# Some aspects of a mixture model for estimating the boundary of a set of data

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This paper discusses a method for estimating the parameters of the boundary of a set of points for which the y variable is bounded above. The boundary may be linear, for example, in which case a scatterplot of the data may have a triangular appearance. An example is obtained by plotting cube root of food volume in an animal's incompletely filled stomach against the animal's length; full stomachs constitute the upper boundary, while other volumes fall between 0 and the boundary, depending on how full or empty a stomach may be.

Our method is to fit a mixture of an ordinary regression model and a variate having an unknown mixing distribution, which represents the variation of another unobserved factor such as the proportionate fullness of the stomach, for example. The mixing distribution is discretized and the number of mixing classes is estimated by Akaike's procedure. The method is found to be stable and reliable for simulated sets of data, and is illustrated by application to three data sets. Examples of occurrence of the problem in various areas of ecology, and in other areas, are given.

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#### Introduction

In certain studies in ecology, and in many other areas, data of the following type arise. Two variables, y and x, are related, but the variation of y is restricted by a boundary (which we take to be the upper boundary). The boundary may be approximately linear, and the observations of y for a given value of x may be distributed over a range from 0 to the boundary, rather than approximately symmetrically around some value, as in the ordinary regression model. Thus there is a "varying factor" (or factors), which tends to move some points away from the boundary. Such data present a roughly triangular form when the y and x coordinates of each data point are plotted on a graph. More generally, the boundary may be nonlinear and the scatterplot of y versus x covers a region of the x-y plane.

For such data, interest often lies in estimating the parameters of the boundary line and in estimating the variation around it. The boundary may represent a maximum or upper bound to y which is achievable when the varying factor is not present, and be of interest in itself; or it may be important to compare the boundary lines, statistically, between two or more sets of data.

Figure 1 of Maller *et al.* (1983), reproduced as Figure 1 here, is an example of such a data set, in which y is the cube root of the observed stomach volume of a western rock lobster and x is its carapace length (see also Fig. 3

of the present paper). The values of y are distributed from a maximum value, representing lobsters whose foreguts were full at the time of capture, to zero, when lobsters were caught at times before they had commenced feeding. These data are typical of the stomach contents of fish and other animals which are sampled under field conditions, since there is usually no way to control for fullness of stomach. It is important in these studies to identify in an objective way animals which have a large proportion of the stomach filled, since the inclusion of animals with small proportions filled could introduce serious bias or unreliability, e.g., in calculating dietary components. Statistically, the problem is to fit a line to the upper envelope of the data.

This type of problem is not restricted to fisheries research. In forestry, a good example of the kind of data we are interested in occurs in Ward (1982, Fig. 5), who plots the relationship between girth and age of junipers. Given optimum conditions, there seems to be a roughly linear relationship between girth and age of tree, but many trees are small for their age (even being only perhaps 20 % of their apparent optimum size). Here the "varying factors" represent the often suboptimal environmental conditions to which a tree may be exposed, and the boundary represents the maximum girth obtainable by a juniper having the best possible conditions. Ward comments (p. 922) that the (ordinary) regression of girth versus age should be "done with cau-

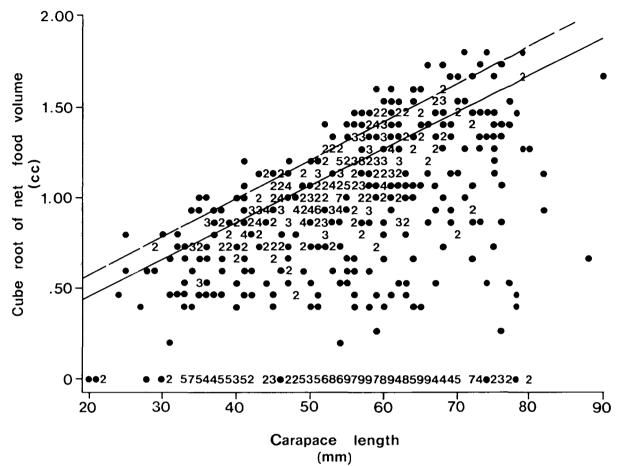


Figure 1. Cube root of net foregut volume (cc) of 543 western rock lobsters plotted against carapace length (mm). Lines shown are fitted by the trimming method (full line) and likelihood method (broken line). Reproduced from: R. A. Maller, E. S. de Boer, L. M. Joll, D. A. Anderson, and J. P. Hinde. 1983. Determination of the maximum foregut volume of western rock lobsters (*Panulirus cygnus*) from field data. Biometrics, 39: 543-552. With permission from The Biometric Society.

tion" even within localities, and should not be used at all where there is "extreme variation". The method we present enables us to estimate girth as a function of age independent of other varying factors.

The problem we are discussing has been clearly recognized by Jarvis (1976), in relating stomatal conductance of leaf canopies to various independent variables (see Figs. 10 and 11 of his paper). He comments that "provided enough measurements have been taken to cover the variable space, the upper limit of a scatter diagram indicates the response to the particular independent variable when the other variables are not limiting". The boundaries in Jarvis' data are nonlinear. Another linear example occurs in Wilson et al. (1986, Fig. 3), who relate yield of tropical grasses sown in various sites to daily maximum and minimum temperatures. Their material "suggests that growth is initiated at a minimum temperature and is optimum at about 30°C daily maximum temperature". Here the "varying factor" is (or includes) the "site" of observations, and its corresponding minimum and maximum daily temperatures, while the boundary is again the optimum growth achievable. Applications of this type of study to growth of marine plants suggest themselves.

A good opportunity to test our methods came with some data of Rabinowitz et al. (1985, Fig. 1), who measured the weight of seedlings of prairie grass as a function of harvest date. Since not all seeds germinate at the same time, plants at a given harvest date are a variety of ages, and a plot of weight versus (chronological) age has a triangular appearance. Rabinowitz et al. used the "trimming" method of Maller et al. (1983) to estimate the "true" regression of weight on age, and compared it with the actual regression of weight on age, obtained by recording also the actual age of a seedling (see Fig. 2 of Rabinowitz et al. (1985)). Here the "boundary" is the actual regression of weight on age, and the "varying factor" is the effect of knowing only the chronological rather than the actual age of a seedling. Assuming linearity, Rabinowitz et al. obtained excellent agreement between the two regressions, and we discuss another analysis of this data set later.

A beautiful meteorological example is given by Wendler and Kodama (1986, Fig. 1), who plot global radiation flux in Fairbanks, Alaska, as a function of month of year. The "varying factor" here is cloud cover; on a cloudless day, maximum flux measurements are achieved, falling to close to zero fluxes for very overcast days. The "boundary" for this data is obviously sinusoidal rather than linear. Scott (1979, Fig. 5) has a similar plot of total radiance at Port Hacking, NSW. For an astronomical example, see Seki and Hasegawa (1986, Fig. 1), who plot interstellar polarization against extinction magnitude for about 1400 stars, obtaining a roughly linear boundary. Here the varying factor seems to be mostly degree of alignment of intervening dust grains with the galactic magnetic field.

Returning to fisheries research, other examples occur in Salmon and Hyatt (1983, Fig. 5; clutch sizes of fiddler crabs as a function of female carapace width), in Hines and Pearce (1982, Fig. 4; depth of refuge versus shell length of abalones), in Michaletz *et al.* (1987, Fig. 4; size of ingested zooplankton prey versus mouth gape for four fish species), and in Smith (1983, Fig. 4; length of prey tadpoles versus length of predators). Here the upper boundaries are fairly obvious physical limitations in terms of the size of the species studied, and the "varying factors" are the random factors influencing clutch size, depth of refuge available, or available prey size. Similar comments apply to data of Bryant and Westerterp (1983, Fig. 4), who plot size of insect prey versus foraging distance of house martins.

In Maller *et al.* (1983), two methods for estimating relationships of the above kind were given. The present paper is a continuation of that paper, in which the "mixture method" of that paper is extended, and its use is demonstrated in the analysis of data. For a general reference to mixture distributions see Everitt and Hand (1981).

The model assumed is a generalization of an ordinary regression model in which a set of points  $y_i$  with covariate vector  $x_i$  is related by

$$y_i/p = \alpha + \beta x_i + \varepsilon_i \tag{1}$$

where  $\alpha$  and  $\beta$  are parameters to be estimated. In terms of our previous terminology, the random amount p by which each point y is displaced downwards represents the "varying factors", for example the unobserved proportionate fullness of a lobster's stomach. In (1),  $\varepsilon_i$ represents independent normal  $(0,\sigma^2)$  error terms, where  $\sigma^2$  is unknown and to be estimated. Note that (1) and the calculations in the following section are easily generalized to the multiple or polynomial regression case.

In general, the distribution of p is unknown and must also be estimated from the data. From this point of view the problem is one of incomplete data and so falls into a class of problems identified by Dempster *et al.* (1977) and associated with the "EM algorithm". In Maller *et al.* (1983), Anderson and Hinde, following Laird (1978), suggested estimating the unobserved mixing distribution of p nonparametrically, by assuming that p has a discrete distribution with masses  $\pi_j$  at points  $m_j$ ,  $0 \le m_1 \le ... \le m_k \le 1$ , where  $m_j$  are given and  $\pi_1, ..., \pi_k$ and k are to be estimated. The likelihood equations derived from (1) with this mixing distribution were solved iteratively by an EM method for a fixed value of k (actually k = 10 was chosen). The procedure seemed to converge but required a very large number of iterations.

One aim of the present paper is to suggest a computationally improved method of fitting with faster convergence, which makes it feasible to study simulations of the data. With these, the distributions of the estimators of  $\beta$  and  $\sigma^2$  and especially the choice of the parameter k are examined. The Akaike (1973) information criterion is introduced as a means of deciding on the optimal number of classes k, and shown to work well in simulations. The method is also illustrated with two new data sets on stomach volumes (of ghost crabs and marron) and with the prairie grass data of Rabinowitz *et al.* 

#### Numerical procedures

Given (1) and assuming that the distribution of  $\varepsilon_i$  is normal  $(0,\sigma^2)$ , the discretized log likelihood of the sample  $y_1, \dots, y_n$  is

log L

$$= \sum_{i=1}^{n} \log \left\{ (2\pi\sigma^2)^{-\frac{1}{2}} \sum_{j=1}^{k} m_j^{-1} \exp[-(y_i/m_j - \mu_i)^2/2\sigma^2] \pi_j \right\} (2)$$
$$= \sum_{i=1}^{n} \log \left[ (2\pi\sigma^2)^{-\frac{1}{2}} \sum_{j=1}^{k} m_j^{-1} e_{ij} \pi_j \right], \text{ say,}$$
(3)

where  $\mu_i = \alpha + \beta x_i$ . Maximizing this subject to

$$\sum_{j=1}^{n} \pi_j = 1$$

gives for  $\pi_i$  the equations

$$\pi_{j} = n^{-1} \sum_{i=1}^{n} \left\{ \frac{-m_{j}^{-1} e_{ij} \pi_{j}}{\sum_{j=1}^{k} m_{j}^{-1} e_{ij} \pi_{j}} \right\}, \ 1 \le j \le k,$$
(4)

which can be used to update a new value of  $\pi_j$  on the left given a previous set of  $\pi_j$ ,  $1 \le j \le k$ , on the right. Differentiation of log L with respect to  $\beta$  gives another likelihood equation:

$$\beta = \sum_{i=1}^{n} (x_i - \bar{x}) y_{ia} / \sum_{i=1}^{n} (x_i - \bar{x})^2$$
(5)

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where

$$\mathbf{y}_{ia} = \mathbf{y}_i \hat{\mathbf{E}}(\mathbf{p}^{-1} | \mathbf{y}_i)$$

and

$$\hat{E}(p^{-1}|y_i) = \left(\sum_{j=1}^{k} m_j^{-2} e_{ij} \pi_j\right) / \left(\sum_{j=1}^{k} m_j^{-1} e_{ij} \pi_j\right).$$

Similarly, equations for  $\alpha$  and  $\sigma^2$  can be found. Note that  $\beta$  occurs implicitly in  $y_{ia}$ , so (5) is not an explicit solution for  $\beta$ .

Anderson and Hinde's suggested method of solution was to insert "old" values of  $\beta$ ,  $\pi_i$  and  $\sigma^2$  on the RHS of (4), (5) and a corresponding equation for  $\sigma^2$ , and obtain "new" values of  $\beta$ ,  $\pi_i$ , and  $\sigma^2$  from the LHS of those equations. Starting values for the procedure were the "trimming" estimates given as the other method in Maller et al. (1983). This procedure seemed to converge to a stable set of estimates but required a very large number of iterations (often more than 300 for the lobster data), and was very time consuming. We suggest an improvement of this method as follows. Equation (4) is still used to update new values of  $\pi_i$  on the LHS by inserting old estimates in the RHS. Given these estimates of  $\pi_i$ , Equation (5) is "solved" for an estimate of  $\beta$  by a Newton-Raphson procedure, to a sufficient degree of accuracy, and similarly for  $\sigma^2$ . These values are then inserted in  $e_{ii}$ , new values of  $\pi_i$  produced from (4), and the procedure repeated. Again, the "trimming" estimates and a simple histogram estimate of the distribution of p are used as starting values. Upon convergence, if it occurs, a set of estimates  $\hat{\beta}$ ,  $\hat{\sigma}^2$ , and  $\hat{\pi}_i$  is obtained. The new procedure converged in most cases considered, produced much faster convergence (often up to 6 times as fast), and also revealed that the old procedure, although increasing the likelihood of each step, still had not reached a maximum. Standard errors of the estimates conditional on the values of  $\pi_i$  and k are now available from the second derivative matrix of the log likelihood.

The main advantage of the procedure, however, is that simulations of the model assumed to be generating the data are now feasible, and we can use these to study the properties of the estimates. In fact these properties turn out to be very good, at least for reproducing the known values in simulated data, and seem to give reasonable estimates for data similar to the lobster data, at least inasmuch as can be judged by comparisons between sets of data. The most problematical point is the choice of k. For this we propose to use the Akaike (1973) information criterion, defined as

The model with minimum AIC is the chosen model. The AIC penalizes the likelihood estimate for the number of parameters, and selects a compromise model, with the highest likelihood for the least number of parameters; Stone (1977) gives a useful discussion of the AIC method and its connection with cross-validation.

We demonstrate that the AIC reaches a minimum for many sets of simulated data and for the data of Morris (1977), and Thompson (1988), and provides very good estimates for the simulated data. In the case of the Rabinowitz *et al.* (1986) data, we are able to reproduce the "actual" estimates very closely.

# Simulations

In Maller *et al.* (1983) the cube root of foregut volume (in cc) of the western rock lobster (*Panulirus cygnus*) was found to be related to its carapace length (in mm) approximately as follows:

$$y_i/p = \alpha + \beta x_i + \varepsilon_i \tag{6}$$

where  $\alpha = 0$ ,  $\beta = 0.02$ , and  $\varepsilon$  is normal with mean 0 and variance  $(0.14)^2$ . In this section, simulations of the model (1) are examined. For the main set of simula-

Table 1. Results from 1000 simulations of the method applied to  $y_i/p = \alpha + \beta x_i + \varepsilon_i$  where  $\alpha = 0, \beta = 0.02, \varepsilon_i$  is N(0,(0.14)<sup>2</sup>), and p has distribution (7). The number of discrete mixing intervals is k, and the standard errors of a, b, and s were calculated from the simulations.

k	а	SE(a)	b	SE(b)	s	SE(s)	log L	$-\frac{1}{2}(AIC)$
5	-0.02	0.03	0.0190	0.0006	0.199	0.016	-146.5	-154.5
6	-0.01	0.03	0.0195	0.0005	0.175	0.005	-102.4	-111.4
7	-0.01	0.03	0.0197	0.0005	0.160	0.005	-91.40	-101.4
8	-0.01	0.03	0.0199	0.0005	0.155	0.005	-93.68	-104.7
9	-0.01	0.03	0.0198	0.0005	0.157	0.006	-93.64	-105.6
10	-0.01	0.03	0.0198	0.0005	0.154	0.006	-85.75	- 98.8
11	-0.00	0.03	0.0198	0.0005	0.147	0.005	-79.39	- 93.4
21	0.00	0.03	0.0199	0.0005	0.140	0.005	-76.67	-100.7
41	0.00	0.03	0.0199	0.0005	0.139	0.006	-76.50	-120.5
61	0.00	0.03	0.0199	0.0005	0.139	0.006	-76.49	-160.8
81	0.00	0.03	0.0199	0.0005	0.139	0.006	-76.79	-140.8

tions, 110 realizations of (6) were chosen with n = 1000,  $x_i$  having a uniform distribution on [30, 80] and p having distribution

$$0.5 \,\delta_1 + 0.5 \,\mathrm{U} \left[ 0.2, 1 \right] \tag{7}$$

where  $\delta_i$  denotes a point mass at 1 and U[a,b] is the uniform distribution on [a,b]. Thus 50% of the lobsters had full stomachs, but no stomachs less than 20% full occurred. Starting values for the iterative procedure were the true values from (6) and a simple histogram estimate of the distribution of p.

Table 1 shows the estimates a,b,s of  $\alpha = 0$ ,  $\beta = 0.02$ ,  $\sigma = 0.14$ , their standard errors over the 110 realizations, and the average log likelihood of the 110 realizations. The new procedure converged in over 95% of cases. The table suggests that values of  $k \le 6$  provide biased estimates, especially for  $\sigma$ , while k = 11 produces excellent estimates. These are the minimum AIC estimates. Q-Q plots showed that the distributions of a and b

were very closely approximated by normal distributions for k > 6.

The whole procedure was repeated for n = 100 with similar results, although the variability of the estimates was correspondingly higher. Here the maximum of log L occurred for about k = 40. It was noticed that the average of the estimates of  $\sigma$  progressively decreased as k increased (it was 0.1217 for k = 41), although it was never significantly less than 0.14. The same trend is evident in Table 1, although it is small, probably owing to the increasing number of parameters which are being estimated as k increases; for samples of the order of n = 100, there are  $\leq 5$  observations per cell expected when  $k \geq 20$ . This represents "overfitting", and is penalized by the AIC procedure.

We might expect the mixing distributions to be poorly estimated by the nonparametric method. Figure 2 shows the mean, maximum, and minimum mixing cumulative distributions for 110 realizations of model (6) with n = 250, fitted with k = 11. The estimates seem reason-

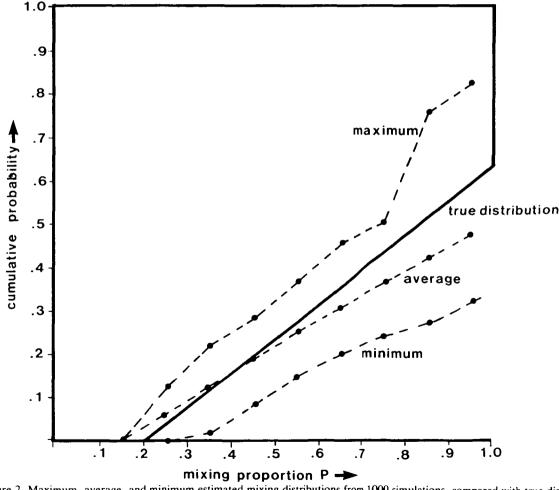


Figure 2. Maximum, average, and minimum estimated mixing distributions from 1000 simulations, compared with true distribution.

able although variability is high. (Of course "averaging" the estimated distributions may not be a good way of displaying them.) A number of checks on the above results were done, mostly for the case n = 100. Similar data were generated with mixing distribution

$$U(0.2,1);$$
 (8)

i.e., all lobsters were downweighted to some extent. The fitting procedure was modified to allow a parameter for the fitting of some probability mass at 1 (Table 1 was generated in this way) or not. Trying various combinations (data generated with or without mass at 1)  $\times$  (data fitted with or without mass at 1) gave predictable results.

Some of the simulations with N = 1000 were repeated

with different starting values for a, b, or s<sup>2</sup>. For starting estimates as far away as a = -0.25, b = 0.016 or s = 0.12, the Newton-Raphson procedure occasionally did not converge, especially for small values of  $k(k \le 6)$ . But usually it did, and the estimates recovered were the same as those in Table 1 to the order of accuracy of the fitting procedure (more iterations were required on average, of course). Convergence in the other data sets could be obtained by changing the starting estimates; an adequate choice is usually the "trimming estimates" of Maller *et al.* (1983), which are simple to calculate.

As a final test, the method was applied to a simulated set of least-squares data with n = 100,  $\alpha = 0$ ,  $\beta = 0.02$ ,  $\sigma = 0.14$ , and with *no* mixing distribution. The estimates produced by the procedure varied, as k was varied, over the ranges 0.002 to -0.001 for a, 0.0202 to 0.0209 for b,

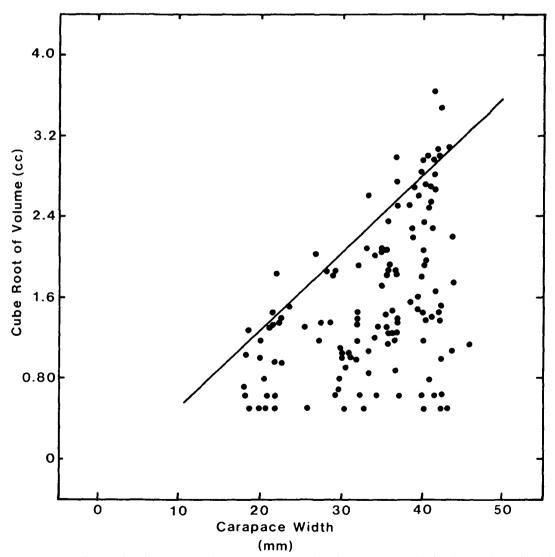


Figure 3. Cube root of stomach volume (cc) of 136 ghost crabs plotted against carapace width (mm). The line is fitted by the methods of the present paper.

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0.146 to 0.139 for s, and 50.45 to 50.36 for log L. The least-squares estimates for the data were a = 0.002, b = 0.0202, s = 0.148, and the Akaike procedure selected k = 1; exactly these values, to the accuracy of the calculations.

## Applications to data

(1) Figure 3 shows the cube root of stomach volume of 136 male and female ghost crabs as a function of carapace width (Morris, 1987). (The volumes as plotted have been rescaled by a mesh-size factor of 0.4, which is irrelevant for our purposes.) Table 2 lists the estimates of  $\alpha$ ,  $\beta$ , and  $\sigma$  obtained for various values of k, together with the maximized likelihood and  $-\frac{1}{2}(AIC)$  for the data in Figure 3. The minimum AIC occurs at k = 8, corresponding to estimates a = 0.25, b = 0.077, s = 0.32. The line with parameters a and b is shown plotted in Figure 3. A separate regression for females gave a = -0.45, b = 0.086, suggesting no significant differences between sexes, as judged by the standard errors given in Table 2.

(2) Dr Rabinowitz kindly supplied the data on which her Figures 1 and 2 are based. Rabinowitz *et al.* (1986) obtained for the regression of log weight on *actual* age the estimates a = 0.54 (SE 0.02), b = 0.856 (SE 0.0008), s = 0.23, whereas the method of the present paper, applied to log weight and *chronological* age, produced minimum AIC estimates at k = 20 of a = 0.69 (SE 0.03), b = 0.0855 (SE 0.0015), s = 0.22 (SE 0.01), in excellent agreement except for a slightly lower value of a in Rabinowitz *et al.* estimates. (But they used the trimming method of Maller *et al.* (1983) as a "robustifying" tool in their regression, and this is known to produce estimates of  $\alpha$  which are slightly low (Maller *et al.*, 1983.).)

(3) Using as an example some data kindly supplied by Thompson (1988), we demonstrate how to test for whether downward displacement of points has actually occurred. Thompson's data are 92 observations on gut weight of the marron *Cherax tenuimanus*, taken as y variable, versus carapace length of the animal, taken as x variable.

Fitting by the method of this paper gave k = 4 as the minimum AIC value, and the estimates for k = 4 together with the estimates for an ordinary least-squares regression of y on x (k = 1) are given in Table 3. (Gut weight was cube root transformed before analysis, and one outlying value was removed.)

Minus twice the difference in log likelihood between the two fits has the value 6.10, which we take as approximately  $\chi^2$  with 3 d.f., since there are four parameters (the four mixing proportions) fitted when k = 4. Since this value is not significant, the data are adequately described by k = 1, i.e., a simple regression of y on x. This is borne out by plots of the data which show little displacement.

# Acknowledgement

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Table 2. Result of applying the method to the data of Morris (1987). Standard errors of a, b, and s were calculated from the second derivative of the log likelihood.

k	а	SE(a)	b	SE(b)	S	SE(s)	log L	$-\frac{1}{2}(AIC)$
1	-0.09	0.27	0.048	0.008	0.69	0.04	-143.0	-147.0
3	-0.17	0.27	0.062	0.008	0.56	0.05	-132.5	-138.5
4	-0.40	0.28	0.086	0.008	0.58	0.05	-128.0	-135.0
5	0.04	0.28	0.056	0.008	0.53	0.05	-131.4	-139.4
6	0.05	0.27	0.060	0.008	0.45	0.04	-125.8	-134.8
7	-0.21	0.20	0.069	0.006	0.36	0.03	-116.3	-126.3
8	-0.25	0.19	0.077	0.005	0.32	0.03	-114.1	-125.1
ĝ.	-0.50	0.20	0.080	0.006	0.36	0.03	-118.1	-130.1
10	-0.29	0.20	0.074	0.006	0.32	0.03	-118.6	-131.6

Table 3. Result of applying the method to the data of Thompson (1988). Standard errors of a, b, and s were calculated from the second derivative of the log likelihood.

k	а	SE(a)	b	SE(b)	S	SE(s)	log L	$-\frac{1}{2}(AIC)$
1	0.25	0.07	0.027	0.001 5	0.18	0.01	29.72	25.7
4	0.26	0.07	0.028	0.001 3	0.13	0.01	32.77	25.8

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