

Nonlinear Regression Models and Applications in Agricultural Research

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ABSTRACT

Nonlinear regression models are important tools because many crop and soil processes are better represented by nonlinear than linear models. Fitting nonlinear models is not a single-step procedure but an involved process that requires careful examination of each individual step. Depending on the objective and the application domain, different priorities are set when fitting nonlinear models; these include obtaining acceptable parameter estimates and a good model fit while meeting standard assumptions of statistical models. We propose steps in fitting nonlinear models as described by a flow diagram and discuss each step separately providing examples and updates on procedures used. The following steps are considered: (i) choose candidate models, (ii) set starting values, (iii) fit models, (iv) check convergence and parameter estimates, (v) find the “best” model among competing models, (vi) check model assumptions (residual analysis), and (vii) calculate statistical descriptors and confidence intervals. The associated feedback mechanisms are also addressed (i.e., model variance homogeneity). In particular, we emphasize the first step (choose candidate models) by providing an extensive library of nonlinear functions (77 equations with the associated parameter meanings) and examples of typical applications in agriculture. We hope that this contribution will clarify some of the difficulties and confusion with the task of using nonlinear models.

IN DATA ANALYSIS, we often ask the following questions: Which is the best model to describe our data? Which is the best statistical index to judge the goodness of fit? How do we choose among competing models? There are no simple answers to these questions. Here we attempt to provide agronomists with a general framework on how to approach these questions appropriately. Our specific objectives are: (i) to provide a succinct overview of nonlinear models and to develop a guideline to understand the family of functions used in agricultural applications; (ii) to indicate techniques to modify nonlinear models and how to cope with multiple nonlinear models; (iii) to discuss key methodological issues on parameter estimation, model performance, and comparison; and (iv) to demonstrate step-by-step analysis of experimental data using a nonlinear regression model. The structure follows the flow diagram in Fig. 1. We start with the definition of nonlinear regression models and discuss their main advantages and disadvantages. Then we present 77 nonlinear functions (including those in supplemental tables) with references to applications in agriculture. We offer an updated overview of methodologies to fit models, choose starting values, assess goodness of fit, select the best models, and evaluate residuals. Finally, we reanalyse experimental data on biomass growth with time (Damasatos et al., 2009).

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NONLINEAR REGRESSION MODELS

Definition

In general, statistical models used in agricultural applications can be described with the following notation:

$$y = f(x, \theta) + \epsilon$$

where y is the response variable, f is the function or model, x are the inputs, θ denotes the parameters to be estimated, and ϵ is the error. Each parameter can be evaluated for whether it is linear or not; if the second derivative of the function with respect to a parameter is not equal to zero, then the parameter is nonlinear. Thus a given function (f) can have a mix of linear and nonlinear parameters.

Why Should We Use Nonlinear Models?

The main advantages of nonlinear models are parsimony, interpretability, and prediction (Bates and Watts, 2007). In general, nonlinear models are capable of accommodating a vast variety of mean functions, although each individual nonlinear model can be less flexible than linear models (i.e., polynomials) in terms of the variety of data they can describe; however, nonlinear models appropriate for a given application can be more parsimonious (i.e., there will be fewer parameters involved) and more easily interpretable. Interpretability comes from the fact that the parameters can be associated with a biologically meaningful process. For example, one of the most widely used nonlinear models is the logistic equation (Eq. [2.1] in Table 1). This model describes the pervasive S-shaped growth curve. The parameters have a clear meaning (see Table 1) and units associated with their definition. The asymptotic parameter (Y_{asym}) has units equal to the response variable (Y), the inflection point (x_m) has units equal to the independent variable (x), and the

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