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Empirical comparison of iterative methods in logistic models based on three real experiments and simulated data

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SUMMARY

The estimation of unknown parameters in a logistic model with multinomial distribution is usually carried out using iterative methods: the Newton-Raphson or Fisher scoring method. These methods often differ in the number of iterations, which is connected with the type of model used. In this paper these two iterative methods are compared empirically. Data from three real experiments were used for the analysis. Each experiment was described by a different logistic model. Additionally, calculations were carried out for two experiments expanded with simulated data.

Key words: ear emergence, grain contamination, Fisher scoring method, hatchability of chicks, logistic model, maximum likelihood method, Newton-Raphson method

1. Introduction

One of the problems which arises in statistical analysis is the estimation of unknown parameters. The estimation of regression parameters in a logistic model which belongs to the broad class of generalized linear models (McCullagh and Nelder, 1989) can be carried out by various methods. We can seek estimators of parameters using geometrical methods (Agresti, 1984 p. 228; Bakinowska and Kala, 2002b): the least squares method (LS), or the weighted least squares method (WLS). If the joint distribution of the observed variables is known, we can estimate the vector of unknown parameters using the maximum likelihood method, under some assumptions (McCullagh and Nelder, 1989 p. 114; Bakinowska, 2004; Bakinowska and Kala, 2002a). The main problem is to solve the maximum likelihood equation, which is non-linear. Its solution can be sought using iterative methods (McCullagh and Nelder, 1989, p. 42; McCulloch and Searle, 2001 p. 105). One of these is the Newton-Raphson method (N-R) based on the Hessian matrix of likelihood function. This method is simplified if the matrix of second derivatives of the likelihood function is replaced by its expectation, which leads to the Fisher information matrix. This approach is known as the Fisher scoring method (FS) (see McCulloch and Searle, 2001 p. 143, compare Bakinowska 2004).

For the statistical description of experiments we can use various types of logistic model. These include the regression logistic model (Rao and Toutenburg, 1999 p.313; Agresti, 1984 p. 105), the logistic model with logit-link function (Agresti, 1984 p. 104; McCullagh and Nelder 1989 p. 31; Cramer, 2003 p. 13), and the logistic model with multinomial distribution where the units are classified according to an ordinal scale (Agresti, 1984 p. 1; Atkinson and Zocchi, 1999) or according to a nominal scale (Atkinson and Zocchi, 1999; compare Bakinowska and Kala 2001) or according to a hierarchical scale (McCullagh and Nelder 1989 p. 161; Atkinson and Zocchi, 1999).

In this paper two iterative methods, the Newton-Raphson method and the Fisher scoring method, are compared empirically for various logistic models. The data for the analysis came from three real experiments. Additionally two analyses based on simulated data were carried out. In the first experiment the logistic regression model with covariates was considered (Bakinowska, 2004). The observed units were classified according to an ordinal scale. In the second experiment the observed units were classified according to a hierarchical scale (Bakinowska and Kala, 2001). In the third experiment contrasts were used to compare varieties of winter rye (compare Bakinowska and Kala, 2007). Additionally, in the two last examples, simulated data were analyzed.

The determination of estimates of unknown parameters was carried out using programs written in Turbo Pascal 7.0 (Marciniak, 1994). In all the analyses the estimator of vector $\boldsymbol{\beta}_0$ obtained using the simple least squares method (LS) was the starting point of the iterations. The condition to stop the iterative procedure was the difference: $\left|\boldsymbol{\beta}_n - \boldsymbol{\beta}_{n-1}\right| = 0.00001$.

2. Analysis of degree of grain contamination

2.1. Material and method

In Bakinowska (2004), a laboratory experiment was presented which aimed to establish the influence of gas concentration on the degree of grain contamination. There were three levels of gas concentration, each applied in three replications. The degree of contamination was determined by the number of corks on each grain. In this experiment the probability that a single grain will be contaminated by a given number of corks was calculated. The grains were classified in $k = 6$ separate categories (corresponding to the columns of Table 1 in Bakinowska, 2004). The results of classification for the i^{th} pot form a random vector $\mathbf{y}_i$ which follows the multinomial distribution $\mathbf{y}_i \sim M(m_i, \boldsymbol{\pi}_i)$ (where $i = 1,\ldots, 9$ is the object number, m_i is the number of units (grains) which were classified, and $\boldsymbol{\pi}_i$ is the vector of probabilities corresponding to the i^{th} object). The vector $\mathbf{y}_i$ was variable depending on the gas concentration (x_i). The probability was calculated using the logistic transformation described in Bakinowska (2011). In the regression model, the linear regression function and then the quadratic regression function were used. The unknown parameters were estimated using two iterative methods: (FS) and (N-R).

Table 1. Estimates of coefficients of linear regression in the logistic model

Parameters	Starting $\boldsymbol{\beta}_0$	FS (7)	N-R (5)
β_{01}	-1.027761	-1.000980	-1.000980
β_{11}	0.002532	0.002451	0.002451
β_{02}	0.147073	0.149743	0.149743
β_{12}	0.002339	0.002145	0.002145
β_{03}	0.986325	0.980773	0.980773
β_{13}	0.001603	0.001011	0.001011
β_{04}	1.959639	1.810271	1.810271
β_{14}	-0.000417	-0.000253	-0.000253
β_{05}	2.906989	2.482906	2.482906
β_{15}	-0.002245	0.001014	0.001013

2.2. Results

The results of comparison of the number of iterations for these two methods are presented in Tables 1–4. Alongside the name of a method is the number of iterations realized. Tables 1 and 2 concern linear regression. Table 1 contains the estimates of parameter vectors $\boldsymbol{\beta}_0$ and $\boldsymbol{\beta}_n$ (where n is the number of realized iterations). We can notice that the number of iterations for the Fisher scoring method was 7, and for Newton-Raphson 5. The estimates obtained are similar. In Table 2 estimates of individual probabilities of successive categories are given. The estimates were the same.

Table 2. Estimates of individual probabilities in the logistic model (linear regression)

Category	Independent variable	FS (7), N-R (5)	Independent variable	FS (7), N-R (5)	Independent variable	FS (7), N-R (5)
1	x_1=10	.273592	x_2=50	.293499	x_3=100	.319532
2		.269103		.270400		.270538
3		.186568		.173275		.156780
4		.129827		.120689		.109466
5		.064563		.068601		.073526
6		.076347		.073537		.070159

Table 3. Estimates of coefficients of quadratic regression in the logistic model

Parameters	Starting $\boldsymbol{\beta}_0$	FS (4)	N-R (5)
β_{01}	-0.531303	-0.524021	-0.524021
β_{11}	-0.029065	-0.028862	-0.028862
β_{21}	0.000283	0.000281	0.000281
β_{02}	0.707885	0.705642	0.705642
β_{12}	-0.033354	-0.033192	-0.033192
β_{22}	0.000320	0.000318	0.000318
β_{03}	1.528928	1.523048	1.523048
β_{13}	-0.032931	-0.032604	-0.032604
β_{23}	0.000309	0.000302	0.000302
β_{04}	2.699417	2.641407	2.641405
β_{14}	-0.047500	-0.048742	-0.048742
β_{24}	0.000422	0.000432	0.000432
β_{05}	3.857756	3.420443	3.420442
β_{15}	-0.062756	-0.052361	-0.052360
β_{25}	0.000542	0.000476	0.000476

For comparison, the same set of data was analyzed using the logistic model with quadratic regression. Table 3 contains these estimates of parameter vectors $\boldsymbol{\beta}_0$ and $\boldsymbol{\beta}_n$. The number of iterations for the Fisher scoring method was 4, and for Newton-Raphson 5. In Table 4 estimates of individual probabilities of successive categories are given. The estimates were the same for these two methods. The entry 0.273592 in Table 2 row 1 denotes the probability that for a gas concentration of 10ppm the grain will not be contaminated. Similarly the entry 0.269103 in Table 2 row 2 denotes the probability that for a gas concentration of 10ppm the grain will be contaminated one time. The other probabilities are interpreted analogously.

Table 4. Estimates of individual probabilities in the logistic model (quadratic regression)

Category	Independent variable	FS (4), N-R (5)	Independent variable	FS (4), N-R (5)	Independent variable	FS (4), N-R (5)
1		0.31333		0.22000		0.35333
2		0.28667		0.24000		0.28333
3	x_1=10	0.17333	x_2=50	0.19667	x_3=100	0.14667
4		0.12667		0.12667		0.10667
5		0.05000		0.09667		0.06000
6		0.05000		0.12000		0.05000

3. Analysis of hatchability of chicks

3.1. Material and method

The second experiment concerned the hatchability of chicks (Niemiec et al. (1994)), and is described in the paper of Bakinowska and Kala (2001). In this experiment six flocks, each containing 11 hens and 1 rooster, of the Rhode Island Red strain, aged 54 weeks, were divided into three groups and fed on diets containing different amounts of ochratoxin A. The control group (I) was fed with a standard mixture without ochratoxin A, while groups (II) and (III) were given the same diet with 2.1 and 4.1 ppm of ochratoxin A respectively. Eggs laid by the hens of each group were placed in incubators. In each group, among the incubated eggs (m) there were recorded the number of unfertilized eggs (y_1), the number of fertilized eggs in which the embryos died before hatching (y_2), and eggs from which chicks hatched (y_3) (compare Bakinowska and Kala, 2001). We can assume that we are considering six independent objects s=6 (three doses of toxin each replicated twice) and three separated categories k=3.

3.2. Results

The results of the comparison of number of iterations for the two methods are presented in Tables 5–6. In Table 5 the vectors of coefficients $\boldsymbol{\beta}_0$ and $\boldsymbol{\beta}_n$ of linear regressions are presented, and in Table 6 the respective estimates of vectors of probabilities $\boldsymbol{\pi}$ are given.

Table 5. Estimates of coefficients of linear regression in the logistic model

Parameters	Starting $\boldsymbol{\beta}_0$	FS (11)	N-R (11)
β_{01}	-1.404708	-3.145248	-3.145248
β_{11}	0.014783	-0.043293	-0.043293
β_{02}	-0.839397	-1.899499	-1.899500
β_{12}	0.259462	0.486231	0.486231

Table 6. Estimates of individual probabilities in the logistic model (linear regression)

Category	Independent variable	FS (11), N-R (11)	Independent variable	FS (11), N-R (11)	Independent variable	FS (11), N-R (11)
1		0.041279		0.037827		0.034799
2	x_1=0	0.088886	x_2=2.1	0.255679	x_3=4.1	0.488695
3		0.869835		0.706494		0.476506

The number of iterations for the Fisher scoring method is 11, and for Newton-Raphson it is also 11. The estimates were the same. The entry 0.041279 in Table 6 row 1 denotes the probability that the egg for a dose of toxin of 0ppm the egg will be unfertilized. Similarly the entry 0.088886 in Table 6 row 2 denotes the probability that for a dose of toxin of 0ppm the egg will be fertilized, but the embryo will die before hatching. The entry 0.869835 in Table 6 row 3 denotes the probability that for a dose of toxin of 0ppm the chicks will hatch. The other probabilities are interpreted analogously for other doses of toxin.

4. Analysis of time points of ear emergence

4.1. Material and method

The third example concerned various time points of ear emergence in winter rye. This experiment was carried out at COBORU (Research Centre for Cultivar Testing in Słupia Wielka) in the years 2000–2001. There were 83 varieties tested in 2000, and 50 in 2001. The observations were carried out at 7 time points (categories) for three replications (plots) every second day for 60 chosen plants (Table 7). At each time point the number of plants with ear emergence was recorded. Because some cells were empty, the categories were combined. At least 4 separate categories were considered. In this paper three chosen varieties are used for analysis (SMH 1398, RAH 1598, LPH 34) as an illustration of comparison between the iterative methods. In the analysis, variety SMH 1398 was compared with RAH 1598, and variety SMH 1398 with LPH 34. The observed data was analyzed using a logistic model. The adopted model can be written in the following form (see Miller et al. 1993, compare Bakinowska and Kala 2007):

$$\log\frac{\gamma_{ji}}{1-\gamma_{ji}} = \theta_j + \tau_i, \quad j = 1,2,\ldots,k-1, \quad i = 1,2,\ldots,s,$$

where θ_j is the border (cutpoint) of the *j*-th category, τ_i is the effect of the *i*-th treatment (hence $\theta_j + \tau_i$ means the cutpoint of the *j*-th category for the *i*-th treatment), and γ_{ji} is the *j*-th cumulative probability corresponding to units of the *i*-th treatment (variety), $\gamma_{ji} = \pi_{1i} + \pi_{2i} + \ldots + \pi_{ji}, \quad j = 1, 2, \ldots, k-1.$

Table 7. Number of eared plants

Variety	Category			
	1	2	3	4
SMH 1398	7	11	24	18
	12	7	33	8
RAH 1598	5	15	25	15
	17	15	21	7
LPH 1398	20	13	17	10
	27	14	16	3

4.2. Results

The results of the comparison of numbers of iterations are given in Table 8. The vector of unknown parameters $\boldsymbol{\beta}$ consists of cutpoints θ_j and contrasts ρ_1 (comparison of SMH 1398 with RAH 1598) and ρ_2 (comparison of SMH 1398 with LPH 34). In our example the relation between effects and contrasts can be written as: $\rho_1 = \tau_{\text{SMH}} - \tau_{\text{RAH}}$, $\rho_2 = \tau_{\text{SMH}} - \tau_{\text{LPH}}$. Assuming that the effects τ_i , $i = 1, 2, 3$, of varieties sum to zero we get:

$$\tau_{\text{SMH}} = \tfrac{1}{3}\rho_1 + \tfrac{1}{3}\rho_2 \ , \ \tau_{\text{RAH}} = -\tfrac{2}{3}\rho_1 + \tfrac{1}{3}\rho_2 \ , \ \tau_{\text{LPH}} = \tfrac{1}{3}\rho_1 - \tfrac{2}{3}\rho_2 \ .$$

In Table 8 the vectors of coefficients $\boldsymbol{\beta}_0$ and $\boldsymbol{\beta}_n$ are presented. The number of iterations for the Fisher scoring method was 4, and for Newton-Raphson 3. The estimates obtained by the Fisher scoring method do not differ from the estimates obtained by Newton-Raphson.

Table 8. Estimates of cutpoints and contrasts in the logistic model

Parameters	Starting $\boldsymbol{\beta}_0$	FS (4)	N-R (3)
θ_1	-1.276442326	-1.187535	-1.187535
θ_2	-0.205753477	-0.188530	-0.188530
θ_3	1.727948845	1.672704	1.672703
ρ_1	-0.257583876	-0.349281	-0.349281
ρ_2	-1.156311639	-1.185298	-1.185298

5. Analysis of examples with simulated data

5.1. Example 1

For the experiment concerning the degree of grain contamination a new level of gas concentration x_4=20 was added, and corresponding numbers of corks on each grain were simulated. The number of objects was 12, after adding one level on three replications. For this example, based partly on real data and partly on simulated data, two iterative methods were applied. The number of iterations for the linear regression model for the Fisher scoring method was 6, and for Newton-Raphson 4. The numbers of iterations for the quadratic regression model were 6 (FS) and 5 (N-R).

5.2. Example 2

In the experiment concerning hatchability of chicks, a new dose of toxin was added, namely 3.1, and the corresponding values of $y_{1,}$ y_2 and y_3 were simulated. The number of iterations for the linear regression model for the Fisher scoring method was 12, and for Newton-Raphson 11. Meanwhile the numbers of iterations for the quadratic regression model were 17 (FS) and 10 (N-R).

5.3. Example 3

The experiment concerning analysis of time points of ear emergence was extended to include the variety denoted by the symbol 3332-R. For analysis of the data, eight treatments (objects) were used. The number of iterations for the Fisher scoring method was 5, and for Newton-Raphson 4.

6. Conclusions

In most cases the number of iterations was smaller in the Newton-Raphson method than in the Fisher scoring method. However, the numbers of iterations are comparable. The estimates of unknown parameters were similar too. The structure of the Hessian of log-likelihood function in a logistic model with multinomial distribution is very complex. The Fisher scoring method (in which the Fisher information matrix is used) can be more convenient. This matrix is simpler (see Bakinowska 2004). For a more complex structure of data the number of iterations was larger (see the example in paragraph 3). We can expect that for a large number of tested objects the number of iterations may be large.

To compare these two methods, the numbers of iterations for all examples are given in Table 9. It is easy to see that the number of iterations changes somewhat in comparison with experiments with a smaller number of treatments. This occurs more frequently for the Fisher scoring method.

Table 9. All numbers of iterations

Experiment	Method	Number of treatments	Number of iterations: FS	Number of iterations: N-R
§ 2	Linear regression	3	7	5
§ 3	Linear regression	3	11	11
§ 4	Analysis of variance	3	4	3
§ 5.1	Linear regression	4	6	4
§ 5.2	Linear regression	4	12	11
§ 5.3	Analysis of variance	4	5	4
§ 2	Quadratic regression	3	4	5
§ 5.1	Quadratic regression	4	6	5
§ 5.2	Quadratic regression	4	17	10

To compare these two methods in the third example, the number of treatments, number of categories and the number of replications were successively and separately increased. Modification of the number of categories and replications has little influence on the number of iterations. However, for a higher number of treatments, the number of iterations was higher chiefly for the Fisher scoring method. We conclude that although the Newton-Raphson method was the most complex, it was frequently faster than the Fisher scoring method.

REFERENCES

Agresti A. (1984): Analysis of Ordinal Categorical Data. Wiley, New York.

Atkinson A.C., Zocchi S.S. (1999): Optimum experimental designs for multinomial logistic models. Biometrics 55: 437–444.

Bakinowska E. (2004): Analyzing experiments by generalized linear models. Listy Biometryczne - Biometrical Letters 41: 37–49.
Bakinowska E., Kala R. (2001): O modelach logistycznych. Roczniki Akademii Rolniczej w Poznaniu: 3–9.
Bakinowska E., Kala R. (2002a): Maximum Likelihood Estimation for Multivariate Categorical Data. Listy Biometryczne – Biometrical Letters 39: 29–40.
Bakinowska E., Kala R. (2002b): Metody Estymacji w Uogólnionym Modelu Liniowym. Colloquium Biometrycze 32: 241–251.
Bakinowska E., Kala R. (2007): An application of logistic models for comparison of varieties of seed pea with respect to lodging. Biometrical Letters 44: 143–154.
Cramer J.S. (2003): Logit Models from Economics and Other Fields. Cambridge University Press.
Marciniak A. (1994): Turbo Pascal 7.0 z Elementami Programowania. Wydawnictwo Nakom.
McCullagh P., Nelder J.A. (1989): Generalized Linear Models. 2nd. ed. Chapman and Hall, London.
McCulloch CH.E., Searle S.R. (2001): Generalized, Linear, and Mixed Models. Wiley, New York.
Miller M.E., Davis CH.S., Landis J.R. (1993): The analysis of longitudinal polytomous data: generalized estimating equations and connections with weighted least squares. Biometrics 49: 1033–1044.
Niemiec J., Borzemska W., Goliński P., Karpińska E., Szeleszczuk P., Celeda T. (1994): The effect of ochratoxin A on egg quality, development of embryos and the level of toxin in eggs and tissues of hens and chicks. Journal of Animal and Feed Sciences 3: 309–316.
Rao C.R., Toutenburg H. (1999): Linear Models. 2nd ed. Springer-Verlag, New York.