A maximum-likelihood estimator of food retention time in ruminants

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(*Received 7 June 1971 – Accepted 4 October 1971*)

1. A method for estimating the retention time of foodstuffs in the alimentary tract of the ruminant is given which utilizes the logistic function. This method results in a maximum-likelihood estimator that has known statistical properties.

2. An example is presented in which the logistic function was fitted to an excretion curve and found to provide a very good fit.

The rate of passage of foodstuffs through the alimentary tract of the ruminant has been studied extensively. Castle (1956) and Coombe & Kay (1965) have each suggested a method for estimating the retention time for a marker substance to pass through a specified section of the gut. The former calculated the retention time by adding together the times of excretion from 5 to 95% at intervals of 10%, taken from the graph, and dividing the sum by ten; the latter calculated retention time

$$\bar{R} = \Sigma(MT)/\Sigma M,$$

where T was the length of time between dosing and excretion in the faeces, and M was the total amount of marker in that collection. Neither of these methods, however, results in an estimator that has any known statistical properties.

This paper presents an alternative method for estimating the retention time as well as estimating the maximum rate of passage of the foodstuffs through the alimentary tract and the statistical properties of these maximum-likelihood estimators.

ESTIMATION AND PROPERTIES

Past studies by Balch (1950) and Castle (1956) have indicated that the cumulative excretion curves for many experiments of this kind are sigmoid in shape. A particular form of the two-parameter logistic function due to Krause, Siegel & Hurst (1967) is

$$\eta_t = \frac{100}{1+\exp[-R(t-\tau)/25]}, \tag{1}$$

where η_t is the percentage of marker excreted from initial administration to time t.

The parameters in formula 1 possess a physical interpretation. The parameter R is the maximum value of the derivative of η_t with respect to t. Thus, R is the maximum rate of passage of the marker through the ruminant. Similarly, τ is the time required for one-half of the marker to be excreted. The maximum value of the derivative of η_t with respect to t, or R, occurs at time $t = \tau$ which implies that the maximum rate of passage occurs at the time when one-half of the marker has been excreted. One can also think of τ as the median time of excretion since one-half of the marker is eliminated in τ units of time following the initial administration. The maximum-likelihood estimator of τ, call it $\hat{\tau}$, estimates the same quantity as the $\bar{R}$ value calculated by Castle (1956).

The parameters are estimated by the method of maximum likelihood. This is accomplished by letting $Y_t = \eta_t + \epsilon_t$, where the random variables ϵ_t, $t = 1, 2, \ldots, n$, are assumed to be stochastically independent and normally distributed with mean zero and variance σ^2. Further, it is assumed that σ^2 is independent of t (homoscedastic). Thus, Y_t is normally distributed with mean η_t and variance σ^2.

The actual estimates of the parameters are obtained by finding the simultaneous solution of a Taylor's series approximation of the maximum-likelihood equations:

$$\Sigma(Y_t - \eta_t)\frac{\partial \eta_t}{\partial R} = 0 \quad \text{and} \quad \Sigma(Y_t - \eta_t)\frac{\partial \eta_t}{\partial \tau} = 0. \tag{2}$$

These solutions, call them $\hat{R}$ and $\hat{\tau}$, are obtained by a computer program utilizing the standard Newton–Raphson iterative technique. (A list of this Fortran IV program and instructions for using it are available upon request from the first author.)

The estimate of σ^2, $\hat{\sigma}^2$, is then obtained by using these values $\hat{R}$ and $\hat{\tau}$ in

$$\hat{\sigma}^2 = \frac{1}{n-2}\Sigma\left[Y_t - \frac{100}{1+\exp[-\hat{R}(t-\hat{\tau})/25]}\right]^2. \tag{3}$$

The asymptotic variance–covariance matrix of the maximum-likelihood estimators $\hat{\sigma}^2$, $\hat{R}$, and $\hat{\tau}$ is given by the inverse of the following matrix:

$$V^{-1} = \begin{bmatrix} \frac{n}{2\sigma^2} & 0 & 0 \\ 0 & \frac{16}{\sigma^2}\sum_t \frac{[(t-\tau)\exp[-R(t-\tau)/25]]^2}{[1+\exp[-R(t-\tau)/25]]^4} & \frac{-16}{\sigma^2}\sum_t \frac{R(t-\tau)\exp[-2R(t-\tau)/25]}{[1+\exp[-R(t-\tau)/25]]^4} \\ 0 & \frac{-16}{\sigma^2}\sum_t \frac{R(t-\tau)\exp[-2R(t-\tau)/25]}{[1+\exp[-R(t-\tau)/25]]^4} & \frac{16}{\sigma^2}\sum_t \frac{R^2\exp[-2R(t-\tau)/25]}{[1+\exp[-R(t-\tau)/25]]^4} \end{bmatrix}. \tag{4}$$

The iterative procedure that the computer program uses to obtain the estimates of R and τ utilizes empirical values of V^{-1}. Thus, an estimate of the variance–covariance matrix of the estimators is available at the end of the estimation procedure.

The statistical properties of the maximum-likelihood estimators are discussed by Patton & Krause (1972). Results reported there indicate that the estimators are unbiased and uncorrelated if the observations are taken at times that are symmetric about time τ in interval $(0, 2\tau)$. Further, the distribution of each estimator is approximately normal. A well-designed experiment to ensure a small correlation between $\hat{R}$ and $\hat{\tau}$ would involve an *a priori* estimate of τ and utilize data recorded at nearly symmetric intervals about that estimate. For example, suppose an *a priori* estimate of τ is 30 h. If the process is observed at 20 h it should also be observed at 40 h – or at 15 h and 45 h.

In other words, symmetry here refers to having an observation the same distance above τ as another observation is below τ. If a prior estimate of τ is not available from previous studies, it is suggested that observations be taken at constant intervals so that when τ is estimated from the data, the observations will be approximately symmetric about τ.

The approximate normality of the estimators coupled with the easily obtained (from the computer program) estimates of the variances and the robustness of the standard t test indicates that the application of t statistics (referring here to the standard tests on means utilizing Student's t distribution) for testing suitable hypotheses and setting confidence intervals on the unknown parameters would be appropriate. The near-zero correlation of the estimators indicates that, for most practical purposes, the test concerning the individual parameters R and τ would be independent. Thus, attention could be focused on either parameter without reference to the effect of the other.

AN EXAMPLE

This form of the logistic function was fitted to an excretion curve obtained in an experiment by Martz, Asay, Wormington, Leddicote & Daniels (1969). The data were already collected when this problem was presented to the authors so that no control of the selection of times of the observations was possible.

The data given below were fed into the computer program. (The only additional information that must be supplied to the program is a starting value for R and a starting value of τ.) The column headed by t gives the time in hours from the time of initial administration and the corresponding value in the 'actual' column gives the percentage of the marker substance that was eliminated in time t. The 'estimated' column gives the percentage of marker substance excreted estimated by the fitted logistic function. The estimated parameters are $\hat{R} = 3{\cdot}1079$ and $\hat{\tau} = 25{\cdot}2439$. Thus the fitted function is:

$$\hat{\eta}_t = \frac{100}{1+\exp[-3{\cdot}1079(t-25{\cdot}2439)/25]}. \tag{5}$$

t	Actual	Estimated	Actual − estimated
15	22·1	21·9	0·2
24	45·7	46·1	−0·4
27	56·0	55·4	0·6
30	63·8	64·4	−0·6
33	70·9	72·4	−1·5
38	86·6	83·0	3·6
48	92·1	94·4	−2·3
52	95·8	96·5	−0·7
73	99·2	99·7	−0·5

$\hat{\sigma}^2 = 3{\cdot}18$. Coefficient of determination $= 0{\cdot}995$.

The standard errors of these estimates, obtained from V^{-1}, of R, τ and σ^2 are 0·135, 0·296 and 0·841 respectively. The estimator $\hat{\sigma}^2$ is uncorrelated with $\hat{R}$ and $\hat{\tau}$, and the correlation between $\hat{R}$ and $\hat{\tau}$ is 0·35. This last correlation would have been much smaller if the experiment had been designed such that the observations were taken at times roughly symmetric about τ.

In this example, $\hat{\tau} = 25{\cdot}2439$ h is the time from initial administration until one-half of the marker substance has been excreted as well as the time at which the rate of passage of the marker through the ruminant is a maximum. This maximum rate of passage is R or, in this example, 3·1079%.

The known statistical properties of the estimators $\hat{R}$ and $\hat{\tau}$ make it possible to test hypotheses about R and τ or set confidence limits on R and τ by using ordinary t tests.

The use of the inverse sine transformation is frequently desirable when the variance of the error term is related to the binomial variance. However, a small Monte Carlo study of 300 samples of size fifteen with a variance of the form of a binomial variance with $n = 100$ indicated no appreciable increase in the accuracy of the estimates when the transformation was used. Thus, the inverse sine transformation of the data does not appear to be necessary in this estimation problem.

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Printed in Great Britain