An application of logistic models for comparison of varieties of seed pea with respect to lodging

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SUMMARY

In the paper a logistic model for the analysis of threshold traits observed at several time points is discussed. The theoretical considerations are illustrated with the use of data from a real experiment concerning the lodging of three varieties of seed pea. In the analysis three estimation procedures, following from the least squares principle, were used and compared.

Key words: logistic model, threshold models, weighted least squares method

1. Introduction

In experimental research various traits are observed. Usually they are represented by continuous or discrete random variables. Nevertheless, there are traits, which are naturally continuous in character, but the results of their observations are statements about the membership of the studied unit in a definite category, as in the case of discrete random variables. Such traits include for example physical or mental state of patients, inclination to disease, resistance to frost or resistance of cereals to lodging. The continuous nature of such traits is hidden and only the results of classification of observed units are analyzed in detail.

For example, the states of patients, recorded during medical treatment, can be recorded as poor, good or excellent. Another example is lodging, conventionally related not to a single plant but to whole plots, which is usually expressed using the 9-point grading scale.

The relation of the hidden continuous random variable with a discrete ordinal scale is determined by the separation points of successive categories. In literature

the separation points are called thresholds (Misztal et al., 1989) or cutpoints (see Miller et al., 1993), and the traits are called threshold traits.

The probability of success is associated with each category. For an experimenter who carries out an experiment, in which the studied threshold trait is lodging, it may be interesting not only to estimate unknown probabilities of individual categories or cumulative probabilities, but above all to consider the possibility of their comparison for various treatments, for example, for various varieties of cereals.

The aim of the paper is to present a method of analyzing of such probabilities by the use of a logistic model in application to lodging data. The sought probabilities can be estimated using various methods under different model assumptions. Three of them, based on the least squares principle, are shown and compared in the paper. The theoretical considerations are illustrated by the analysis of data taken from a real experiment.

2. A model for observations

To begin with, let us assume that the studied threshold trait represents a hidden continuous random variable. Moreover, let the domain of this random variable be divided by k-1 unknown numbers θ_j , j=1,2,...,k-1,

$$-\infty < \theta_1 < \theta_2 < \ldots < \theta_{k-1} < \infty$$

into k separate parts representing successive categories. And finally, let F be the cumulative distribution function of the hidden continuous random variable. Then the value of F at the point θ_i is the cumulative probability,

$$F(\theta_j) = \pi_1 + \pi_2 + ... + \pi_j, \tag{1}$$

where π_l denotes the probability of success of the *l*-th category.

Now we will assume that in the experiment there are s groups, each including m_i , i = 1,2,...,s, homogeneous units, which are classified in k separate categories. Classification of all units is repeated at several time points. Of course with the passing of time the values of variables which characterize each group are changing which can influence the decision about the membership of each unit in a particular category.

Let \mathbf{z}_i be a vector of variables characterizing the *i*-th group of units. They are called covariate variables, or shortly, covariates. Moreover, let π_{jic} be the probability of success of the *j*-th category for units of the *i*-th group classified at

the c-th time point, and let $\gamma_{jic} = \pi_{1ic} + \pi_{2ic} + ... + \pi_{jic}$ be the j-th cumulative probability. This probability is connected with the threshold point θ_{jc} modified by the unknown effects of covariates, describing the i-th group. This relation takes the form

$$F^{-1}(\gamma_{iic}) = \theta_{ic} + \mathbf{z}_i^T \tau_i, \tag{2}$$

where τ_i is a vector of unknown effects of covariates. The component $\mathbf{z}_i^T \tau_i$ represents here the total period-group effect, which, when different from zero, moves specifically the cutpoint θ_{ic} .

During the experiment the data are collected. For each group they comprise the number of successes of each category in each period as well as the values of covariates in each period. Sometimes the values of a given covariate may be the same for all periods. This is so, for example, when the covariate is a dummy variable indicating the group membership.

The results of classification of all m_i units with respect to k disjoint categories are usually modeled with the use of the multinomial distribution. For the i-th group in period c such distribution is determined by the number m_i and a vector

$$\boldsymbol{\pi}_{ic} = (\pi_{1ic}, \pi_{2ic}, \dots, \pi_{kic})^T,$$

where the probabilities $\pi_{1ic}, \pi_{2ic}, \dots, \pi_{kic}$ sum up to one.

The natural unbiased estimator of the probability vector $\mathbf{\pi}_{ic}$ is the vector \mathbf{p}_{ic} of observed frequencies. Its dispersion matrix takes the form (see Mardia et al., 1979, p.57)

$$D(\mathbf{p}_{ic}) = \frac{1}{m_i} (\boldsymbol{\pi}_{ic}^{\delta} - \boldsymbol{\pi}_{ic} \boldsymbol{\pi}_{ic}^{T}), \tag{3}$$

where π_{ic}^{δ} is a $k \times k$ diagonal matrix with elements of the vector π_{ic} on its diagonal.

Now, let \mathbf{p}_i be a vector composed of all observations corresponding to the *i*-th group, i.e.

$$\mathbf{p}_i = (\mathbf{p}_{i1}^T, \mathbf{p}_{i2}^T, ..., \mathbf{p}_{ii}^T)^T.$$

If the vectors \mathbf{p}_{ic} , c=1,2,...,t, are considered as independent, then the dispersion matrix of random vector \mathbf{p}_i , $D(\mathbf{p}_i) = \mathbf{V}_i$, is a $ck \times ck$ block-diagonal,

where blocks on the main diagonal have the form (3). Otherwise, when we cannot assume the independence, the sub-blocks apart from the diagonal in $D(\mathbf{p}_i)$ are of the form

$$Cov(\mathbf{p}_{ic}, \mathbf{p}_{ic'}) = \frac{1}{m_i} (\mathbf{\Pi}^{i(cc')} - \boldsymbol{\pi}_{ic} \boldsymbol{\pi}_{ic'}^T),$$
(4)

where the pr-th element of a $k \times k$ matrix $\Pi^{i(cc')}$ is the probability that the unit at the time point c will be of the category p and at the time point c' will be classified to the category r.

It is easy to notice that the vector $\mathbf{\gamma}_{ic}$ of cumulative probabilities,

$$\mathbf{\gamma}_{ic} = (\gamma_{ic}, \gamma_{2ic}, ..., \gamma_{kic})^T$$

follows from π_{ic} by a simple linear transformation. Moreover, because $E(\mathbf{p}_{ic}) = \pi_{ic}$ for c = 1, 2, ..., t, then $E(\mathbf{p}_i) = \pi_i$, where

$$\pi_i = (\pi_{i1}^T, \pi_{i2}^T, ..., \pi_{it}^T)^T$$

is a vector of all probabilities corresponding to all categories in all periods. In consequence, the left hand side of (2) applied to all j = 1, 2, ..., k-1 and c = 1, 2, ..., t represents the mapping of the expectation of the observed vector \mathbf{p}_i into a new vector $\mathbf{\eta}_i$, which by the right hand side of (2) is modeled in the form

$$\mathbf{\eta}_{i} = \mathbf{\theta} + \mathbf{Z}_{i} \mathbf{\tau}_{i}, \tag{5}$$

where $\boldsymbol{\theta}$ is a vector of unknown thresholds, \mathbf{Z}_i is a matrix of values of covariates, while $\boldsymbol{\tau}_i$ is the vector of unknown parameters. The mapping $\boldsymbol{\pi}_i \rightarrow \boldsymbol{\eta}_i$ is known as a link function whereas the relation (5) fulfils the assumptions of the generalized linear models (McCullagh and Nelder, 1989).

3. The link function and estimation

Various models, belonging to the class of generalized linear models, differ mainly in forms of the link function (see McCullagh and Nelder, 1989, p.30 or Lindsey, 1997, p.19). If in the equality (1) it is assumed that F is the distribution of the standard normal random variable, then the resulting model is termed as probit. However, the estimation of parameters in such a case encounters

numerical problems connected with inversion of the distribution function of the standard normal variable. It is easier to find a solution of (1) by assuming that F is the standard logistic distribution (see Rao and Toutenburg 1999, p.316), which has a simple form of the inverse function. Such a model is termed as logistic (see Agresti 1984, p.104).

In the analysis of categorical data the logistic models have wide applications (see McCullagh and Nelder, 1989). As referenced by Miller et al. (1993), Koch et al. (1989) apply this model to describe a clinical trial of a new treatment for a respiratory disorder in which 111 patients, assigned into two groups and visited four times during the following-up period, were classified with respect to 5-point ordinal scale.

The logistic model corresponding to the equality (2) takes the form

$$\eta_{jic} = \log \frac{\gamma_{jic}}{1 - \gamma_{jic}} = \theta_{jc} + \mathbf{z}_{i}^{T} \mathbf{\tau}_{i}, \quad j = 1, 2, ..., k - 1, \quad c = 1, 2, ..., t,$$
(6)

where η_{jic} follows from the logistic transformation of the cumulative probability γ_{jic} . This set of equations can be written in compact form as

$$\mathbf{\eta}_i = \mathbf{C}_i^T \log(\mathbf{L}_i \mathbf{\pi}_i) = \mathbf{\theta} + \mathbf{Z}_i \mathbf{\tau}_i, \tag{7}$$

where

$$\mathbf{\eta}_i = (\eta_{1i1}, \eta_{2i1}, ..., \eta_{k-1, i, t})^T$$

is a t(k-1)-dimensional column vector, which is the image of π_i in the logistic transformation. The matrix \mathbf{L}_i in (7) is block-diagonal with t blocks \mathbf{L}_{ic} , each \mathbf{L}_{ic} being a binary matrix which postmultiplied by π_i gives the sums γ_{jic} and $1-\gamma_{jic}$. The symbol $\log(\mathbf{L}_i\pi_i)$ denotes a vector of logarithms, whereas \mathbf{C}_i^T is, alike \mathbf{L}_i , a block diagonal matrix, where each of the blocks \mathbf{C}_{ic}^T , c = 1, 2, ..., t, is a matrix of contrasts corresponding to the differences of logarithms in (6).

Because \mathbf{p}_i is asymptotically normal,

$$\mathbf{p}_{i} \sim N(\boldsymbol{\pi}_{i}, \mathbf{V}_{i})$$

the random variable $\eta(p_i)$ is asymptotically normal as well (see Rao, 1973, p.388 or Agresti, 1984, p.247),

$$\eta(\mathbf{p}_i) \sim N(\eta(\boldsymbol{\pi}_i), \mathbf{G}_i \mathbf{V}_i \mathbf{G}_i^T),$$

where G_i is a matrix of partial derivatives

$$\mathbf{G}_i = \frac{\partial \mathbf{\eta}_i}{\partial \mathbf{\pi}_i}$$

determined at $\pi_i = \mathbf{p}_i$. Actually, the matrix \mathbf{G}_i is block-diagonal with blocks of the form (see Grizzle et. al. 1969)

$$\mathbf{G}_{ic} = \frac{\partial \mathbf{\eta}_{ic}}{\partial \boldsymbol{\pi}_{ic}} = \mathbf{C}_{ic}^T \mathbf{D}_{ic}^{-1} \mathbf{L}_{ic}, \tag{8}$$

where $\mathbf{D}_{ic} = (\mathbf{L}_{ic}\boldsymbol{\pi}_{ic})^{\delta}$.

Now, let

$$\mathbf{\eta}(\mathbf{p}) = (\mathbf{\eta}^T(\mathbf{p}_1), \mathbf{\eta}^T(\mathbf{p}_2), \ldots, \mathbf{\eta}^T(\mathbf{p}_s))^T,$$

let X stand for a matrix of the form

$$\mathbf{X} = (\mathbf{1}_s \otimes \mathbf{I}_{t(k-1)} : diag \mathbf{Z}_i),$$

and let β be a vector of all parameters,

$$\boldsymbol{\beta} = (\boldsymbol{\theta}^T, \boldsymbol{\tau}_1^T, \boldsymbol{\tau}_2^T, \dots, \boldsymbol{\tau}_n^T)^T.$$

Then the model for all observations from all groups can be written as

$$E(\mathbf{\eta}(\mathbf{p})) = \mathbf{X}\mathbf{\beta}, \quad D(\mathbf{\eta}(\mathbf{p})) = \mathbf{\Sigma},$$
 (9)

where Σ is a block-diagonal matrix. Its blocks, being the dispersion matrices of $\eta(\mathbf{p}_i)$, i=1,2,...,s, are of the form $\mathbf{G}_i\mathbf{V}_i\mathbf{G}_i^T$, where the structure of \mathbf{V}_i depends on the assumptions about the vectors \mathbf{p}_{ic} , c=1,2,...,t. If they are considered as not independent, then the formula (4) must be used. Note, that these matrices are expressed through more elementary probabilities than those forming the vectors π_{ic} . In effect the use of (4) requires much more detailed description of the results of the conducted experiment.

The equations given in (9) form a basis for estimation of the parameters contained in the vector $\boldsymbol{\beta}$. Under normality, the estimate of $\boldsymbol{\beta}$ can be obtained by the maximum likelihood principle, which, however, leads to a system of nonlinear equations. It can be solved by the Newton-Raphson method or, after slight

modification, by the Fisher scoring method (see McCulloch and Searle 2001, p.105 and 143). Much less elaborated methods follow directly from the simple or weighted least squares approach.

In the first case, the dispersion structure of the model is completely ignored, and the estimator of β takes the standard form

$$\boldsymbol{\beta}_{SLS} = (\mathbf{X}^T \mathbf{X})^{-1} \mathbf{X}^T \boldsymbol{\eta}(\mathbf{p}),$$

provided that X is of full column rank.

In the second case, instead of the unknown dispersion matrix Σ , its sample counterpart can be set. Its form depends on the assumptions about the vectors \mathbf{p}_{ic} , c=1,2,...,t, as well as on the data collected. Let \mathbf{S}_0 denote the sample dispersion matrix when the random vectors \mathbf{p}_{ic} , c=1,2,...,t, are considered as independent and let \mathbf{S} stand for the same matrix but without this simplifying assumption. Anyway, to assure the non-singularity of \mathbf{S} or of \mathbf{S}_0 it suffices to choose in (8) as \mathbf{C}_{ic} , c=1,2,...,t, i=1,2,...,s, the matrices of full row ranks. In result the two weighted least squares estimators take the forms

$$\boldsymbol{\beta}_{WLS0} = (\mathbf{X}^{T}(\mathbf{S}_{0})^{-1}\mathbf{X})^{-1}\mathbf{X}^{T}(\mathbf{S}_{0})^{-1}\boldsymbol{\eta}(\mathbf{p}), \quad \boldsymbol{\beta}_{WLS} = (\mathbf{X}^{T}\mathbf{S}^{-1}\mathbf{X})^{-1}\mathbf{X}^{T}\mathbf{S}^{-1}\boldsymbol{\eta}(\mathbf{p}),$$

respectively.

The dispersion matrix of these estimators can also be evaluated in a similar way, i.e.

$$D(\boldsymbol{\beta}_{SLS}) = (\mathbf{X}^T \mathbf{X})^{-1} \mathbf{X}^T \mathbf{S} \mathbf{X} (\mathbf{X}^T \mathbf{X})^{-1},$$

and

$$D(\boldsymbol{\beta}_{WLS0}) = (\mathbf{X}^T(\mathbf{S}_0)^{-1}\mathbf{X})^{-1}.$$

Of course, if the collected data are sufficiently rich then S_0 can be replaced by S as well.

4. An example

In an experiment carried out at the Research Centre for Cultivar Testing in Słupia Wielka 14 varieties of seed pea were tested with respect to lodging. The lodging was determined on a 9-point ordinal scale: 9 - stems are standing, ..., 1 - stems are lying. Each of the varieties was repeated on 20 plots and the observations were recorded successively five times during the experiment. To

simplify the illustration the neighboring categories were combined into three only and only three varieties (KOS, PRH1599, POMORSKA) were chosen. The number of periods was also reduced to three. The data obtained are presented in Table 1.

Table 1. Results of classification of 60 plots at each of three time points									
KOS									
	c = 2 $c = 3$								
		cat. I	cat. II	cat. III			cat. I	cat. II	cat. III
	cat. I	5	5	4		cat. I	2	5	7
c = 1	cat. II	0	4	1	c = 1	cat. II	0	1	4
	cat. III	0	0	1		cat. III	0	0	1
								c = 3	
							cat. I	cat. II	cat. III
						cat. I	2	3	0
					c = 2	cat. II	0	3	6
						cat. III	0	0	6
PRH1599									
			c = 2					c = 3	
		cat. I	cat. II	cat. III			cat. I	cat. II	cat. III
	cat. I	5	1	6	<i>c</i> = 1	cat. I	1	4	7
c = 1	cat. II	0	2	5		cat. II	0	1	6
	cat. III	0	0	1		cat. III	0	0	1
								c = 3	
							cat. I	cat. II	cat. III
						cat. I	1	4	0
					c = 2	cat. II	0	1	2
						cat. III	0	0	12
				POMO	RSKA				
	-		c = 2					c = 3	
		cat. I	cat. II	cat. III			cat. I	cat. II	cat. III
c = 1	cat. I	16	1	1	<i>c</i> = 1	cat. I	12	4	2
	cat. II	0	1	0		cat. II	0	0	1
	cat. III	0	0	1		cat. III	0	0	1
	c = 3								
						,	cat. I	cat. II	cat. III
						cat. I	12	3	1
					c = 2	cat. II	0	1	11
						cat. III	0	0	2

According to the notation of Section 3 we have s = 3 groups (varieties), t = 3time points in which the observations were carried out, and k = 3 separate categories concerning the levels of lodging. In result, the vector $\boldsymbol{\theta}$ in the model (7) has now the form

$$\mathbf{\theta} = (\theta_{11}, \, \theta_{21}, \, \theta_{12}, \, \theta_{22}, \, \theta_{13}, \, \theta_{23})^T,$$

where θ_{jc} denotes a cutpoint of the *j*-th category for the *c*-th time point. The vector of covariates for each variety reduces here only to one dummy variable indicating the group membership. In consequence $\mathbf{Z}_i = \mathbf{1}_6$ for i = 1,2,3, while the matrix \mathbf{X} and the vector $\boldsymbol{\beta}$ in (9) take the forms:

$$\mathbf{X} = (\mathbf{1}_3 \otimes \mathbf{I}_6, \mathbf{I}_3 \otimes \mathbf{1}_6), \quad \boldsymbol{\beta} = (\boldsymbol{\theta}^T, \tau_1, \tau_2, \tau_3)^T, \tag{10}$$

where τ_i is the effect of *i*-th variety.

It is easy to notice that the matrix X in (10) is not of full column rank. This inconvenience can be avoided by replacing the three group effects τ_1 , τ_2 , τ_3 by two contrasts

$$\rho_{(1)} = \tau_1 - \tau_2, \quad \rho_{(2)} = \tau_1 - \tau_3.$$

Assuming that the group effects sum to zero, the original parameters can be expressed uniquely in terms of contrasts by the following equations

$$3\tau_1 = \rho_{(1)} + \rho_{(2)}, \quad 3\tau_2 = -2\rho_{(1)} + \rho_{(2)}, \quad 3\tau_3 = \rho_{(1)} - 2\rho_{(2)}.$$
 (11)

In result, the replacement of the 18×3 submatrix $\mathbf{1}_3 \otimes \mathbf{I}_6$ in \mathbf{X} with the 18×2 matrix of form

$$\frac{1}{3} \begin{pmatrix} 1 & 1 \\ -2 & 1 \\ 1 & -2 \end{pmatrix} \otimes \mathbf{1}_6$$

completes the reparametrization of the model.

Using the collected data, the estimates of cutpoints θ_{ji} and contrasts $\rho_{(1)}$ and $\rho_{(2)}$ where obtained by the simple least squares (SLS) method as well as by two weighted least squares methods (WLS⁰, WLS). The results are presented in Table 2. In the last two rows the values of the Wald statistic (see McCulloch and Searle 2001, p.24), for testing hypotheses concerning the separate contrasts, are also given.

	SLS	(S.D.)	WLS ⁰	(S.D.)	WLS	(S.D.)	
θ_{11}	1.150	(0.334)	1.287	(0.311)	1.357	(0.314)	
θ_{21}	2.944	(0.592)	2.876	(0.566)	2.632	(0.515)	
θ_{12}	-0.270	(0.307)	-0.188	(0.299)	-0.152	(0.280)	
θ_{22}	0.880	(0.334)	0.807	(0.303)	0.880	(0.297)	
θ_{13}	-1.579	(0.449)	-1.213	(0.348)	-1.180	(0.349)	
θ_{23}	0.045	(0.290)	0.083	(0.286)	0.147	(0.263)	
$ ho_{(1)}$	0.481	(0.590)	0.521	(0.370)	0.718	(0.494)	
$ ho_{\!\scriptscriptstyle (1)}$	-1.597	(0.679)	-1.876	(0.423)	-1.895	(0.607)	
Z_1	0.66		1.9	99	2.11		
Z_2	5.53*		19.7	0**	9.74**		

Table 2. Estimates of parameters

First observe that the WLS⁰ and WLS methods provide the estimates which are more similar than that following from the SLS method. On the other hand the estimates of thresholds obtained by the WLS method in majority cases appeared to be more precise, in terms of their standard deviations, than those following from the WLS⁰ method, which in turn are better than those obtained by the SLS method. However, in the case of estimates of contrasts $\rho_{(1)}$ and $\rho_{(2)}$, which are of main interest, the WLS⁰ method appeared to be the most precise. This can indicate that the more elaborate approach does not always lead to more precise estimates. On the other hand, the better performance of WLS⁰ can be caused by simplifying assumptions on the model describing the collected data which, in the case of the experiment under consideration, are not fully justified.

Coming to details, first note that the estimate of $\rho_{(1)}$ is non-negative, i.e. $\tau_2 \le \tau_1$, however, the difference between the effects τ_2 and τ_1 appeared to be not significant ($\alpha = 0.05$). On the other hand, the contrast $\rho_{(2)}$ is negative and significant, which means that $\tau_1 < \tau_2$. Thus we can conclude that the third variety, POMORSKA, differs significantly from the other two, which behave similarly.

The conclusion above can be expressed in terms of probabilities which provide a direct interpretation. According to the equality (6), the cumulative probability γ_{iic} takes the form

$$\gamma_{jic} = \frac{\exp(\theta_{jc} + \tau_i)}{1 + \exp(\theta_{ic} + \tau_i)},\tag{12}$$

where the effect τ_i can be obtained through the equations (11). The estimates of these probabilities are presented in Table 3.

Table 3. Estimates of cumulative probabilities

		KOS	PRH1599	POMORSKA
		i = 1	i = 2	i = 3
Γ	j = 1, c = 1	0.685	0.574	0.915
SLS	j = 2, c = 1	0.929	0.890	0.985
	j = 1, c = 2	0.345	0.245	0.722
	j = 2, c = 2	0.624	0.507	0.891
	j = 1, c = 3	0.124	0.081	0.412
L	j = 2, c = 3	0.419	0.308	0.781
		KOS	PRH1599	POMORSKA
		i = 1	i = 2	i = 3
	j = 1, c = 1	0.697	0.578	0.938
	j = 2, c = 1	0.919	0.870	0.987
WLS^0	j = 1, c = 2	0.345	0.238	0.775
	j = 2, c = 2	0.588	0.459	0.903
	j = 1, c = 3	0.159	0.101	0.553
	j = 2, c = 3	0.409	0.291	0.819
		KOS	PRH1599	POMORSKA
_		i = 1	i = 2	i = 3
WLS	j = 1, c = 1	0.724	0.561	0.946
	j = 2, c = 1	0.904	0.821	0.984
	j = 1, c = 2	0.367	0.221	0.794
	j = 2, c = 2	0.620	0.443	0.915
	j = 1, c = 3	0.172	0.092	0.580
	j = 2, c = 3	0.439	0.276	0.839

The detailed inspection of the obtained values confirms the differences between the estimation methods, however, irrespective of the method used, differences between corresponding extreme probabilities are smaller than those between moderate probabilities. This is due to the non-linearity of the transformation (12). On the other hand, the weighted least squares methods (WLS⁰, WLS) provided probabilities which differentiate varieties more definitely than the least squares method. This is especially visible for probabilities at the second and third time point, and concerns distinct as well as similar varieties. In any case, in all methods the third variety, POMORSKA, appeared to be the most resistant to lodging.

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