beta_n \in u^t\hat{\beta}_n \pm d_{n,u}\hat{\sigma}_{n,u}/n^{1/2}) - \Psi[\zeta_q{}^{1/2}(1-\alpha)]| = 0, \qquad (3.11)$$

where $\zeta_q(1-\alpha)$ is the $(1-\alpha)$-th quantile of χ^2- distribution with q degrees of freedom. Moreover $\hat{H}_n^{-1}(1-\alpha)$ tends in P_n probability to $H^{-1}(1-\alpha)$, where $H(\cdot)$ is the cumulative distribution function of χ^2-distribution with q degrees of freedom.

For practical purposes, a stochastic approximation to the simultaneous confidence intervals suggested above is available, which makes this idea widely applicable.

Stochastic Approximation to (3.7)

(i) Given the original data $Z_n = \{(Y_i, X_i{}^t); i = 1, \cdots, n\}$, draw B_n conditionally independent bootstrap samples $Z^*_{n,1}, \cdots, Z^*_{n,B_n})$, each of size n, from the fitted model $\hat{P}_n$.

(ii) For every u in $\mathcal{U}$, form $\hat{H}^*_{n,u}$, the left continuous cumulative distribution function of the bootstrapped roots $\{R^*_{n,u,j} = R_{n,u}(Z^*_{n,j}, \hat{\theta}_n) : 1 \le j \le B_n\}$. Glivenko- Cantelli theorem tells us that this cumulative distribution function approximates $\hat{H}_{n,u}$. A detailed account of Glivenko-Cantelli theorem can be found in, for example, Billingsley(1979).

(iii) For every value of j, let

$$s_{n,j.} = \sup_u \hat{H}^*_{n,u}(R^*_{n,u,j}) = \sup_u[\text{rank}(R^*_{n,u,j}) - 1], \qquad (3.12)$$

the rank being calculated among the B_n possible values of its argument.

(iv) Form $\hat{H}^*_n$, the left continuous cumulative distribution function of the values compute in (iii), $\{s_{n,j} : 1 \le j \le B_n\}$. This cumulative distribution function approximates $\hat{H}_n$ by Glivenko-Cantelli theorem.

(v) Find c^*_n, the largest $(1-\alpha)$-th quantile of $\hat{H}^*_n$.

(vi) Find $d^*_{n,u}$, the largest c^*_n-th quantile of $\hat{H}^*_{n,u}$, which approximates $d_{n,u}$.

(vii) Define the simultaneous confidence intervals by analogy with the previous ones as follows;

$$u^t\hat{\beta}_n \pm d^*_{n,u}\hat{\sigma}_{n,u}/n^{1/2}. \qquad (3.13)$$

Let Q_n denote the joint distribution of $(Z_n, Z^*_{n,1}, \cdots, Z^*_{n,B_n})$ when Z_n has the distribution P_n. Formally

$$Q_n(A) = \int_A \hat{P}_n^{B_n}(dz^*)P_n(dz) \tag{3.14}$$

for every measurable subset A in the range of $(Z_n, Z^*_{n,1}, \cdots, Z^*_{n,B_n})$. Note that z^* can be written as

$$z^* = (z^*_1, \cdots, z^*_{B_n}), \tag{3.15}$$

where z_j^* takes values in $R^{p+1} \times R^n$ Euclidean space.

The following theorem states that the stochastic approximation version just described gives similar results to Theorem 3.1. It is also an easy consequence of Theorem 4.2 in Beran(1988).

Theorem 3.2. Besides the assumptions in Theorem 3.1, suppose that B_n tends to ∞ as n increases. Then for the stochastic approximation versions of the simultaneous confidence intervals given by (3.13), the same results as those in Theorem 3.1 also hold with respect to Q_n probability.

4. SIMULATION

A Monte Carlo study is provided to compare the ordinary asymptotic methods with the bootstrap in terms of coverage probabilities of simultaneous confidence intervals. Note that the ordinary Edgeworth expansion argument is not available in this logistic regression model due to the lattice structure of the response Y_i's, see for example, Feller(1971, p.539). Usually an analytic comparison of confidence intervals is based on the Edgeworth type expansions. See, for example, Hall(1986a, 1988), Beran(1987), etc. for this line of argument. Therefore it is an interesting situation to compare the conventional methods with bootstrap methods when the expansion argument is not available.

In this study, the number of parameters are 2, so our model is given by

$$\log p_i/(1 - p_i) = \beta_0 + \beta_1 x_i, \tag{4.1}$$

where $Y_i|X_i = x_i$ has a Bernoulli distribution with parameter p_i. Simultaneous confidence intervals for the components β_0 and β_1 will be constructed. Since only two statements are concerned simultaneously, the most popular conventional method can be that of Bonferroni's. Also, Scheffe's method is another possible candidate, which is supposedly very conservative.

Uniform distribution over the interval (0, 1) is taken as the distribution of X_i, which will be standardized during the simulation. To find the maximum likelihood estimators, the algorithm given in McCullagh and Nelder(1990) is used with subroutines *ssifa* and *ssisl* in *linpack* library to solve the simultaneous equation. To generate uniform random numbers *g05caf* function in *NAG* mathematical library is used.

To compute coverage probabilities in the ordinary asymptotics, it can be easily checked that; the critical values are given by 1.960394 ($\alpha = 0.1$), and 2.241845 ($\alpha = 0.05$) for Bonferroni's method, and they are given by $\zeta_2^{1/2}(.90) = 2.145966$, and $\zeta_2^{1/2}(.95) = 2.447747$ for Bonferroni's method. The functions *qnorm* , and *qchisq* in *S* are used to calculate these values.

The stochastic approximation algorithm described in section 3 is used for the computation of the bootstrap coverage probabilities, since no closed form expression of $\hat{H}_{n,u}$ is available. The number of bootstrap replications, B_n, are set at both 99 and 1,000. See Hall(1986b) for the use of the number of replications 99. Smaller numbers of replications like 19 do not seem to give correct coverage probabilities. Due to frequent occurrences of singular covariance matrices, sample sizes n are set at 100, 200, and 400. For sorting and ranking, *m01ajf* and *m01anf* functions in *nag* mathematical library are used with a little modification.

In each case, the number of replications are set at 1000, so the standard errors attached to each simulated coverage probabilities are around $(0.9 \times 0.1/1000)^{1/2} \approx 0.01$ or so. Throughout C_{Bonf} denotes asymptotic methods based on Bonferroni's, $C_{Scheffe}$ denotes asymptotic methods based on Scheffe's, and $C_{B_{99}}$ and $C_{B_{1000}}$ denote bootstrap methods with the number of bootstrap resampling 99 and 1000, respectively.

Table 1 compares critical values obtained by each method. As previously explained, the critical values for C_{Bonf} and $C_{Scheffe}$ are found from the standard tables, and the critical values for $C_{B_{99}}$ and $C_{B_{1000}}$ are calculated by averaging the critical values obtained at each replication, which uses the stochastic approximation algorithm described in section 3. As we have already expected, Bonferroni method gives smaller critical values than Scheffe's. The bootstrap methods give critical values which vary from case to case. For bootstrap methods with resampling size 99, the standard errors attached to the estimated critical values are ranging from 0.17 to 0.4, while the standard errors with resampling size 1000 are ranging from 0.05 to 0.27.

Table 2 compares the estimated coverage probabilities. Each method should be compared in terms of both overall coverage probability and balancedness. Scheffe's method gives very conservative confidence intervals as expected, since this method is intended for the simultaneous intervals for all the linear combinations. In case of normal error linear regression models, which can be regarded as the case when $n = \infty$ with known error variance, we expect the marginal coverage probabilities for Scheffe's method to be .968124 and .985624 when $\alpha = 0.10$ and $\alpha = 0.05$ respectively, and we can check this out from a couple of cases in the table. Note the excellent performance of Bonferroni method when the number of statements is small (in this case, 2). In case of normal error linear models, we expect that the overall coverage probabilities would be at least 0.90 and 0.95 for $\alpha = 0.10$ and $\alpha = 0.05$, respectively, and we can see that the errors in coverage probabilities are relatively small.

Table 3 summarizes errors for each method in overall coverage probabilities. Both $C_{B_{99}}$ and $C_{B_{1000}}$ give reasonably good coverage probabilities. Unfortunately, the rate of bias reduction is not detectable in this study.

To compare balancedness, Imbalance of each method is computed for each case, which in this case is just an absolute value of difference in each marginal probabilities. See Beran(1990) for this new terminology. Table 4 summarizes Imbalance of each methods. $C_{B_{99}}$ and $C_{B_{1000}}$ give more stable Imbalance than the other two in that in two cases out of six, $C_{Scheffe}$ and C_{Bonf} give Imbalance of more than 0.02 while the other two methods do not. But it is not so clear to see which one is the best method in terms of Imbalance.

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Tables

Table 1: Critical Values

$1-\alpha$		.90			.95		
n		100	200	400	100	200	400
$C_{Scheffe}$		2.1460	2.1460	2.1460	2.4477	2.4477	2.4477
C_{Bonf}		1.9604	1.9604	1.9604	2.2418	2.2418	2.2418
$C_{B_{99}}$	β_0	1.8875	1.9380	1.9493	2.1522	2.2088	2.1350
	β_1	2.1937	2.1407	2.1074	2.5274	2.4503	2.4069
$C_{B_{1000}}$	β_0	1.8726	1.8991	1.9229	2.1352	2.1668	2.2011
	β_1	2.1658	2.1015	2.0910	2.5114	2.4135	2.4000

Table 2: Estimated Coverage Probabilities

$1-\alpha$		.90			.95		
n		100	200	400	100	200	400
$C_{Scheffe}$	β_0	.977	.957	.967	.994	.981	.984
	β_1	.950	.967	.954	.971	.981	.979
	β_0, β_1	.929	.926	.925	.966	.963	.964
C_{Bonf}	β_0	.951	.945	.949	.987	.974	.972
	β_1	.930	.950	.932	.962	.971	.961
	β_0, β_1	.886	.898	.888	.950	.947	.938
$C_{B_{99}}$	β_0	.936	.946	.955	.966	.975	.979
	β_1	.951	.950	.955	.980	.974	.973
	β_0, β_1	.895	.900	.915	.947	.952	.953
$C_{B_{1000}}$	β_0	.941	.939	.953	.966	.975	.980
	β_1	.951	.950	.939	.980	.974	.966
	β_0, β_1	.898	.896	.899	.955	.944	.950

Table 3: Errors in Overall Coverage Probabilities

$1-\alpha$	.90			.95		
n	100	200	400	100	200	400
$C_{Scheffe}$	.029	.026	.025	.016	.013	.014
C_{Bonf}	.014	.002	.012	.000	.003	.012
$C_{B_{99}}$	.005	.000	.015	.003	.002	.003
$C_{B_{1000}}$	.002	.004	.001	.005	.006	.000

Table 4: Imbalance

$1-\alpha$	.90			.95		
n	100	200	400	100	200	400
$C_{Scheffe}$	.027	.010	.013	.023	.000	.005
C_{Bonf}	.021	.005	.003	.025	.003	.011
$C_{B_{99}}$	.017	.004	.000	.014	.001	.006
$C_{B_{1000}}$	.010	.011	.014	.014	.001	.014