

TR/05/85

March 1985

Properties of Estimators of  
Parameters in Logistic Regression Models.

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z1486051

## Summary

Properties of various types of estimators of the regression coefficients in linear logistic regression models are considered. The estimators include those based on maximum likelihood, minimum chi-square and weighted least squares. Theoretical approximations to the biases of the estimators are developed. The results of a large scale simulation investigation evaluating the moment properties of the estimators are presented for the case of a logistic model with a single explanatory variable.

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## 1. Introduction

In the statistical analysis of binary data when explanatory variables are present, the logistic regression model plays a central role. To introduce the model, let  $Y_1, Y_2, \dots, Y_g$  represent  $g$  independent binomial random variables where  $Y_i$  represents the number of successes in a set of  $n_i$  independent trials. For the  $i$ th group, let  $x_{i1}, \dots, x_{ik}$ , denote the values on  $k$  explanatory variables which are thought to influence the individual trial probability of success, denoted by  $P_i$ , for the  $i$ th group,  $i=1, \dots, g$ . For this situation, the linear logistic regression model is

$$\text{Log} (P_i / Q_i) = \sum_{j=1}^k \tilde{x}_{ij} \tilde{\beta}_j, \quad i = 1, \dots, g \quad (1.1)$$

where  $Q_i = 1 - P_i$  and

$$\tilde{x}_{ij} = (1, x_{i1}, \dots, x_{ik}), \quad \tilde{\beta}' = (\beta_0, \beta_1, \dots, \beta_k) \quad (1.2)$$

The regression coefficients in  $\tilde{\beta}$  are usually all unknown and there are a number of well-known methods for estimating them (see Berkson, (1955)) which we now review.

### (i) Maximum Likelihood

The most commonly used method of estimation is probably maximum likelihood (ML), since these estimates can now be routinely obtained using statistical packages such as GLIM (Baker and Belder 1978),

The kernel of the log-likelihood may be written as

$$\Gamma(\tilde{\beta}) = \sum_{i=1}^g n_i \{ p_i \tilde{x}_{i0} \tilde{\beta} - \log(1 + e^{\tilde{x}_{i0} \tilde{\beta}}) \} \quad (1.3)$$

where  $p_i = y_i/n_i$  denotes the observed proportion of successes in the  $i$ th group. In matrix form the first and second order derivatives of the log-likelihood are given by

$$\frac{\partial L(\tilde{\beta})}{\partial(\tilde{\beta})} = \begin{bmatrix} \sum_i n_i X_{i0} (p_i - p_i) \\ \sum_i n_i X_{i1} (p_i - p_i) \\ \vdots \\ \sum_i n_i X_{ik} (p_i - p_i) \end{bmatrix} \quad (1.4)$$

$$\frac{\partial R(\beta)}{\partial \tilde{\beta}} = \begin{bmatrix} \sum_i n_i x_{i0} \left( q_i^2 \frac{p_i}{Q_i} - p_i^2 \frac{Q_i}{p_i} \right) \\ \sum_i n_i x_{i1} \left( q_i^2 \frac{p_i}{Q_i} - p_i^2 \frac{Q_i}{p_i} \right) \\ \sum_i n_i x_{ik} \left( q_i \frac{p_i}{Q_i} - p_i^2 \frac{Q_i}{p_i} \right) \end{bmatrix}$$

$$\frac{\partial^2 R(\beta)}{\partial \tilde{\beta} \partial \tilde{\beta}'} = \tilde{X}' \tilde{V}_2 \tilde{X} \quad (1.13)$$

Where

$$\tilde{V}_2 = \text{diag} \left( \left( n_i \left( p_i^2 \frac{Q_i}{p_i} + q_i^2 \frac{p_i}{Q_i} \right) \right) \right) \quad (1.14)$$

If we put

$$\tilde{D}_2 = \left( \frac{\partial R(\beta)}{\partial \tilde{\beta}} \right)_{\tilde{\beta} = \hat{\tilde{\beta}}_2} \quad \tilde{V}_2 = \left( \tilde{V}_2 \right)_{\tilde{\beta} = \hat{\tilde{\beta}}_2} \quad (1.15)$$

then  $\hat{\tilde{\beta}}_2$  is given by the solution of the  $k+1$  equations given by

$$\tilde{D}_2 = 0 \quad (1.16)$$

An iterative solution can again be found using a Newton-Raphson approach similar to that outlined for the maximum likelihood estimation procedure. The calculations are conveniently performed using GLIM as follows. If we let

$$Y_{i1} = n_i p_i^2, \quad Y_{i2} = n_i q_i^2 \quad (1.17)$$

$$\mu_{i1} = \exp \left( \tilde{X}_i' \tilde{\beta} \right) \quad \mu_{i2} = \exp \left( - \tilde{X}_i' \tilde{\beta} \right) \quad (1.18)$$

then from (1.11), minimization of  $R(\beta)$  is equivalent to minimization of

$$R^*(\beta) = \sum_i (y_{i1} \mu_{i1}^{-1} + Y_{i2} \mu_{i2}^{-1}) \quad (1.19)$$

Minimisation of  $R^*(\beta)$  is seen to be equivalent to maximisation of the log-likelihood when the  $\{y_{i1}\}$  and  $\{y_{i2}\}$  are treated as observations on independent exponentially distributed random variables with means  $\mu_{i1}$  and  $\mu_{i2}$  respectively. To use GLIM, the data are entered as  $g$  pairs of vectors of observations, the vectors for the  $t$ th pair being

$$\frac{(n_i + 1)(n_i + 2)}{n_i^3 (p_i + n_i^{-1})(q_i + n_i^{-1})} = w_i^{*-1} \quad \text{say} \quad (1.27)$$

A modified WLS estimate is therefore given by the value of  $\beta$  which minimizes

$$S^*(\beta) = \sum_{i=1}^g W_i^* (Z_i^* - X_i^* \beta)^2 \quad (1.28)$$

for which the solution is

$$\hat{\beta}_{\sim 4} = (X' W^* X)^{-1} X' W^* Z^* \quad (1.29)$$

where  $Z^* = (Z_1^*, \dots, Z_g^*)$  and  $W^* = \text{diag}((n_i(p_i + n_i^{-1})(q_i + n_i^{-1}) / (1 + n_i^{-1})(1 + 2n_i^{-1})))$ .

If we let  $N = \sum_{i=1}^g n_i$  and assume that with fixed  $g$

$$\lim_{n_i \rightarrow \infty} n_i / N = \lambda_i, \quad i = 1, \dots, g \quad (1.30)$$

where  $0 < \lambda_i < 1$ , then if the logistic regression model is correct, it is well-known that

$$N^{1/2}(\hat{\beta}_{\sim} - \beta) \xrightarrow{d} MN(0, (X' V X)^{-1}) \quad (1.31)$$

where  $V = \text{diag}((\lambda_i p_i q_i))$  and we use  $\hat{\beta}_{\sim}$  to denote any estimator from the set  $\{\hat{\beta}_{\sim 1}, \hat{\beta}_{\sim 2}, \hat{\beta}_{\sim 3}, \hat{\beta}_{\sim 4}\}$  follows that the four estimators all have the same asymptotic properties with

$$E_a(\hat{\beta}_{\sim}) = \beta, \quad \text{cov}_a(\hat{\beta}_{\sim}) = (X' V X)^{-1} \quad (1.32)$$

In section 2, we develop approximations to the biases of the estimators correct to order  $N^{-1}$ . In section 3, the results of a fairly large scale simulation investigation to compare the moment properties of the estimators for a number of sample sizes and parameter configurations when there is a single explanatory variable are presented. These results considerably extend the findings made by Berkson (1955) who considered the particular case  $g = 3$ ,  $n_i = 10$ ,  $i = 1, 2, 3$  and showed that the simple WLS method was more efficient than the ML and MCS methods of estimation under a number of success probability configurations.

## 2. Approximate Biases of Estimators

In this section we develop approximations to order  $N^{-1}$  for the biases of the ML, MCS and WLS estimators. Initially it is convenient to consider a general class of estimation procedures in which the estimates  $\hat{B}_1, \hat{B}_2, \dots, \hat{B}_k$

(i) Maximum Likelihood

putting

$$\phi = \sum_i n_i \left\{ p_i \log \frac{Q_i}{P_i} - \log Q_i \right\} \quad (2.10)$$

we obtain

$$U_r = - \sum_i x_{ir} n_i (p_i - P_i), \quad V_{rs} = \sum_i x_{ir} x_{is} n_i P_i Q_i \quad (2.11)$$

$$W_{rst} = \sum_i x_{ir} x_{is} x_{it} n_i P_i Q_i (Q_i - P_i) \quad Z_{srtu} = \sum_i x_{ir} x_{is} x_{it} x_{iu} n_i P_i Q_i (1 - 6p_i + 6P_i^2) \quad (2.12)$$

The derivatives higher than first order are all constants and are  $O(N)$  so

$A_{rst}$  is  $O(N^{-2})$ . and  $B_{rs, tu}$  and  $C_{rstu}$  are  $O(N^{-3})$ . We also have

$$E(U_r) = 0 \quad (2.13)$$

$$E(U_r U_s) = \sum_i n_i P_i Q_i x_{ir} x_{is} = I_{rs} \text{ say} \quad (2.14)$$

where  $I_{rs} = V_{rs}$  is the  $(r,s)$ th element in the information matrix and

$$E(U_r U_s U_t) = - \sum_i x_{ir} x_{is} x_{it} n_i P_i Q_i (Q_i - P_i) = -W_{rst} \quad (2.15)$$

Since  $E(U_r U_s U_t)$  is  $O(N)$ , the last two terms in (2.5) which are neglected in (2.9) are  $O(N^{-2})$ . Hence the bias of the ML estimator correct to  $O(N^{-1})$  is

$$\begin{aligned} b_r^{(1)} &= - \frac{1}{2} \sum_s \sum_t I_{st} \sum_a \sum_b \sum_c I^{ra} I^{sb} I^{tc} W_{rst} \\ &= - \frac{1}{2} \sum_s \sum_t \sum_u I^{rs} I^{tu} W_{stu} \end{aligned}$$

$$\text{using } \sum_c \sum_d I^{ac} I^{bd} I^{cd} = I^{ab}$$

$$(2.16)$$

(ii) Minimum Chi-Square

Putting

$$\phi = \sum_i n_i (P_i - P_i)^2 / P_i Q_i \quad (2.17)$$

we obtain

$$U_r = \sum_i n_i x_{ir} \left\{ \frac{(2P_i - 1)(P_i - P_i)^2}{P_i Q_i} - 2(P_i - P_i) \right\} \quad (2.18)$$

$$V_{rs} = 2 \sum_i x_{ir} x_{is} n_i \left[ P_i Q_i - 2(P_i - 1)(P_i - P_i) + \left\{ \frac{2(P_i - 1)^2 + 1}{4} \right\} \frac{(P_i - P_i)^2}{P_i Q_i} \right] \quad (2.19)$$

$$W_{rst} = \sum_i x_{ir} x_{is} x_{it} n_i \left\{ \frac{(2P_i - 1)(P_i - P_i)^2}{2P_i Q_i} - (P_i - P_i) \right\} \quad (2.20)$$

Since  $V_{rs}$  is independent of  $\beta$ ,  $W_{rst}$ ,  $Z_{rstu}$  and all higher order derivatives are zero, we have from (2.5)

$$\begin{aligned}\hat{\beta}_r - \beta_r &= -\sum_s V^{rs} U_s \\ &= -\sum_s \lambda^{rs} U_s + \sum_s \sum_t \sum_u \lambda^{rt} \lambda^{su} U_s (V_{tu} - \lambda_{tu})\end{aligned}\quad (2.34)$$

using the same approximation as in (2,22), where

$$\lambda_{rs} = E(V_{rs}) = 2 \sum_i (n_i - 1) P_i Q_i x_{ir} x_{is} \quad (2.35)$$

Standard calculations using Taylor series approximations gives

$$E \left[ p_i q_i \left\{ \log \left( \frac{p_i}{q_i} \right) - \log \left( \frac{P_i}{Q_i} \right) \right\} \right] = \frac{Q_i - P_i}{2n_i} + 0 \left( \frac{1}{n_i^2} \right) \quad (2.36)$$

and

$$\begin{aligned}E \left[ n_i p_i q_i \left\{ \log \left( \frac{p_i}{q_i} \right) - \log \left( \frac{P_i}{Q_i} \right) \right\} \left\{ n_i p_i q_i - (n_i - 1) P_i - Q_i \right\} \right] \\ = n_i P_i Q_i (Q_i - P_i) + 0(1)\end{aligned}\quad (2.37)$$

Hence

$$E(U_s) = \sum_i x_{is} (Q_i - P_i) + 0(N^{-1}) \quad (2.38)$$

and

$$E\{U_s (V_{tu} - \lambda_{tu})\} = -4 \sum_i x_{is} x_{it} x_{iu} n_i P_i Q_i (Q_i - P_i) + 0(1) \quad (2.39)$$

Using these results in (2.34) and noting that  $\lambda^{rs} = \frac{1}{2} I^{rs} + 0(N^{-2})$ , we obtain for the bias of the WLS estimator

$$b_r^{(3)} = \frac{1}{2} \sum_s I^{rs} \sum_i x_{is} (Q_i - P_i) - \sum_s \sum_t \sum_u I^{rt} I^{su} \sum_i x_{is} x_{it} x_{iu} n_i P_i Q_i (Q_i - P_i) \quad (2.40)$$

Thus to order  $N^{-1}$ , the biases of the MCS and WLS estimators are equal. The bias of the ML estimator will be greater than the biases of the MCS and WLS estimators if

$$3 \sum_s \sum_t \sum_u I^{rt} I^{su} \sum_i x_{is} x_{it} x_{iu} n_i P_i Q_i (Q_i - P_i) > \sum_s I^{rs} \sum_i x_{is} (Q_i - P_i) \quad (2.41)$$

### 3. Moment Properties Of The Estimators

In order to investigate the properties of the ML, MCS, WLS and MWLS estimators, a large scale simulation investigation was made for the case of a single explanatory variable with equally spaced values. Without loss of generality, the linear logistic regression model was taken as

$$\log(P_i/Q_i) = \beta_0 + \beta_1(i-1). \quad i = 1, \dots, g \quad (3.1)$$

For the MCS estimators, the biases to  $O(N^{-1})$  are

$$E(\hat{\beta}_0^{(2)} - \beta_0) = \frac{1}{2} \{I^{11} \sum_i (Q_i - P_i) + I^{12} \sum_i x_i (Q_i - P_i)\} + 2E(\hat{\beta}_0^{(1)} - \beta_0) \quad (3.7)$$

$$E(\hat{\beta}_1^{(2)} - \beta_1) = \frac{1}{2} \{I^{21} \sum_i (Q_i - P_i) + I^{22} \sum_i x_i (Q_i - P_i)\} + 2E(\hat{\beta}_1^{(1)} - \beta_1) \quad (3.8)$$

the same results holding for the biases of the WLS estimators.

In table 2, the biases of the estimators obtained by simulation are given together with the approximation by (3.4), (3-5), (3.7) and (3.8). The results show that the absolute values of the biases for the MWLS estimators were consistently larger than those of the other three estimators. The bias advantage of the WLS estimator compared with the MWLS estimator is in agreement with the suggestions made by Hitchcock (1962). In the case of  $\beta_1$  it is seen that the ML estimates were systematically too high while the other three methods gave negative biases in nearly all cases.

Table 2

Biases  $\times 10^2$  of estimators for configurations shown in table 1.

a)  $\beta_0$

Configuration	ML	Approx(3.4)	MCS	WLS	Approx(3.7)	MWL
n=25	(i)	-9.31	-5.10	-1.52	2.05	9.18
	(ii)	-4.29	-2.35	-1.86	-1.37	2.41
	(iii)	2.14	0.30	1.66	2.67	0.12
n=25	(iv)	-2.87	-2.50	6.67	9.82	15.80
	(v)	-0.92	-0.64	0.35	0.63	2.03
	(vi)	-0.07	0.14	-0.99	-0.40	-2.38
n=50	(i)	-3.21	-2.55	0.61	1.48	6.60
	(ii)	-0.13	-1.17	0.90	1.02	3.11
	(iii)	0.16	0.15	-0.14	0.14	-0.66
n=50	(iv)	-0.21	-1.25	4.29	5.12	9.82
	(v)	-1.48	-0.32	-0.79	-0.69	0.16
	(vi)	-0.04	0.07	-0.57	-0.35	-1.05
n=100	(i)	-1.48	-1.28	0.35	0.66	3.59
	(ii)	-0.73	-2.35	-0.15	-0.12	0.98
	(iii)	-0.54	0.07	-0.70	-0.61	-0.86



Table 3

Variances of estimators for configurations shown in table 1.

a) $\beta_0$ 

Configuration	ML	MCS	WLS	MWLS	Approx(3.3)	
n=25	(i)	0,2118	0,1848	0,1768	0.1581	0.1889
	(ii)	0.1143	0.1083	0.1070	0.0974	0.1143
	(iii)	0.1272	0.1187	0.1190	0.1073	0.1176
n=25	(iv)	0.1127	0.0998	0.0983	0.0858	0,1018
	(v)	0.0603	0.0560	0.0552	0.0517	0.0586
	(vi)	0.0661	0.0617	0.0620	0.0560	0.0688
n=50	(i)	0.1017	0.0957	0.0940	0.0863	0.0944
	(ii)	0.0597	0.0581	0.0579	0.0551	0.0571
	(iii)	0.0627	0.0607	0.0605	0.0573	0.0588
n=50	(iv)	0.0538	0.0513	0.0510	0.0467	0.0509
	(v)	0.0282	0.0273	0.0273	0.0262	0.0293
	(vi)	0.0383	0.0372	0.0370	0.0351	0.0344
n=100	(i)	0.0480	0.0464	0.0459	0.0437	0.0472
	(ii)	0.0301	0.0297	0.0296	0.0289	0.0286
	(iii)	0.0319	0.0316	0.0315	0.0306	0.0294
n=100	(iv)	0.0270	0.0264	0.0264	0.0251	0.0255
	(v)	0.0141	0.0139	0.0139	0.0136	0.0146
	(vi)	0.0174	0.0172	0.0172	0.0167	0.0172

b) $\beta_1$  (variances  $\times 10^2$ )

Configuration	ML	MCS	WLS	MWLS	Approx(3.3)	
n=25	(i)	2.5560	2.2950	2.2240	2.0080	2.5013
	(ii)	1.8980	1.7930	1.7740	1.6120	1.9580
	(iii)	3.7530	3.1790	3.2030	2.7190	3.1078
n=25	(iv)	0.3037	0.2721	0.2668	0.2408	0.2903
	(v)	0.2476	0.2278	0.2234	0,2065	0.2360
	(vi)	0.3098	0.2758	0.2761	0.2390	0.3386

Table 4

Mean square errors and efficiencies of estimators relative to the ML estimators for configurations shown in table 1.

Configuration	a) $\beta_0$				Efficiencies			
	ML	Mean Square MCS	WLS	MWLS	MCS	WLS	MWLS	
n=25	(i)	0.2205	0.1851	0.1772	0.1665	119.1	124.4	132.4
	(ii)	0.1161	0.1087	0.1072	0.0980	106.8	108.3	118.5
	(iii)	0.1277	0.1190	0.1197	0.1073	107.3	106.7	119.0
n=25	(iv)	0.1135	0.1043	0.1079	0.1108	108.8	105.2	102.4
	(v)	0.0604	0.0560	0.0552	0.0521	107.9	109.5	115.9
	(vi)	0.0661	0.0618	0.0620	0.0566	107.0	106.6	116.8
n=50	(i)	0.1027	0.0957	0.0942	0.0907	107.3	109.0	113.2
	(ii)	0.0597	0.0582	0.0580	0.0560	102.6	102.9	106.6
	(iii)	0.0627	0.0607	0.0605	0.0574	103.3	103.6	109.2
n=50	(iv)	0.0538	0.0531	0.0536	0.0564	101.3	100.4	95.4
	(v)	0.0284	0.0273	0.0273	0.0262	104.0	104.0	108.4
	(vi)	0.0383	0.0372	0.0371	0.0352	103.0	103.2	108.8
n=100	(i)	0.0482	0.0464	0.0460	0.0450	103.9	104.8	107.1
	(ii)	0.0302	0.0297	0.0296	0.0290	101.7	102.0	104.1
	(iii)	0.0319	0.0316	0.0315	0.0307	101.0	101.3	103.9
n=100	(iv)	0.0270	0.0269	0.0270	0.0278	100.4	100.0	97.1
	(v)	0.0141	0.0139	0.0139	0.0137	101.4	101.4	102.9
	(vi)	0.0174	0.0172	0.0172	0.0167	101.2	101.2	104.2
(b) $\beta_1$ (mean square errors x $10^2$ )								
n=25	(i)	2.6311	2.3040	2.2240	2.0293	114.2	118.3	129.7
	(ii)	1.9311	1.7970	1.7752	1.6353	107.5	108.8	118.1
	(iii)	3.7684	3.2160	3.3745	2.9735	117.2	111.7	126.7
n=25	(iv)	0.3051	0.2767	0.2783	0.2685	110.3	109.6	113.6
	(v)	0.2491	0.2238	0.2255	0.2192	108.9	110.5	113.6
	(vi)	0.3099	0.2897	0.3099	0.2888	107.0	100.0	107.3

## Acknowledgement

We wish to thank Mr. Dennis Scrimshaw for many helpful discussions during the course of this work.

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