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An evaluation of the efficiency of plant protection products via nonlinear statistical methods – a simulation study

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SUMMARY

A nonlinear statistical approach was used to evaluate the efficiency of plant protection products. The methodology presented can be implemented when the observations in an experiment are recorded as success or failure. This occurs, for example, when following the application of a herbicide or pesticide, a single weed or insect is classified as alive (failure) or dead (success). Then a higher probability of success means a higher efficiency of the tested product. Using simulated data sets, a comparison was made of three methods based on the logit, probit and threshold models, with special attention to the effect of sample size and number of replications on the accuracy of the estimation of probabilities.

Key words: threshold model, logistic model, plant protection, simulated data

1. Introduction

Evaluation of the efficiency of an experimental factor is an important element of agricultural research. It is essential to know what level of implemented treatment ensures the optimal gain. The observations collected in plant protection experiments are various in nature, and can be measured as quantitative traits and analyzed using linear statistical methodology, where the effect of using a herbicide is expressed for example as plant biomass or height (Finney, 1979). However, the observed response can also be coded on a discontinuous scale, or on a time scale when the data are treated as event times (Burgos et al., 2013, Ritz et al., 2013). A special case is where observations are collected in a binary manner, i.e. as a sequence of failures and successes. For

example, an individual weed may be evaluated as destroyed or not, and similarly, an individual insect may be classified as alive or not. Although nonlinear statistical methods have been widely developed over recent decades, the analysis of such data sets is not easy.

The aim of this paper is to compare some of the nonlinear statistical approaches used in evaluating the efficiency of plant protection products, with special attention to planning a proper experimental design. The essential assumption in these methods, based on a generalized linear model and threshold model, is the existence of an unobservable and continuous variable, named liability, whose values determine the observed categorical trait. It is supposed that the efficiency is influenced by many unknown factors, similar to disease-resistance, but their effect is observed on a binary scale. The compared methods are illustrated using simulated data sets.

2. Material

Let us assume that four plant protection products were evaluated according to the following schema: each product was applied in the same dose to 100 (or 1000) individuals, and only two types of result were observed: the individual weed or insect was destroyed (this observation was recorded as a success and coded as 1) or it was still alive (recorded as a failure and coded as 0).

To simulate the successes and failures we used a standard normal random variable z. To model the differences between products we interpreted a result with z less than fixed c_i (i = 1,2,3,4) as representing a success (coded as 1) of the i-th product. This procedure was repeated n = 100 (or n = 1000) times, and the obtained sequence of ones and zeros was treated as one replication or as a series of k replications, k = 2,4,5 (or k = 2,5,10), each of size 100/k (1000/k). The data were simulated for two sets of parameters c_i. The first was more compact, while the other was more widely spread. The assumed values of parameters in these two sets and the numbers of successes obtained are presented in Tables 1 and 2 respectively.

Table1. True values of parameters and numbers of successes in a simulation of 100 observations per treatment

Sample	Assumed parameter – first set				Assumed parameter – second set			
size	**0.5**	**-0.3**	**0.7**	**-0.2**	**-1.7**	**-0.6**	**0.9**	**1.5**
100	74	47	71	40	6	35	81	94
50	38	24	38	25	4	16	42	49
50	36	23	33	15	2	19	39	45
25	19	9	17	11	1	7	19	25
25	19	15	21	14	3	9	23	24
25	17	9	16	9	2	8	19	22
25	19	14	17	6	0	11	20	23
20	15	7	14	7	1	5	15	20
20	16	12	14	14	3	9	17	20
20	11	20	15	6	1	4	15	17
20	16	8	15	8	1	7	18	18
20	16	13	13	5	0	10	16	19

Table 2. True values of parameters and numbers of successes in a simulation of 1000 observations per treatment

Sample	Assumed parameter – first set				Assumed parameter – second set			
size	**0.5**	**-0.3**	**0.7**	**-0.2**	**-1.7**	**-0.6**	**0.9**	**1.5**
1000	686	378	752	406	33	258	808	944
500	349	191	366	202	23	131	401	473
500	337	187	386	204	10	127	407	471
200	148	80	145	78	15	58	165	190
200	129	75	149	82	4	49	156	190
200	138	75	146	88	5	55	158	187
200	141	70	156	77	4	51	164	188
200	130	79	156	81	5	45	165	189
100	74	41	74	41	6	26	85	94
100	74	38	71	37	9	32	80	96
100	64	38	73	45	1	27	77	93
100	65	37	76	37	3	22	79	97
100	72	37	72	42	4	24	80	93
100	66	38	74	46	1	31	78	94
100	69	33	79	36	2	26	82	92
100	72	37	77	41	3	25	82	96
100	65	38	76	38	2	18	83	95
100	65	41	80	43	2	27	82	94

From a practical point of view, the logit, probit and threshold models differ in terms of the input data representation. In the logit and probit models the input data are the frequencies (empirical probabilities of success), while in the threshold approach there is a sequence of zeros and ones. An interesting question is whether the final results depend on the number of replications. Therefore several variants of the data were analyzed.

3. Methods

The generated data sets were analyzed using the generalized linear model with logit and probit link functions, and the threshold model. The implemented methods are well-known in the literature, and so only some essential points will be noted here.

The generalized linear model used in this study can be written as

$$\mathrm{E}(\eta(f_{ij})) = \alpha_i + \beta_j, \quad i = 1, 2, 3, 4, \quad j = 1, \ldots, k \tag{1}$$

where E denotes the expectation operator, $\eta(f_{ij})$ is a (so-called) link function, f_{ij} is the observed probability of success of the *i*-th product in the *j*-th replication, and α_i and β_j are unknown parameters representing products (treatments) and replications respectively (McCullagh and Nelder, 1989, Agresti, 1984).

If the link function has the form:

$$\eta(\pi_{ij}) = \log\frac{\pi_{ij}}{1-\pi_{ij}}, \tag{2}$$

where π_{ij} is a probability of success corresponding to the *i*-th treatment (herbicide or pesticide) in the *j*-th replication, the equality (1) with π_{ij} replaced by f_{ij} is called the logit model (Rao and Toutenburg, 1999; Bakinowska and Kala, 2007, McCullagh and Nelder, 1989).

If the link function in the model (1) is of the form:

$$\eta(\pi_{ij}) = \Phi^{-1}(\pi_{ij}), \tag{3}$$

where Φ^{-1} denotes the inverse of the standard normal cumulative distribution function (and $\pi_{ij} = f_{ij}$), then equality (1) is called the probit model (Rao and Toutenburg, 1999).

In the threshold model it is supposed that the effects of treatments are related to some unobservable continuous random variable *w*. The comparison of its values with a given threshold leads to dichotomous events or a threshold trait. The threshold model can be written as

$$w = \beta_i + e, \quad i = 1, 2, 3, 4, \tag{4}$$

where β_i is a fixed threshold corresponding to the *i*-th treatment (product), and *e* is the error standard normal random variable. This means that the standard deviation of *e* is the unit of the random variable *w*. Therefore the effectiveness of the treatments is here considered as the threshold trait with two categories of observed values (Falconer, 1960).

The computations were performed in SAS (Statistical Analysis System, SAS Inst. 1997) using the *logistic glm* procedure (with the *logit* link function for the logit model, and with the *probit* link function for the probit model), and using a program developed by authors for the threshold model. In this latter case, Bayesian methods with the Gibbs sampling algorithm were used for the estimation of model parameters. In the animal science literature there are well-known formulae for the ordinary threshold model with repeated observations for one treatment (Sørensen et al., 1995, Moliński et al., 2003). This approach was implemented here. In the Gibbs sampling procedure, the prior distributions were assumed to be an improper distribution for fixed effects and standard normal distribution for errors. The estimation was performed based on the conditional posterior distribution, which for the parameter β_i was normal with mean equal to the solution of the appropriate mixed model equations (Sørensen and Gianola, 2002).

In each analysis, the Gibbs sampler generated 10 000 runs. The first 2000 were discarded as a burn-in period. Moreover, to avoid autocorrelation within the generated sequences, only every tenth result was used.

4. Results

Using the results of estimation from the logit, probit and threshold models, estimates of probability of success for each product can be established. In the case of the logit model

$$\hat{\pi}_{ij} = \frac{\exp(\hat{\mu}_{ij})}{1+\exp(\hat{\mu}_{ij})},$$

where $\hat{\mu}_{ij}$ is the best linear unbiased estimator of $\alpha_i + \beta_j$. Under the probit model

$$\hat{\pi}_{ij} = \Phi(\hat{\mu}_{ij}),$$

while for the threshold model

$$\hat{\pi}_{ij} = \Phi(\hat{\beta}_{ij}),$$

where Φ is the cumulative distribution function of the standard normal random variable.

By means of a similar formula,

$$\pi_i = \Phi(c_i),$$

the true probabilities of success, characterizing the products, can also be calculated. The true and estimated probabilities derived from the simulated data are presented in Tables 3 and 4.

From a practical point of view, one of the most interesting results of the statistical analysis is the decision as to which product is the most effective. This information follows directly from the estimated probabilities. Since in our study the theoretical (true) probabilities are known, the main question concerns consistency between the estimated and true probabilities.

Table 3. True and estimated probabilities of success for the case with 100 observations per treatment

Model	Treatments					Treatments			
	1	2	3	4		1	2	3	4
	1 x 100					1 x 100			
threshold	0.740	0.471	0.709	0.401	threshold	0.059	0.349	0.811	0.942
logit	0.739	0.469	0.709	0.400	logit	0.060	0.350	0.810	0.940
probit	0.740	0.470	0.710	0.400	probit	0.060	0.350	0.810	0.940
	2 x 50					2 x 50			
logit	0.701	0.419	0.668	0.351	logit	0.053	0.322	0.791	0.933
probit	0.699	0.421	0.668	0.352	probit	0.050	0.320	0.788	0.931
	4 x 25					4 x 25			
logit	0.725	0.446	0.694	0.375	logit	0.058	0.348	0.813	0.941
probit	0.723	0.447	0.694	0.376	probit	0.054	0.339	0.806	0.938
	5 x 20					5 x 20			
logit	0.750	0.476	0.720	0.404	logit	0.066	0.387	0.844	0.953
probit	0.750	0.477	0.717	0.405	probit	0.064	0.374	0.835	0.954
true	**0.691**	**0.382**	**0.758**	**0.421**	**true**	**0.044**	**0.274**	**0.816**	**0.933**

Table 4. True and estimated probabilities of success for the case with 1000 observations per treatment

Model	Treatments					Treatments			
	1	2	3	4		1	2	3	4
	1 x 1000					1 x 1000			
threshold	0.686	0.378	0.752	0.406	threshold	0.033	0.258	0.808	0.944
logit	0.686	0.378	0.752	0.406	logit	0.033	0.258	0.808	0.944
probit	0.686	0.378	0.752	0.406	probit	0.033	0.258	0.808	0.944
	2 x 500					2 x 500			
logit	0.687	0.380	0.753	0.408	logit	0.032	0.252	0.803	0.942
probit	0.688	0.380	0.753	0.408	probit	0.031	0.251	0.802	0.942
	5 x 200					5 x 200			
logit	0.688	0.380	0.754	0.408	logit	0.031	0.247	0.800	0.941
probit	0.688	0.380	0.754	0.408	probit	0.030	0.248	0.800	0.941
	10 x 100					10 x 100			
logit	0.703	0.396	0.766	0.425	logit	0.033	0.260	0.811	0.945
probit	0.703	0.396	0.767	0.425	probit	0.032	0.258	0.809	0.945
true	**0.691**	**0.382**	**0.758**	**0.421**	**true**	**0.044**	**0.274**	**0.816**	**0.933**

5. Conclusions and discussion

Before analyzing the results, let us note the differences between the sets of initial parameters which determine the true probabilities. In the first set (0.5, -0.3, 0.7, -0.2) the range R = |0.5-(-0.2)| = 0.7, while in the set (-1.7, -0.6, 0.9, 1.5) the range is more than four times larger. In consequence, drawing inferences with respect to the first set is much more difficult. This observation is confirmed by the fact that in the case n = 100 the estimated probabilities differ significantly from their true counterparts, irrespective of the method used. The differences were so great that even the ranking of products based on the estimated probabilities differs from that based on true probabilities. This does not occur in the case n = 1000 or for the second set of initial parameters.

To draw more precise conclusions, the absolute values of the differences between true and estimated probabilities were calculated. As expected, better accuracy of estimation was achieved for data with n = 1000 individuals per treatment. Moreover, in the logit and probit approaches, replications can improve the results. The best estimates were obtained for two and four replications in the case n = 100 and for two and five replications in the case n = 1000, but only in the first set of initial parameters. When the parameters were taken from the second set, the best results were obtained for ten replicates (almost the same results were also obtained for one replicate in the probit method).

The above considerations lead to the conclusion that the method based on a generalized linear model with two, three or four replications of size n = 100 will produce satisfactory results.

The proposed methodology can be easily expanded to situations with more than two categories. One advantage here is the avoidance of frequency transformation to normal distribution. Similar modeling (a threshold model) has previously been used to analyze the efficiency of herbicides based on real data (Skotarczak et al., 2002), to research the lodging of cereals (Bakinowska and Kala, 2007), and to analyze downy mildew infection of field pea varieties

(Bakinowska et al., 2012). The results obtained following the Bliss transformation of data, when compared with those obtained from the threshold model analysis, showed consistency and produced the same ranking of herbicides (Skotarczak et al., 2002).

REFERENCES

Bakinowska E., Kala R. (2007): An application of logistic models for comparison of varieties of seed pea with respect to lodging. Biometrical Letters 44(2): 143–154.

Bakinowska E., Pilarczyk W., Osiecka A., Wiatr K. (2012): Analysis of downy mildew infection of field pea varieties using the logistic model. Journal of Plant Protection Research 52(2): 264–270.

Burgos N.R., Tranel P.J., Streibig J.C., Davis V.M., Shaner D., Norsworthy J.K., Ritz C. (2013): Review: confirmation of resistance to herbicides and evaluation of resistance levels. Weed Science 61(1): 4–20.

Falconer D.S. (1960): Introduction to quantitative genetics. Ronald Press Co, New York.

Finney D.J. (1979): Bioassay and the practice of statistical inference. International Statistical Review 47(1): 1–12.

Moliński K., Szydłowski M., Szwaczkowski T., Dobek A., Skotarczak E. (2003): An algorithm for genetic variance estimation of reproductive traits under a threshold model. Archives of Animal Breeding 46(1): 85–91.

McCullagh P., Nelder J.A. (1989): Generalized linear models. 2nd. ed., Chapman and Hall, London.

Rao C.R., Toutenburg H. (1999): Linear Models. 2nd ed. Springer-Verlag, New York.

Ritz C., Pipper C.B., Strebig J.C. (2013): Analysis of germination data from agricultural experiments, European Journal of Agronomy 45: 1–6.

SAS Institute (1997): SAS/STAT software: Changes and enhancements through release 6.12. SAS Inst., Cary, NC, USA.

Sørensen D.A., Andersen S, Gianola D., Kørsgaard I. (1995): Bayesian inference in threshold models using Gibbs sampling. Genetics Selection Evolution 27: 229–249.

Sørensen D.A, Gianola D. (2002): Likelihood, Bayesian and MCMC methods in quantitative genetics. Springer-Verlag, New York.

Skotarczak E., Molińska A., Moliński K. (2002): Zastosowanie modelu progowego do oceny skuteczności działania wybranych herbicydów. Colloquium Biometryczne 32: 125–132.