Estimating Richards Function Parameters by Marquardt's Algorithm

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ABSTRACT

We address the problem of determining the Richards growth function parameters by Marquardt's nonlinear fitting algorithm. This growth function's parameters are directly related to its S-shaped form, and are therefore biologically relevant for growth comparison studies. We have developed a fitting program which estimates values for the four parameters of the Richards function and we present applications of this method for fish and cephalopod growth data.

KEYWORDS: nonlinear fitting algorithms, S-shaped curves, parameter estimation, Richards function, Marquardt's algorithm.

INTRODUCTION

The motivation for this work came from growth comparison studies in plants and fish. Experimental data of this type becomes stationary after a certain time describing an S-shaped curve. In 1959 Richards proposed a function as a growth model (Richards, 1959) which has been widely used in plant comparison studies (Namkoong and Matzinger, 1975; Neals and Nichols, 1978; Causton and Venus, 1981; Rose and Charles Edwards, 1981).

The most popular nonlinear sigmoid curves with less than five parameters are the well-known logistic, Gompertz (1825), Nelder (generalised logistic) (1961), von Bertalanffy (1957) and Richards function (1959). The latter function not only generalises the logistic function, but it also generalises the von Bertalanffy equation (Richards, 1959; von Bertalanffy, 1957).

It has been widely used to model plant growth, because its parameters or their combination, have geometrical or biologically meaning (Causton and Venus, 1981; Del Riego and Dodson, 1987, 1990; Namkoong and Matzinger, 1975; Summerfelt and Hall, 1987. The von Bertalanffy equation parameters have also geometrical meaning, and have been used in many fish growth studies Bagenal, 1973; Beverton and Holt, 1957; Gulland, 1983; Namkoong and Matzinger, 1975; Ricker, 1975). However there are cases, like (Forsythe and van Heukelen, 1987), where von Bertanffly's fit has also been found inadequate to model the early growth cycle.We decided to use Marquardt's (1963) algorithm to estimate the four parameters of the Richards growth function for a set of data because this method overcomes many problems inherent in other fitting methods (Box *et al.*, 1969). This algorithm has been employed in many commercial subroutines but generally within complex programs. This poses a constraint for many investigators, because it is a difficult procedure to program (Marquardt, 1963; Conway *et al.*, 1970; Namkoong and Matzinger, 1975). Our idea was to produce a simple, independent executable program which could run on any PC-computer. We include a detailed description of Marquardt's algorithm which may be helpful for those who would like to apply this method to other functions. The authors would like to thank J. Chavarría for codifying our fitting program.

Marquardt's algorithm was also used by Namkoong and Matzinger (1975) to fit their data to the Richards function but their approach is different from ours because they approximated the three parameters of the differential equation which defines the Richards function, not the function itself. On the other hand, the estimation approach of Causton and Venus (1981) employs the logarithm of the Richards function using the Newton-Raphson algorithm.

RICHARDS FUNCTION AND MARQUARDT'S ALGORITHM

Richards Function

The standard form for the Richards function is given by:

$$L(t) = \frac{\alpha}{(1 \pm e^{\beta - \kappa t})^{1/\eta}}$$

where α and κ are positive constants, β is a constant and $-1 \leq \eta$ 0 and the sign in the equation corresponds to the sign of η.

To apply this function as a model for growth, take any living organism. *a* represents its limiting size; it is the first parameter used to compare the growth of individuals in the same species, or between two species. Note that the initial size predicted by this function is $L(0) = \alpha\ (1 + e^{\beta})^{-1/\eta}$. Less direct, but more important, are the parameters η and κ, directly related to the rate at which each individual or species is growing. In practice, we find that if we keep α, and the quotients β/η and κ/η constant, different values of β, κ, and η can give curves of quite similar appearance and fit. Accordingly, the parameters α, β/η, κ/η, and η seem better to represent curves of different appearances (Del Riego and Dodson, 1987, 1990). Perhaps it is for this geometrical reason that using different arguments, on the one hand Richards and on the other Causton and Venus, proposed these and other quotients in their growth studies (Causton and Venus, 1981).

We claim that this function can also be applied to fish growth studies in an effective manner. Observe that Richards function gives a very good fit to fish data (see Figures 2, 3 and 4), even at the early growth cycle. To our knowledge Richards equation has not been used before in fish studies, because the preferred model is still von Bertalanffy equation. We hope to convice you that this Richards model is a suitable comparison tool.

MARQUARDT'S ALGORITHM APPLIED TO RICHARDS FUNCTION

Marquardt's Strategy

Let (t_i, Y_i), $i=1,\dots,m$ denote the experimental data to be fitted. We will consider in the sequel that the Richard's function L depends not only on the time t_i, but also on the four parameters, *i.e.*

$$Y_i \quad L_i = L(t_i, \alpha, \beta, \kappa, \eta)$$

The four estimated parameters (A, b, k, n) are obtained by a least minimum squares method, that is to say, they minimize the function

$$\phi = \sum_{i=1}^{m} (Y_i - L(t_i, \alpha, \beta, \kappa, \eta))^2$$

The non-linearity in Richard's function makes it impossible to calculate its parameters directly by this equation. They are usually obtained by either of the two main classical minimal squares estimation procedures:

- the Taylor series expansion
- the Gradient or Steepest Descent.

They both determine the value of the parameter vector

$$\mathbf{p} = (p_1, p_2, p_3, p_4) = (A, b, k, n)$$

by successive corrections of size $\delta = (\delta_1, \delta_2, \delta_3, \delta_4)$, that is to say,

$$\mathbf{p} = \mathbf{p} + \delta$$

The difference in both methods lies in the manner in which they evaluate δ.

Let δ_T and δ_G the correction vectors for the Taylor and Gradient methods respectively. Marquardt (1963) proposed a new way to evaluate the vector which we will denote by δ_M . His main strategy centers around the right choosing of a parameter λ 0 such that

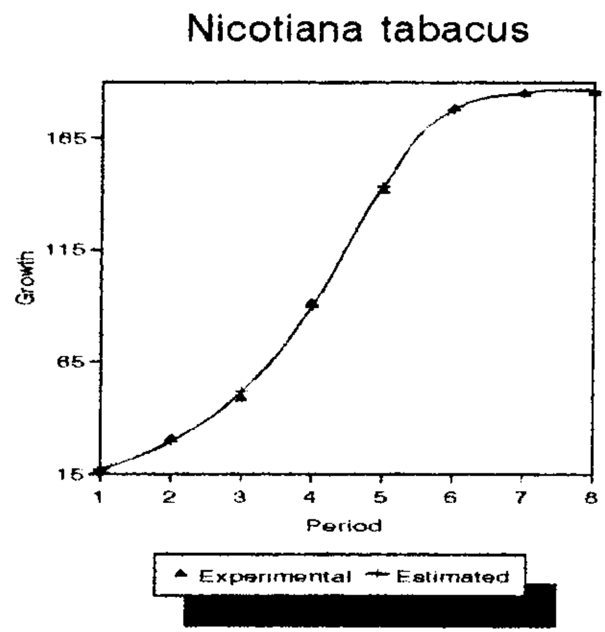

Figure 1. Stationary Data.

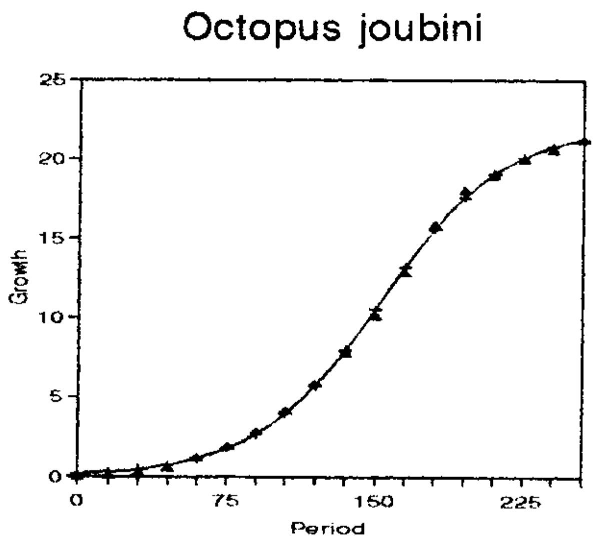

Figure 2. Almost Stationary Data.

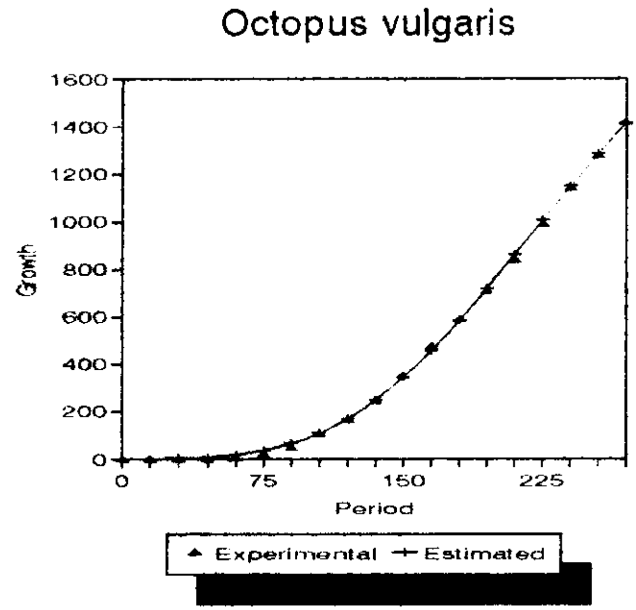

Figure 3. Non-Stationary Data.

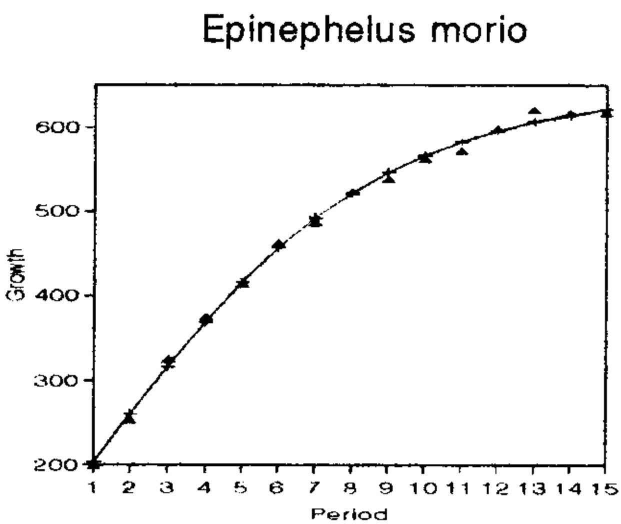

Figure 4. Almost Stationary Data.

$$\delta_M = \delta(\lambda)$$

It turns out that δ_M constitutes an optimal interpolation between δ_T and δ_G. Moreover, in the δ_M-neighborhood the truncated linear Taylor series adequately represents Richards non-linear model.

Numerical Algorithm

Denote by $Q_{m\times 4} = \left(\frac{L_i}{p_j}\right)$, and $G_{4\times 1} = (g_j) = \left({}_{i=1}^{m} (Y_i - L_i)\cdot \frac{L_i}{p_j}\right)$

If $Q^T Q = (q_{ij})$, let $Q^*_{4\times 4} = \left(\frac{q_{ij}}{q_{ij} \quad q_{ij}}\right)$, $G^*_{4\times 1} = \left(\frac{g_j}{q_{jj}}\right)$

Initial Values

$\lambda^{(0)} = 10^{-2}$

$\mathbf{p}^{(0)}$, obtained by Hadley's (1978) algorithm.

Once $\lambda^{(r)}$ and $\mathbf{p}^{(r)}$ are known, obtain $\delta^{*(r)}$ as a solution vector to the system of equations defined by:

$$Q^{*(r)} + \lambda^{(r)} I)\, \delta^{*(r)} = G^{*(r)}. \text{ Then } \delta_j(\lambda^{(r)}) = (\delta_j^{*(r)} / \quad q_{jj}^{-2}) \quad j = 1, 2, 3, 4.$$

Evaluate

$$\mathbf{p}^{(r+1)} = \mathbf{p}^{(r)} + \delta(\lambda^{(r)})]$$

and

$$\phi^{(r+1)} = {}_{i=1}^{m} (Y_i - L(t_i, \mathbf{p}^{(r+1)})^2$$

Evaluation of $\lambda^{(r+1)}$: Let

$$\phi(\lambda) = {}_{i=1}^{m} \left(Y_i - \lambda(t_i, \mathbf{p}^{(r)}) - {}_{i=1}^{4} \frac{L_i}{p_j} \delta_j(\lambda)\right)^2$$

compute $\phi(\lambda^{(r)})$. If $\phi(\lambda^{(r)}) \quad \phi^{(r+1)}$, then $\lambda^{(r+1)} = \lambda^{(r)}$. Otherwise, let $\mu > 1$.

Compute $\phi(\lambda^{(r)} / \mu)$. If $\phi(\lambda^{(r)} / \mu) \quad \phi^{(r+1)}$ then $\lambda^{(r+1)} = \lambda^{(r)} / \mu$, else there exists $\omega \quad 1$ such that $\phi(\lambda^{(r)} \mu^{\omega}) \quad \phi^{(r+1)}$. In this case $\lambda^{(r+1)} = \lambda^{(r)} \mu^{\omega}$.

THE FITTING PROGRAM'S PERFORMANCE

The Fitting Program

A Pascal program with manual, embodying Marquardt's algorithm to fit real data to a Richards function was written to run on any PC-compatible computer. The data can be entered either manually or by giving an ASCII file. It produces a printed report and an ASCII output file. This file can thus be imported in a number of graphic packages to obtain the model fitting graphic. The report gives the parameters fittings for the data provided and the correlation matrix between them to assess the errors. It also calculates the parameter quotients described in Causton and Venus, 1981; Del Riego and Dodson, 1990).

The program includes a subroutine based on Hadley's method to obtain the initial values. Of course, using Marquardt's algorithm, we obtain convergence even when the initial values are far from the solution. For a copy of this PC-program and manual please contact the authors.

The Program's Performance

The program ran both with theoretical and experimental S-shaped data. The precision in this last case depends essentially on how stationary they are.

Theoretical Data

As expected, the parameter's values estimated were the actual parameters; an absolute reliability test was applied, which the program performed rather well. We went up to an ε-precision 10^{-7}.

Experimental Data

Stationary or Almost Stationary Data — Figure 1 presents a set of regular data taken from Namkoong and Matzinger (1975). The program obtained the parameters with a precision of $\varepsilon = 10^{-7}$.

The program ran equally well with the *Octopus joubini* data from Forsythe and van Heukelen (1987) in Figure 2 and the fish data from Moe (1969) in Figure 4, even when they are not yet fully stationary. The ε-precision was 10^{-7} for the first set of data, 10^{-2} for the second case. The standard deviation between the experimental values and the estimated ones was almost null for both cases.

Non-Stationary Data — It was rather unexpected that the program ran even in this case, with ε-precision of 10^{-2}. As an example, we present in Figure 3 *Octopus vulgaris* data contained in Forsythe and van Heukelen (1987), which are well spread in the early stage. The difference between the experimental and the estimated data was not significant. Nevertheless, it must be said that when the data are incomplete, even though values of the parameters of the Richards function are obtained, the theoretical predictions based on this particular fit are unreliable. With data for a longer period of time, (that is to say, with more data), the precision will undoubtedly be increased.

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