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CHAPTER 15: NONLINEAR REGRESSION MODELS AND APPLICATIONS

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Nonlinear statistical models continue to be relevant because they have the advantages of simplicity, flexibility, and parsimony when used in the analysis and description of agricultural data. Often nonlinear models can be easier to interpret than other alternatives. These models have been applied to data ranging from leaf-level to landscape-level processes, such as photosynthesis, biomass accumulation, soil CO_2 efflux, and temperature responses. Our objective is to provide a multistep framework that helps with the application of these models with specific considerations in each step. Even though objectives and applications may vary, common priorities should be set when fitting nonlinear models: obtaining acceptable parameter estimates, a good model fit, and meeting standard assumptions of statistical models. 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 indexes and confidence intervals. In particular, we emphasize the first step (choose candidate models) by providing an extensive library of nonlinear functions (77 equations with the associated parameter interpretations) and application examples in agriculture. We hope that this contribution will clarify some of the difficulties and confusion with using nonlinear models.

Despite the wide availability of techniques for modeling the functional relationship between a dependent variable and independent variable(s), traditional nonlinear models continue to be relevant because they have the advantage of having meaningful parameters and being parsimonious. Recent developments in machine learning (such as neural networks) can provide good predictive abilities, but fail to shed light on the underlying processes. Still, one significant challenge in using nonlinear models is related to choosing the most appropriate model. 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. In this chapter, we attempt to provide agrono-

Abbreviations: AIC, Akaike information criterion; BIC, Bayesian information criterion; DOY, day of year; LRT, likelihood ratio test; QQ, quantile–quantile.

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mists 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 guidelines to understand the family of functions used in agricultural applications; (ii) to describe techniques for modifying nonlinear models and how to cope with multiple nonlinear models; (iii) to discuss key methodological issues related to parameter estimation, model performance, and comparisons; and (iv) to demonstrate step-by-step analysis of experimental data using a nonlinear regression model. The chapter follows the structure of the flow diagram illustrated 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 with references to applications in agriculture. The last sections offer an updated overview of methodologies used to fit models, choose starting values, assess goodness of fit, select the right models, and evaluate residuals. Finally we provide an example of fitting a nonlinear model based on experimental data of biomass growth over time (Danalatos et al., 2009).

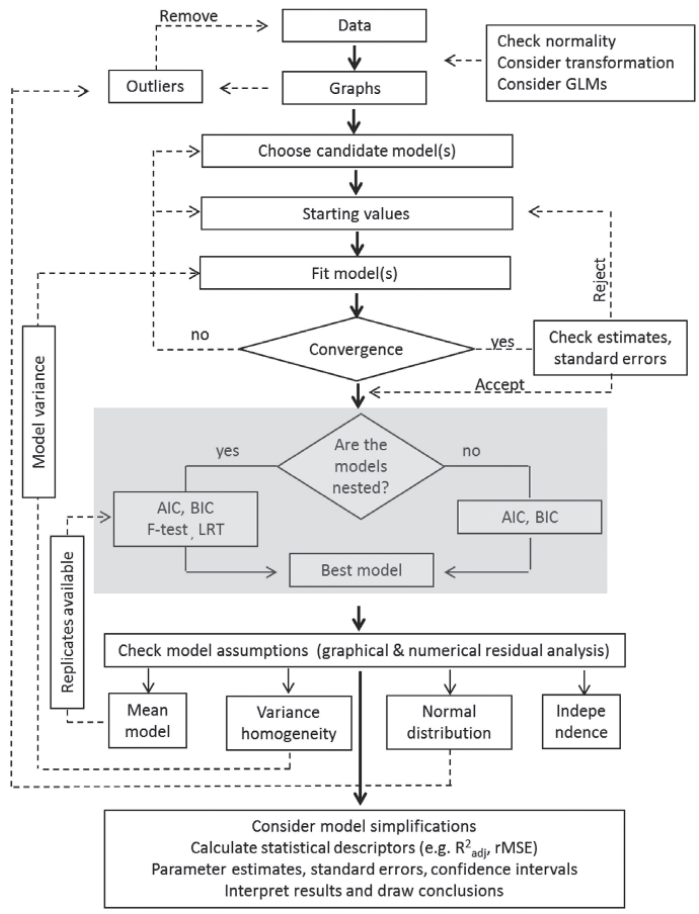


FIG. 1. Suggested workflow in the nonlinear regression analysis. Thick arrows indicate major steps, thin arrows indicate substeps and dashed arrows indicate feedback in nonlinear regression. The shaded part is optional and can be ignored in simple cases. GLM, generalized linear models; LRT, likelihood ratio test; AIC, Akaike information criterion; BIC, Bayesian information criterion.

Nonlinear Regression Model

Definition

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

$$y = f(x, \theta) + \varepsilon \quad [1]$$

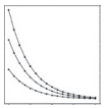
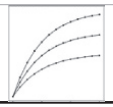
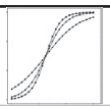
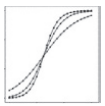
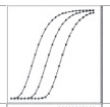
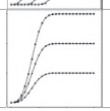
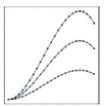
where y is the response variable, f stands for function but can also be thought of as the *model* or *regression function*, x are the inputs, θ denotes the parameters to be estimated, and ε is the error. Each parameter can be evaluated for whether it is linear: if the second derivative of the function 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 benefits of nonlinear models are parsimony, interpretability, and prediction (Bates and Watts, 2007). In general, nonlinear models are capable of accommodating a vast variety of patterns, 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 (t_m) has units equal to the independent variable (t), and the parameter that determines the steepness of the curve (k) has units equal to t. A competing cubic or higher order polynomial model used to describe the same data would have the disadvantages that more parameters will be needed (than just three) and that the parameters will not be easily interpretable (Pinheiro and Bates, 2000). For example, what would be the interpretation of the parameters associated with the x^3, x^4, and x^5 in a five degree polynomial? In addition, when x is a large number the value of x^5 can be extremely large, making the parameter associated with it extremely small and possibly numerically unstable.

The other benefit of using nonlinear regression models is that their predictions tend to be more robust than competing polynomials, especially outside the range of observed data (i.e., extrapolation). Although extrapolation is not considered to be a good practice, when it is necessary to do so, nonlinear models based on functional relationships can have acceptable performance. Nonlinear regression models, however, come at a cost. Their main disadvantages are that they can be less flexible than competing linear models and that generally there is no analytical solution for estimating the parameters. The first point underscores that the choice of the nonlinear model is crucial, thus making it tempting to try a large library of functions and

TABLE 1. Nonlinear regression models. For example fits, see figures in the supplemental material online.

Eq.	Name/reference: form	Schematic graph/ changing parameter		Parameter meaning
Group I: Exponential				
[1.1]	Exponential decay: $Y = Y_o e^{-kt}$		Y_o	Y is the response variable (e.g., soil organic matter), t is the explanatory variable (e.g., time), Y_o is the initial or the maximum Y value, k is a rate constant determines the steepness of the curve.
[1.2]	Exponential rise: $Y = Y_o(1 - e^{-kt})$		Y_o	
Group II: Sigmoid functions				
[2.1]	Logistic (Verhulst, 1838): $Y = \frac{Y_{asym}}{1+e^{-k(t-t_m)}}$		k	Y is the response variable (e.g., biomass), t is the explanatory variable (e.g., time), Y_{asym} or Y_{max} is the asymptotic or the maximum Y value, t_m is the inflection point at which the growth rate is maximized, k controls the steepness of the curve, v deals with the asymmetric growth (if $v = 1$, then Richards equation becomes logistic), a and b are parameters determine the shape of the curve, t_e is the time when $Y = Y_{asym}$, t_c is the critical time for a switch-off to occur (e.g., critical photoperiod), n is a parameter determines the sharpness of the response.
[2.2]†	Richards (1959): $Y = \frac{Y_{asym}}{\left[1+ve^{-k(t-t_m)}\right]^{\frac{1}{v}}}$		k	
[2.3]	Gompertz (1825): $Y = Y_{asym} e^{-e^{-k(t-t_m)}}$		t_m	
[2.4]	Weibull (1951): $Y = Y_{asym}\left(1-e^{-at^b}\right)$		Y_{asym}	
[2.5]‡	Beta (Yin et al., 2003b): $Y = Y_{max}\left(1+\frac{t_e-t}{t_e-t_m}\right)\left(\frac{t}{t_e}\right)^{\frac{t_e}{t_e-t_m}}$		Y_{max}	

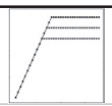
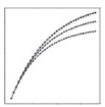
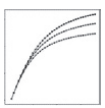
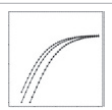
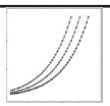
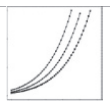
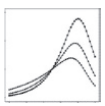
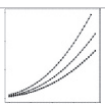
Eq.	Name/reference: form	Schematic graph/ changing parameter		Parameter meaning
[2.6]§	Hill (switch-off) function: $Y = \frac{t_c^n}{t_c^n + t^n}$		t_c	
Group III: Photosynthesis				
[3.1]	Blackman (1905): $Y = \min(Y_{asym}, aI) - R_d$		Y_{asym}	Y is the response variable (net photosynthesis), I is the explanatory variable (irradiance), Y_{asym} is the asymptotic Y value, a is the initial slope of the curve at low I levels, R_d is the dark respiration, θ is a dimensionless curvature parameter when $\theta = 1$ Eq. [3.4] is equivalent to Eq. [3.1] and when $\theta \to 0$ Eq. [3.4] is equivalent to Eq. [3.3].
[3.2] ¶	Asymptotic exponential: $Y = Y_{asym}\left(1 - e^{\frac{aI}{Y_{asym}}}\right) - R_d$		Y_{asym}	
[3.3]¶	Rectangular hyperbola: $Y = \frac{aIY_{asym}}{Y_{asym} + aI} - R_d$		R_d	
[3.4] ¶,#	Non rectangular hyperbola: $Y = \frac{Y_{asym} + aI - \sqrt{\left(Y_{asym} + aI\right)^2 - 4\theta aIY_{asym}}}{2\theta} - R_d$		Y_{asym}	
[3.5]	Modified logistic (Sinclair and Horie, 1989): $Y = Y_{asym}\left[\frac{2}{1 + e^{-k(N - N_{min})}} - 1\right]$		N_{min}	Y is the response variable (light saturated net photosynthesis), N is the explanatory variable (leaf nitrogen), Y_{asym} is the asymptotic Y value, k determines the curvature of the curve, N_{min} is the N value at or below which $Y = 0$.

Table continued.

TABLE 1. Continued.

Eq.	Name/reference: form	Schematic graph/ changing parameter		Parameter meaning
[3.6]††	Farquhar et al. (1980): $Y = \min\left[\frac{V_{\text{cmax}}(C_i - \Gamma^*)}{C_i + K_{\text{mc}}(1 + O/K_{\text{mo}})}, \frac{J(C_i - \Gamma^*)}{4C_i + 8\Gamma^*}\right] - R_{\text{day}}$		V_{cmax}	Y is the response variable (net photosynthesis), C_i is the explanatory variable (intercellular CO_2 concentration), V_{cmax} is the maximum carboxylation capacity, Γ^* is the CO_2 compensation point in the absence of R_d, K_{mc} and K_{mo} are Michaelis–Menten coefficients of Rubisco for CO_2 and O_2, respectively, O is the partial pressure of oxygen (= 210 mbar), J is the photosystem II electron transport rate, R_{day} is the dark respiration occurring in the light.
Group IV: Temperature dependencies				
[4.1]	Van't Hoff (1898) (known as Q_{10} function): $Y = Q_{10}^{\frac{T - T_{\text{ref}}}{10}}$		T_{ref}	Y is the response variable (e.g., respiration), T is the explanatory variable (temperature), T_{ref} is a reference temperature, at which $Y = 1$, Q_{10} is the factor by which the rate of a process (respiration) increases for each 10°C temperature increase, E is the activation energy determines the increase in temperature response, R is the universal gas constant (= 8.314 J K^{-1} mol^{-1}), D is the deactivation energy that determines the decrease in the temperature response, S is the entropy term that determines the transition state of the curve, E_o is an activation-energy-like parameter that is temperature-adjusted, T_x is a fitted temperature parameter in K, T_{min} is the base or minimum temperature for $Y = 0$.
[4.2]	Arrhenius (1889): $Y = e^{\left[\frac{E}{R}\left(\frac{1}{T_{\text{ref}} - 273} - \frac{1}{T - 273}\right)\right]}$		T_{ref}	
[4.3]‡‡	Modified Arrhenius: $Y = e^{\left[\frac{E}{R}\left(\frac{1}{T_{\text{ref}} - 273} - \frac{1}{T - 273}\right)\right]} \left\{\frac{1 + e^{\left[\frac{(T_{\text{ref}} + 273)S - D}{(T_{\text{ref}+273})R}\right]}}{1 + e^{\left[\frac{E}{R} - \frac{D}{(T+273)R}\right]}}\right\}$		E	
[4.4]	Lloyd and Taylor (1994): $Y = e^{E_o\left(\frac{1}{T_{\text{ref}} - 273 - T_x} - \frac{1}{T - 273 - T_x}\right)}$		T_{ref}	

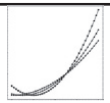
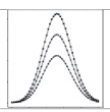
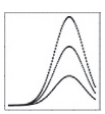
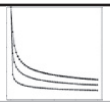
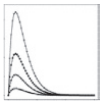
Eq.	Name/reference: form	Schematic graph/ changing parameter		Parameter meaning
[4.5]	Ratkowsky et al. (1982): $Y = \frac{(T - T_{min})^2}{(T_{ref} - T_{min})^2}$		T_{min}	
Group V: Peak or bell shape curves				
[5.1]	Beta (Yin et al. 1995): $Y = \left[\left(\frac{T_c - T}{T_c - T_o}\right)\left(\frac{T - T_b}{T_o - T_b}\right)^{\frac{T_o - T_b}{T_c - T_o}}\right]^c$		T_{ref}	Y is the response variable (e.g., rate of development), T is the explanatory variable (temperature), T_o is the optimum temperature for maximum Y, T_b is the base or minimum temperature for $Y = 0$ T_c is the ceiling or maximum temperature for $Y = 0$ c is a curvature parameter (default $c = 1$).
[5.2]§§	Bell curve: $Y = Y_{asym} e^{\left[a(X - X_o)^2 + b(X - X_o)^3\right]}$		Y_{asym}	Y is the response variable, X is the explanatory variable, Y_{asym} is the asymptotic maximum Y value, X_o is the position of the center of the peak (Y_{asym}), a and b are coefficients controlling the width of the bell.
[5.3]	Gaussian function: $Y = Y_{asym} e^{\left[-0.5\left(\frac{X - X_o}{b}\right)^2\right]}$		Y_{asym}	
Group VI: Others nonlinear equations				

Table continued.

TABLE 1. Continued.

Eq.	Name/reference: form	Schematic graph/ changing parameter		Parameter meaning
[6.1]	Power: $Y = aX^b$		a	Y is the response variable, X is the explanatory variable, a and b parameters defines the shape of the curve and the magnitude of the Y value.
[6.2]	Modified hyperbola: $Y = \frac{aX}{1+bX}$		a	
[6.3]	Michaelis–Menten: $Y = -\frac{\mu X}{X + C_{sat}}$		C_{sat}	Y is the response variable (e.g., denitrification rate), X is the explanatory variable, the substrate (e.g., NO_3), μ is the rate constant, C_{sat} is the half-saturation constant.
[6.4]	Rational function: $Y = \frac{a_1 X^{a_2}}{1 + a_3 X^{a_4}}$		a_1	Y is the response variable, X is the explanatory variable, a_1 and a_3 are parameters defining the magnitude of the Y value, a_2 and a_4 are parameters defining the shape of the curve; if $a_2 = a_4 + 1$, then equation shows a near-linear response; if $a_2 = a_4$, then equation becomes hyperbola; if $a_2 < a_4$, then equation takes a bell-shape; if $a_2 > a_4$ or $a_4 = 0$, the, equation becomes exponential; if $a_2 = 0$, then equation becomes exponential decay.
[6.5]	Ricker curve: $Y = a_1 X e^{-a_2 X}$		a_1	Y is the response variable, X is the explanatory variable, a_1 and a_2 parameters control both the height and the width of the skewed to the right "bell."

† The maximum growth rate for the Richards equation is given in Birch (1999).
‡ The maximum growth rate for the Beta equation is given in Yin et al. (2003b).
§ Cited in Amaducci et al. (2008).
¶ Cited in Goudriaan (1979).
# Goudriaan (1979) and Johnson et al. (2010) used the nonrectangular hyperbola to describe photosynthetic rate response to CO_2.
†† This is simplified version of the Farquhar model. For more details see references in the text.
‡‡ The optimum temperature for this equation is given in Fig. 2.
§§ Cited in Hammer et al. (2009).
Cited in Bril et al. (1994).

choose the model with lowest error. However, it is almost always better to choose a model based on whether it has been used successfully in similar applications and has biologically meaningful parameters (e.g., Table 1).

The lack of analytical solutions has two practical consequences. First, a numerical method needs to be used to find estimates for the parameters, and this implies that convergence of the algorithm needs to be checked (Fig. 1). A lack of convergence often results from the second consideration, which is that these numerical methods require starting values. Choosing a model with biologically meaningful parameters makes the process of choosing starting values easier as the starting values can usually be easily determined from visual inspection of the data (more on this later).

Typical Nonlinear Models and Application Examples

Choosing among competing models for an application is not always a simple task. We have developed a reference table as a guideline to understand the family of functions used in agricultural applications. Table 1 presents 27 common nonlinear equations and Tables 2 through 7 supplements these with 45 additional equations. We classified the equations into six groups. All equations have been used in agricultural applications, and most of the parameters have a meaningful interpretation. The variety of equations in Table 1 reflects the fact that one equation does not suit all processes.

Group I: Exponential

The exponential decay and exponential models, which give rise to maximum functions (Eq. [1.1] and [1.2], Table 1) have been used in a wide spectrum of soil and plant science applications. Both equations have been commonly used to describe light and nitrogen vertical distributions within plant canopies (Monsi and Saeki, 2005), nitrous oxide emission response to nitrogen fertilizer (e.g., Hoben et al., 2011), cumulative soil respiration (e.g., Gillis and Price, 2011), residue or soil organic matter decomposition (Thorburn et al., 2001), photoperiodic sensitivity (e.g., Wang and Engel, 1998), temperature or moisture responses on nitrification (e.g., Ma and Shaffer, 2001), and water infiltration rate (Horton, 1940), and general first-order kinetics processes. It is a simple equation with one major unknown, the rate constant (k), which is also termed *extinction coefficient* in crop physiology or decomposition rate constant in soil science. Also, the ratio $\log(2)/k$ is of importance in soil science because it denotes the mean residence time (e.g., soil organic matter). Equation [1.1] provided the starting point to develop case-specific nonlinear functions. Yin et al. (2000, 2003a) established a nonlinear function to describe leaf area index development as a function of canopy nitrogen content (Eq. [2.8], Table 2). Johnson et al. (2010) developed a flexible nonlinear function for the protein (nitrogen) vertical distribution within plant canopies (Eq. [2.9], Table 2). In soil science, Andren and Paustian (1987) and Gillis and Price (2011) extended Eq. [1.1] to better describe decomposition of straw residue and biochar, respectively (Eq. [2.5], [2.6], and [2.7], Table 2). Lastly, Eq. [1.1], as well as expolinear functions that combine linear and exponential phases (namely Eq. [3.15] and [3.16], Table 3) have also been applied to describe initial parts of growth curves, but not the entire growth curves because the growth profile often reaches an asymptotic value.

TABLE 2. Equations derived from the exponential equation. Numbering continues from Group I of the Table 1.

Eq.	Name and/or reference	Form	Parameter meaning
[2.3]	Parallel or double first order	$Y = fY_o e^{-k_1 t} + (1-f)Y_o e^{-k_2 t}$	Y is the response variable; t is the explanatory variable (e.g., time); Y_o is the initial or maximum Y value; k, k_1 and k_2 are rate constants determines the steepness of the curve (units: time^{-1}); f, f_1, and f_2 are fractions (range: 0–1) that determine the size of each pool; b is a rate constant for the linear component; t_i is the infection point for the logistic component (units: time); t_d is the distance from infection point to 3/4 maximum (units: time).
[2.4]	Triple first order	$Y = f_1 Y_o e^{-k_1 t} + f_2 Y_o e^{-k_2 t} + (1-f_1-f_2)Y_o e^{-k_3 t}$	
[2.5]	Consecutive first order (Andren and Paustian, 1987)	$Y = fY_o e^{-k_1 t} + (1-f)Y_o \left[e^{-k_2 t} + \frac{k_2}{k_1 - k_2}\left(e^{-k_2 t} - e^{-k_1 t} \right) \right]$	
[2.6]	First order plus linear (Gillis and Price, 2011)	$Y = Y_o \left(1 - e^{-kt}\right) + bt$	
[2.7]	First order plus logistic (Gillis and Price, 2011)	$Y = Y_o f \left(1 - e^{-kt}\right) + \frac{Y_o (1-f)}{1 + e^{-\frac{t-t_i}{t_d}}}$	
[2.8]	Leaf area index nitrogen limited equation Yin et al. (2000, 2003a)	$Y_{LAI} = \frac{1}{k_n} \ln\left(1 + \frac{k_n X_N}{n_b}\right)$	Y_{LAI} *and* Y_N are the response variables, leaf area index and nitrogen content, respectively; X_N and X_{LAI} are the explanatory variables, canopy nitrogen content ,and leaf area index, respectively; k_n is the rate constant and determines the steepness of the curve (also called nitrogen extinction coefficient); n_b is the minimum value of nitrogen at or below which leaf photosynthesis under saturated light conditions is zero (usually n_b ranges from 0.25 to 0.80; see review by Archontoulis et al., 2012); Y_o is the initial or maximum Y value, c is a dimensionless coefficient.
[2.9]	Protein or nitrogen distribution within plant canopies (Johnson et al., 2010)	$Y_N = Y_o - \left(Y_o - n_b\right)\left(1 - e^{-k_n X_{LAI}}\right)^c$	

Eq.	Name and/or reference	Form	Parameter meaning
[2.10]	Photoperiodic sensitivity (Wang and Engel, 1998)	$Y = e^{-P_{sen}(X-P_c)}$	Y is the response variable, X is the explanatory variable (photoperiod), P_{sen} is the photoperiod sensitivity coefficient being positive for short-days plants and negative for long days plants, P_c is the critical day-length, around 11 h for short days and 18 h for long days.
[2.11]	Model for water infiltration (Horton, 1940)	$Y = Y_c + (Y_o - Y_c)e^{-kt}$	Y is the response variable (infiltration capacity, mm/h), t is the explanatory variable (time, hours), k is the rate constant representing the rate of decrease, Y_c indicates a final or equilibrium capacity (mm/h) Y_o indicates the initial infiltration capacity (mm/h).

TABLE 3. Additional sigmoid type functions. Numbering continues from Group II of the Table 1.

Eq.	Name and/or reference	Form	Parameter meaning and application
Different version of the logistic equation†			
[3.7]	5-parameter	$Y = Y_{low} + \frac{Y_{asym}}{\left[1 + e^{-k(t-t_m)}\right]^c}$	Y is the response variable (e.g., biomass), t is the explanatory variable (e.g., time), Y_{asym} is the asymptotic Y value, Y_{low} is the initial Y value, t_m is the infection point at which growth rate is maximum, k determines the steepness of the curve, c is a shape parameter.
[3.8]	4-parameter	$Y = Y_{low} + \frac{Y_{asym}}{1 + e^{-k(t-t_m)}}$	
[3.9]	2-parameter	$Y = \frac{1}{1 + e^{-k(t-t_m)}}$	
[3.10]	1-parameter	$Y = \frac{1}{1 + e^{-(t-t_m)}}$	
		Different versions of the beta function‡	
[3.11]	5-parameter; for cases when initial phase is important (Yin et al., 2003b)	$Y = Y_b + (Y_{max} - Y_b)\left(1 + \frac{t_e - t}{t_e - t_m}\right)\left(\frac{t - t_b}{t_e - t_b}\right)^{\frac{t_e - t_b}{t_e - t_m}}$	Y is the response variable, t is the explanatory variable (e.g., time), Y_{max} is the maximum Y value, t_m is the infection point at which growth rate is maximized, t_e is the t value (time) when $Y = Y_{max}$, t_b is the t value when growth starts, Y_b is the Y value at time t_b.

Eq.	Name and/or reference	Form	Parameter meaning and application
[3.12]	2-parameter; for cases when maximum growth rate achieved at the beginning of growth (Yin et al., 2003a)	$Y = Y_{max}\left(2t_e - t\right)\frac{t}{{t_e}^2}$	
[3.13]	2-parameter; for cases when maximum growth achieved toward the end of growth period (Yin et al., 2003a)	$Y = Y_{max}\left(3t_e - 2t\right)\frac{t^2}{t_e^3}$	
[3.14]	3-parameter; Applied to describe leaf senescence; (Yin et al., 2009)	$Y = Y_{max}\left[1 - \left(1 + \frac{t_e - t}{t_e - t_m}\right)\left(\frac{t}{t_e}\right)^{\frac{t_e}{t_e - t_m}}\right]$	
		Expolinear functions for plant growth analysis	
[3.15]	Expolinear (Goudriaan and Monteith, 1990)	$Y = \frac{c_m}{r_m}\log\left[1 + e^{r_m\left(t - t_o\right)}\right]$	Y is the response variable (e.g., biomass), t is the explanatory variable (time), c_m is the maximum growth rate in the linear phase, r_m is the maximum relative growth rate in the exponential phase, t_o is the time when growth begins, Y_{max} is the maximum Y value.
[3.16]	Symmetrical expolinear (Goudriaan, 1994)	$Y = \frac{c_m}{r_m}\log\left[\frac{1 + e^{r_m\left(t - t_o\right)}}{1 + e^{r_m\left(t - t_o - \frac{Y_{max}}{c_m}\right)}}\right]$	

Table continued.

TABLE 3. Continued.

Eq.	Name and/or reference	Form	Parameter meaning and application
Additional generic sigmoid functions			
[3.17]	Levakovic (cited in Zeide, 1993)	$Y = Y_{asym}\left(\frac{t^d}{\beta + t^d}\right)^c$	Y is the response variable (e.g., biomass), t is the explanatory variable (time), Y_{asym} is the asymptotic Y value, β and c determine the start of growth and the inflection point, d controls the shape of the curve.
[3.18]	Korf (cited in Zeide, 1993)	$Y = Y_{asym} e^{-\beta t^{-c}}$	
[3.19]	Special Von Bertalanffly, (1938)§	$Y = Y_{asym}\left[1 - e^{-k(t-t_o)}\right]$	Y is the response variable (e.g., biomass), t is the explanatory variable (time), Y_{asym} is the asymptotic maximum Y value, t_o is the time when growth begins, t_{50} is the time when $Y = 1/2$ of Y_{asym}, k controls the steepness of the curve, v controls the asymmetry and the shape of the curve (for $v = 1$, 2.20 becomes 2.19).
[3.20]	Generalized Von Bertalanffly, (1938)§	$Y = Y_{asym}\left[1 - e^{-k(t-t_o)}\right]^v$	
[3.21]	Log-logistic distribution (Ritz et al., 2013)	$Y = \frac{Y_{asym}}{1 + \exp\left[k\left\{\log(t) - \log(t_{50})\right\}\right]} = \frac{Y_{asym}}{1 + \left(t/t_{50}\right)^k}$	
Inverse sigmoid functions used to quantify water retention curves¶			
[3.22]	van Genuchten (1980)	$\theta_h = \theta_r + \frac{\theta_s - \theta_r}{\left[1 + (ah)^n\right]^{1-\frac{1}{n}}}$	θ_ψ is the volumetric water content (mm/mm), h is the matric potential (kPa), θ_r is the residual water content (mm/mm), θ_s is the saturated water content (mm/mm), a is the inverse of the air entry suction ($a > 0$), n is a measure of the poor-size distribution ($n > 1$).

Eq.	Name and/or reference	Form	Parameter meaning and application
[3.23]	Gardner (1958)	$\theta_h = \theta_r + \frac{\theta_s - \theta_r}{1 + (ah)^n}$	
[3.24]	Brooks and Corey (1964)	$\theta_h = \theta_r + \frac{\theta_s - \theta_r}{(ah)^n}$	
[3.25]	Campbell (1974)	$\theta_h = \theta_s (ah)^n$	

† The 3-parameter logistic equation is given in Table 1 (see Eq. [2.1]).

‡ For additional versions of the beta growth function see Yin et al. (2003b).

§ For a comparison of the two von Bertalanffy (1938) models see Urban (2002).

¶ The R package HydroMe includes the listed water retention equations (see Omuto and Gumbe, 2009).

TABLE 4. Additional equations for photosynthesis. Numbering continues from Group III of the Table 1.

Eq.	Name and/or Reference	Form	Parameter meaning & application
[4.7]	Modified rectangular hyperbola proposed to describe photosynthetic reduction at over-saturated irradiance levels (e.g., photorespiration) (Ye and Zhao, 2010)	$Y = aI\frac{1-\beta I}{1+\gamma I} - R_d$	Y is the response variable (net photosynthesis), I is the explanatory variable (irradiance), a is the slope of the curve when I equals zero, β and γ are coefficients with no clear (biological) meaning.
[4.8]	Modified hyperbola used to describe light saturated photosynthesis response to nitrogen (del Pozo and Dennett, 1999)	$Y = Y_{\text{asym}}\frac{N-N_{\text{min}}}{N+k}$	Y is the response variable (light saturated net photosynthesis), N is the explanatory variable (leaf nitrogen), Y_{asym} is the asymptotic maximum Y value, k determines the curvature of the curve, N_{min} is the N value at or below which $Y = 0$.
[4.9]	Weibull type sigmoid curve used to assess water stress effects on photosynthesis (Vico and Porporato, 2008)	$Y = Y_{\text{asym}}e^{\left[-\left(\frac{-\Psi_L}{d}\right)^b\right]}$	Y is the response variable (e.g., carboxylation rate), Ψ_L is the explanatory variable (water potential), Y_{asym} is the asymptotic Y value, b and d determine the shape of the curve.

TABLE 5. Additional equations for temperature dependencies. Numbering continues from Group IV of the Table 1.

Eq.	Name and/or reference	Form	Parameter meaning & application
[5.6]	Power (e.g., Shibu et al., 2006)	$Y = \left(\frac{T}{T_o}\right)^c$	Y is the response variable, T is the explanatory variable (temperature), T_o is the optimum temperature for maximizing Y, c is a shape factor (usually $c = 2$), a determines the magnitude of the Y value, b determines the shape of the curve.
[5.7]	Logarithmic (e.g., Foereid et al., 2011)	$Y = a + b\log(T)$	
[5.8]	Exponential (e.g., Shibu et al., 2006)	$Y = ae^{bT}$	
[5.9]†	Modified exponential (O'Connell, 1990)	$Y = e^{\left[a+bT\left(1-0.5\frac{T}{T_o}\right)\right]}$	
[5.10]	Bell-shaped 3-parameter; Used to describe photosynthesis response to temperature (Johnson et al., 2010)	$Y = \left[\frac{(1+c)T_o - T_{min} - cT}{(1+c)T_o - T_{min} - cT_{ref}}\right]\left(\frac{T - T_{min}}{T_{ref} - T_{min}}\right)^c$	Y is the response variable (e.g., photosynthesis), T is the explanatory variable (temperature), T_{ref} is a reference temperature, at which $Y = 1$, T_{min} is the minimum temperature for $Y = 0$, T_o is the optimum temperature for maximum Y, c is a shape factor.

† Eq. [5.9] follows an increasing and decreasing pattern like the modified Arrhenius equation (see Eq. [4.3] in Table 1, Fig. 2). It was used by Kirschbaum (1995) to describe soil organic matter decomposition as a function of temperature.

TABLE 6. Additional peak or bell shape equations. Numbering continues from Group V of the Table 1.

Eq.	Name and/or reference	Form	Parameter meaning and application
[6.4]†	Lorentzian 3-parameter	$Y = \frac{a}{1+\left(\frac{X-X_o}{b}\right)^2}$	Y is the response variable, X is the explanatory variable, Y_o is the initial Y value, X_o is the position of the center of the peak, a and b are coefficients controlling the height and width of the peak, c determines the number of peaks ($0 < c < 1$ for one peak).
[6.5] †	Lorentzian 4-parameter	$Y = Y_o + \frac{a}{1+\left(\frac{X-X_o}{b}\right)^2}$	
[6.6]‡	Lognormal 3-parameter	$Y = ae^{-0.5\left[\frac{\log\left(\frac{X}{X_o}\right)}{b}\right]^2}$	
[6.7]	Pseudo–Voigt 4-parameters	$Y = a\left[\frac{c}{1+\left(\frac{X-X_o}{b}\right)^2} + (1-c)e^{-0.5\left(\frac{X-X_o}{b}\right)^2}\right]$	

† Condition $b > 1$.

‡ Condition $0 < b < 1$.

TABLE 7. Additional equations. Numbering continues from Group VI of the Table 1.

Eq.	Name and/or reference	Form	Parameter meaning & application
[7.6]†	Holling type IV (e.g., Bolker, 2008)	$Y = \frac{Y_{asym} X^2}{b + cX + X^2}$	Y is the response variable, X is the explanatory variable, Y_{asym} is the asymptotic Y value, b and c define the position of the peak and the shape of the curve, Y_o is the initial or maximum Y value.
[7.7]‡	Shepherd (e.g., Bolker, 2008)	$Y = \frac{Y_{asym} X}{b + X^c}$	
[7.8]‡	Hassell (e.g., Bolker, 2008)	$Y = \frac{Y_{asym} X}{\left(b + X\right)^c}$	
[7.9]§	2 parameter exponent (e.g., Ratkowsky, 1993)	$Y = Y_o b^X$	
[7.10]	Monod kinetics	$Y = \frac{\mu X}{X + C_{sat}}$	Y is the response variable (e.g., mineralization rate), X is the explanatory variable, the substrate (e.g., OC), μ is the rate constant, C_{sat} is the half-saturation constant, B is the rate of microorganisms (e.g., size of microbial biomass), if $B = 1$, then Monod becomes M–M equation.

† If $c < 0$ the equation takes a peak form; the peak occurs at $X = -2b/c$. This function is called rational function because expresses the ratio of two polynomial functions. It can also take a S-shape (see Bolker, 2008).

‡ If $c > 0$, then equation takes a peak form.

§ If $b > 1$, then Y increases; if $b < 1$ then Y decreases.

Group II: Sigmoid Curves

Sigmoid curves (mathematical functions having an "S" shape) are another important group of nonlinear models. These models are often applied to describe plant height, weight, leaf area index, or seed germination as a function of time, nitrogen application rate, or herbicide dose (e.g., Gan et al., 1996). Sigmoid equations are also used as 0–1 modifiers in process-based models to incorporate the effect of soil moisture or pH effects on soil nitrogen transformation processes (e.g., McGechan and Wu, 2001) and also as a switch-off function in studies assessing plant photoperiodic sensitivity (e.g., Amaducci et al., 2008). Table 1 (Group II) presents common sigmoid functions, and Table 3 provides additional sigmoidal equations, providing increased flexibility (e.g., when maximum growth or inflection point is achieved at the start or at the end of the growth period). Additional equations can be found in Zwietering et al. (1990), Zeide (1993), Leduc and Goelz (2009), and in many statistical textbooks or software manuals (e.g., SigmaPlot, JMP, TableCurve). In general, the suitability of a sigmoid equation to estimate maximum rate of increase or optimum X level for maximizing the Y value is an important research objective (Birch, 1999; Yin et al., 2003b). Each function has its advantages and disadvantages (for a discussion, see Birch, 1999; Yin et al., 2003b), and it is up to the researcher to select the most appropriate one to fit the experimental data. The logistic equation (Eq. [2.1], Table 1) describes symmetric growth having an inflection point at 1/2 of final size (i.e., asymptote). The Gompertz equation has an inflection point that is controlled by its asymptotic value and is at about one-third (1/e = 0.3679), while others like Richards or Weibull or Beta have more flexibility in dealing with asymmetric growth (the inflection point can be at any X value). Having a flexible inflection point is another important feature of a sigmoid curve. For that, Birch (1999), for example, modified the logistic equation (Eq. [2.1], Table 1) to deal with asymmetric growth by adding an extra shape parameter. When growth is known to decrease after a certain period of time, then the β growth function (Eq. [2.5], Table 1) might be a better option. On the other hand, Eq. [2.5] (Table 1) might not predict accurately initial growth, and, in cases when the initial phase should be considered, different versions of the β function should be used (see Eq. [3.11], Table 3). It is important to note that most sigmoid equations assume an initial Y value close to zero at time zero, which is reasonable in most cases; that is, at planting, biomass weight is close to zero.

Group III: Process Specific: Photosynthesis Examples

Photosynthesis is an important biological process involved in plant growth, and its rate is influenced by irradiance, temperature, nitrogen availability, vapor pressure deficit, and CO_2 concentration. Although there are detailed biochemistry models that have been proposed and used (e.g., von Caemmerer and Farquhar, 1981), there is a place for simpler models, especially when the main interest is in comparing different groups or treatments. Different nonlinear functions have been developed to describe photosynthesis response to different environmental variables. Functions to describe photosynthesis response to irradiance have been researched the most (Jassby and Platt, 1976; Goudriaan, 1979). All equations assume that dark respiration (R_d) is independent of light level. Among the equations presented in Table 1, the Blackman (Eq. [3.1]) is the simplest one, and the asymptotic exponential (Eq. [3.2])

and the nonrectangular hyperbola (Eq. [3.4]) are the most common. The rectangular hyperbola (Eq. [3.3], also termed the *Michaelis–Menten equation*) is used less frequently because it suggests that saturation is reached too fast. Currently, discussion on the photosynthetic capacity (Y_{asym}) and efficiency (a) of different plant species is based on the comparison of nonlinear regression estimates; for this, caution should be exercised because similar estimates from different equations can result in different responses (Fig. 2). Equation [3.2] is a simple three-parameter equation widely used in light driven process-based models like SUCROS and Hybrid-maize (Goudriaan and van Laar, 1994; Yang et al., 2004). Equation [3.4] offers more flexibility, and it is more accurate than Eq. [3.2] at the cost of one extra parameter (i.e., θ, curvature parameter). When $\theta = 1$, Eq. [3.4] becomes equivalent to the Blackman equation, and when θ approaches zero, Eq. [3.4] becomes the rectangular hyperbola (Eq. [3.3]). Equation [3.4] comprises the reference equation when the biochemical model of Farquhar et al. (1980) or Collatz et al. (1992) is used in modeling studies. New equations are still being developed and tested (e.g., Eq. [4.7], Table 4).

Photosynthesis response to CO_2 has been quantified empirically using a nonrectangular hyperbola (Goudriaan, 1979; Johnson et al., 2010) and mechanistically using a biochemical model (Farquhar et al., 1980). The biochemical model is based on the Michaelis–Menten kinetics for substrate limited growth and the law of minimum between carboxylation and electron transport rates (Eq. [3.6], Table 1). Although its computation is laborious, this model is widely accepted. For more details on that model, we refer to the original publications (Farquhar et al., 1980; von Caemmerer and Farquhar, 1981) and to model application studies (Medlyn et al., 2002; Archontoulis et al., 2012). Photosynthesis response to leaf N, which is strongly related to Rubisco content, can be modeled using a modified logistic equation

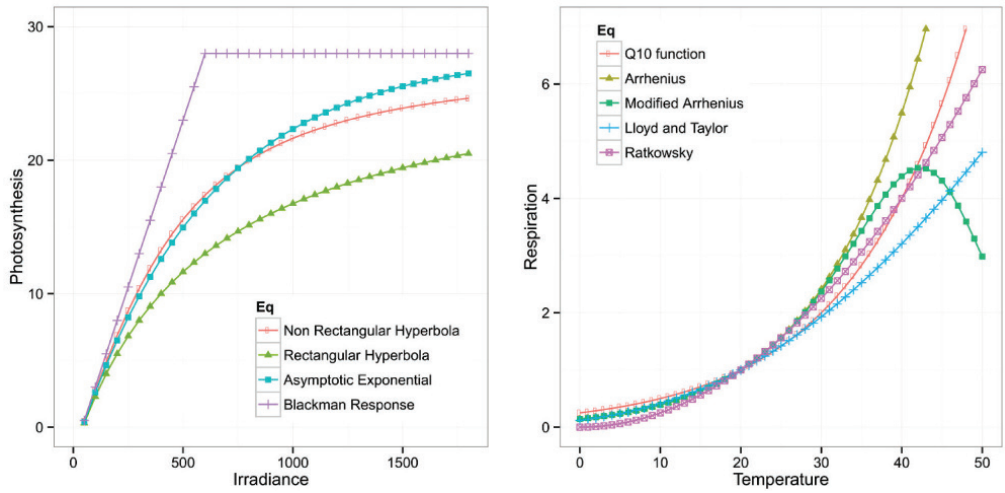


FIG. 2. Nonlinear models for describing photosynthesis response to irradiance (left panel) and respiration response to temperature (right panel). Equations and parameter meaning are given in Table 1. The following parameter values were used for these plots: Y_{asym} = 30 μmol CO_2 $m^{-2}s^{-1}$, a = 0.05 mol CO_2 mol^{-1} photons, θ = 0.7 and R_d = 2 μmol CO_2 $m^{-2}s^{-1}$; Q_{10} = 2, T_{ref} = 20°C, R = 8.314 (J K^{-1} mol^{-1}), E = 65000 (J mol^{-1}), S = 650 (J K^{-1} mol^{-1}), D = 207000 (J mol^{-1}), E_o = 350 (K), T_s = 225 (K), and T_{min} = 0°C. Note that at the reference temperature of 25°C, respiration takes the value of 1. The optimum temperature for the modified Arrhenius equation is: $T_{opt} = D/[S - R\ln(E/D - E)]$ = 42.3°C.

proposed by Sinclair and Horie (1989, see Eq. [3.5], Table 1), but there are alternatives (Eq. [4.8], Table 4). Photosynthesis response to water stress is usually described by sigmoid functions at the leaf level. For instance, Vico and Porporato (2008) utilized a Weibull-type curve (Eq. [4.9], Table 4). Photosynthesis response to vapor pressure deficit has been described by an exponential decay function (e.g., Osorio et al., 2006), but usually more sophisticated approaches are used (Collatz et al., 1992; Yin and Struik, 2009). Photosynthesis response to temperature is discussed below.

Group IV: Plant Responses to Temperature

A multitude of nonlinear regression models have been proposed and tested for modeling temperature dependence of various soil and plant processes (Lloyd and Taylor, 1994; Katterer et al., 1998; Davidson et al., 2006; Shibu et al., 2006; Portner et al., 2010). These include power, logarithmic, exponential, sigmoid, and bell-shape functions (Tables 1 and 5). The van't Hoff or Q_{10} function (i.e., Q_{10} is the factor by which the rate of a process increases for each 10°C temperature increase) is used in many studies, particularly in those addressing leaf or soil respiration rates. A common range for Q_{10} is between 1.4 and 4.9 (a value of 1 indicates no temperature effect) (Tjoelker et al., 2001; Atkin et al., 2005). In the Arrhenius equation, the Q_{10} term has been replaced by the activation energy. Both equations are equivalent, producing similar temperature responses (Fig. 2), but it should be noted that both Q_{10} and E coefficients are temperature range dependent. Usually, narrow temperature measurement ranges result in high and sometimes unrealistic Q_{10} or E estimates. Lloyd and Taylor (1994) noticed limitations of these two functions (i.e., the rate of reaction is not constant across temperatures) and developed a new equation known as Lloyd and Taylor (see Eq. [4.4], Table 1) to fit extensive literature data.

The above temperature functions describe a monotonic increase (Fig. 2). Most likely the rate of a process increases up to an optimum temperature and then drops (due to the lack of appropriate data, the drop is not always apparent). New equations or modifications of existing models have been developed to account for this. For example, the modified Arrhenius function, when compared with the standard Arrhenius equation, includes an additional two-parameter term (see D and S in Eq. [4.3], Table 1, Fig. 2) to capture the decline in the rate of a process at high temperatures (e.g., electron transport rate). If one of the two additional parameters is set to zero, then Eq. [4.3] becomes Eq. [4.2] (Table 1). Practitioners should be aware that this equation is "fragile" and requires careful parameterization (Medlyn et al., 2002; Archontoulis et al., 2012). Johnson et al. (2010) argued that temperature functions based on activation energy of chemical reactions are complex and difficult to apply routinely. They used a modified β function to describe photosynthesis response to temperature (Eq. [5.10], Table 5). Kirschbaum (1995) used a modified exponential temperature function (Eq. [5.9], Table 5) that provides a peak pattern to fit soil organic matter decomposition data. Additional (but difficult to interpret) peak temperature response functions are reported in Portner et al. (2010).

Group V: Bell Curve

In addition to temperature dependencies on photosynthesis, the bell-shape or peak functions are applied in agricultural sciences to describe the rate of phenological

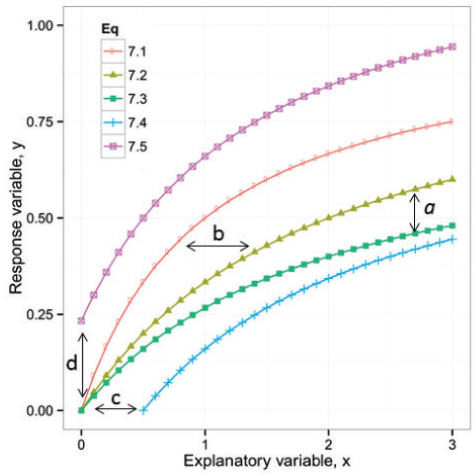
development as a function of temperature (e.g., Yin et al., 1995), the size of a leaf as a function of its rank in a plant (e.g., Hammer et al., 2009), or soil moisture effects on N_2O emissions (e.g., Rafigue 2011). Table 1 lists three commonly used equations (Eq. [5.1–5.3]). More application examples and different types of bell-curve equations can be found in Ma and Shaffer (2001) and in Table 6. In process-based simulation models, researchers have approximated a bell-shape response (viz. rate of development) with a two, three, or four segment (broken) linear regression model (e.g., APSIM; Keating et al., 2003). Typically, these segmented models should be fit using nonlinear methods as well.

Group VI: Others

In allometric studies, the relationships that exist between the growth rates of different plant components are quantified by means of regression analysis. Given the large variability that exists among plant species and plant components, numerous nonlinear models have been utilized to quantify relationships between plant processes, including power (Eq. [6.1], Table 1, e.g., plant N% vs. biomass weight), hyperbolic (Eq. [6.2], Table 1), and sigmoid curves (e.g., Eq. [2.1], Table 1). For application examples, see Vega et al. (2000), Vega and Sadras (2003), and Archontoulis et al. (2010). The Michaelis–Menten equation (Eq. [6.3], Table 1) is well-known and routinely applied to quantify the rate of a process (i.e., denitrification) that is dependent on the substrate (i.e., NO_3). In contrast, Eq. [6.4] is not as common in agronomy, but it appears to be very flexible taking many forms, from linear to exponential to bell-shaped. For example, it was applied to model temperature effects on soil nitrogen mineralization (Bril et al., 1994). The last equation in our reference Table 1 is the Ricker function (Eq. [6.5]), an option for hump-shaped patterns that are skewed to the right (Bolker, 2008).

Manipulating Nonlinear Functions

Sometimes there is a need to modify a "standard" nonlinear function to fit a set of data. This has led to the development of numerous versions of a standard equation (e.g., Birch, 1999; Tsoulakis, 2001; Tables 2, 3, and 4). Using the simplest form of the Michaelis–Menten hyperbolic function (see Eq. [7.1] in Fig. 3), we illustrate simple modification techniques. Equation [7.1] starts at zero when $x = 0$ and increases up to an asymptotic value of 1 as x increases. We can change the horizontal scale of this function by multiplying the variable x by a constant parameter, b, which is called a scale parameter (Bolker, 2008). If $b > 1$, then y saturates faster and if $0 < b < 1$, then y saturates more slowly (Eq. [7.2] in Fig. 3). We can change the vertical scale of the function by introducing a new parameter, a (Eq. [7.3] in Fig. 3). In this case, the asymptote moves from 1 to a. We can shift the whole curve to the right or the left by subtracting or adding a new parameter, c to the x variable (Eq. [7.4] in Fig. 3), which is called the location parameter (Bolker 2008). Similarly we can shift the whole curve up or down by adding or subtracting a new constant value, d, (Eq. [7.5] in Fig. 3). Lastly we can replace x with x^k, where k is a shape parameter, and then the equation can take many forms (exponential, sigmoid, etc.). A close example to the last modification is Eq. [2.6] in Table 1. When we modify nonlinear functions, we should add parameters that have meaningful interpretations.



(#)	Equation	Parameters
7.1	$Y = \frac{x}{1+x}$	-
7.2	$Y = \frac{bx}{1+bx}$	b=0.5
7.3	$Y = a\frac{bx}{1+bx}$	b=0.5, a=0.8
7.4	$Y = a\frac{b(x-c)}{1+b(x-c)}$	b=0.5, a=0.8, c=0.5
7.5	$Y = a\frac{b(x-c)}{1+b(x-c)} + d$	b=0.5, a=0.8, c=0.5, d=0.5

FIG. 3. Example of a nonlinear model modification. Starting with Eq. [7.1], the parameters *a*, *b*, *c*, and *d* were added step-by-step to Eq. [7.1], resulting in four new equations: Eq. [7.2], [7.3], E [7.4], and [7.5]. Horizontal or vertical arrows in the figure panel indicate how additional parameters affect the model.

Combining Nonlinear Functions

Sometimes a single equation is not enough to describe a set of experimental data, and researchers combine more than one equation to fit the data. The Farquhar model of photosynthesis is such an example because it combines two nonlinear models with the law of minimum. The use of the law of minimum is a common technique in modeling to simulate a process (e.g., biochar and tillage effects on soil bulk density, Archontoulis et al., 2016). However, the most common example that fits in this category comes from soil fertility, where researchers fit a quadratic (linear parameters) or quadratic-plus-plateau models to yield vs. nitrogen fertilizer experimental data (Sawyer et al., 2006). However, the estimation of the exact point at which the transition occurs (the optimum N rate, which is of great interest) is usually associated with uncertainty, especially when there are few points to fit the curve (Bachmaier, 2012).

When nonlinear functions are extended or combined to describe a phenomenon, it is important to recognize that there is an upper limit in the number of parameters that can be estimated from standard nonlinear regression analysis. This depends on the complexity of the model and the number of data points. For example, to fit growth curves with three parameters, we need at least four data points. When a process is described by a combination of nonlinear models (e.g., Farquhar model of photosynthesis or generic simulation crop models) then a step-wise parameterization method is usually applied. For application examples, see Miguez et al. (2009) and Archontoulis et al. (2012).

Fitting Nonlinear Models

Presently there are many statistical software packages available for fitting nonlinear models (e.g., SAS, R, JMP, GenStat, MatLab, Sigmaplot, OriginLab, SPSS). Nonlinear parameter estimates can be obtained using different methods (Bates and Watts, 2007); the most common methods are (i) nonlinear least squares, which minimizes

the sum of squared error between observations and predictions, and (ii) the maximum likelihood method, which seeks the probability distribution parameters that make the observed data most likely. For non-normal data such as binomial or counts, generalized linear models should be used (Gbur et al., 2012). Most problems encountered during the use of standard nonlinear regression software functions are due to a poor choice of competing models, equation, or starting values (Fig. 1). The choice of estimation method can affect the parameter estimates (Ruppert et al., 1989), but in general, estimates from least square and from maximum likelihood methods tend to differ only when the data are not normally distributed and are approximately the same when the data follow a normal distribution (Myung, 2003).

Choosing Starting Values

All procedures for nonlinear parameter estimation require initial values. The choice of values influences the convergence of the estimation algorithm. In the worst case, there is no convergence, and in the best case, convergence is reached after a few iterations (Ritz and Streibig, 2005). There is no standard procedure for selecting initial estimates. These are five common methods:

1. If the model has parameters with biological meaning then use information from the literature.
2. Use graphical exploration (see examples).
3. Transform the nonlinear model into a linear one. For instance, log-transformation of Eq. [1.1] yields a linear equation ($\log Y = Y_o - kt$) in which rough estimates of the parameter values can be easily obtained by linear regression. This method is recommended for getting initial estimates and to detect deviations from linearity. These estimates can be used as starting values (Bolker, 2008), but may also be used as final estimates when the variance model is appropriate for $\log Y$ (Ruppert et al., 1989). For more transformation examples, see Zeide (1993), Singh (2006), and Portner et al. (2010).
4. When no clear guidelines exist for choosing starting values, the recommendation is to use a grid search or "brute-force" approach (e.g., PROC NLIN in SAS or nls2 package in R). This grid search can be done by generating an extensive coverage of possible parameter values (and their combinations) and then evaluating the model at each one of these parameter combinations. The numerical method can then be used, starting with the combination that resulted in the best fit (lower mean squared error). The hope is that a sufficiently extensive coverage of the parameter space will result in a combination of parameters that will result in an adequate fit.
5. Use prespecified algorithms: this approach is specific to a given equation and can be used to calculate starting values for a given dataset (e.g., Pinheiro and Bates, 2000; Ritz and Streibig, 2008).

Check Algorithm Convergence

After the initial attempt at fitting a nonlinear model, we recommend that algorithm convergence is evaluated (Fig. 1). Convergence is achieved when a measure (such as the relative offset, change in LOSS function, or maximum change among parameter estimates; Bates and Watts, 2007) is below a certain threshold value (i.e., 10^{-5}),

indicating that the algorithm has found a "best" solution (Fig. 1). If convergence is not achieved, the most likely problems are the poor choice of starting values or that the selected model is not well suited to describe the data. If convergence is achieved, the next step is to evaluate whether the parameter estimates are within a reasonable range. This requires not only evaluating the point estimates but also their standard errors. Unusually large standard errors are a sign of convergence problems, even if convergence was apparently achieved in the previous step. If no problems were encountered up to this point, the analysis can continue by simplifying the model and assessing model assumptions.

Evaluating Model Assumptions

When we are dealing with one model, the next step is to evaluate key model assumptions: normally distributed errors, independent errors, and homogeneous variance for the errors (Fig. 1). This step and the following steps are not unique to nonlinear models but are common to all linear models. Substantial deviations from the assumptions could result in bias (inaccurate estimates) and/or distorted standard errors (Ritz and Streibig, 2008). Violations of these assumptions can be detected from an analysis of the residuals by means of graphical procedures and formal statistical tests. For a more complete analysis, see Ritz and Streibig (2008). Briefly, to check whether the distribution of the measurement errors follows normality, the standardized residual plot is commonly applied (Pinheiro and Bates, 2000). Outliers and many extreme values are common causes for deviations from normality (Fig. 1). Heterogeneity of variance can be detected by looking at the plot of the fitted values over the residuals (absolute residuals: raw residuals stripped of the negative sign; or standardized residuals: raw residuals scaled by the variance; see Example 1). When the residual errors show a trend (e.g., increasing variability as the explanatory variable increases), this can be addressed by modeling the variance as a function of the independent variable or the fitted values (Fig. 1). If variance heterogeneity is ignored, the parameter estimates might not be influenced much, but this may result in severely misleading confidence and prediction intervals (Carroll and Ruppert, 1988). The residuals are assumed to be independent, and when this assumption is violated this is visually evident in a plot of correlations of residuals against "lag" (or units of separation in time or space). Typically, variables measured in time on the same subject (e.g., plant, animal or soil sample) tend to result in autocorrelated residuals which need to be accounted for by modeling the variance covariance matrix of the residuals.

Model Selection Criteria

When dealing with multiple models, the question is how to find the best one among competing models. Depending on the structure of the models, different statistical criteria can be used to find the "best" model: *F* test, Akaike information criterion (AIC), Bayesian information criterion (BIC), or likelihood ratio test (Zucchini, 2000; Burnham and Anderson, 2002; Hoffmann, 2005; Ritz and Streibig, 2008; Lewis et al., 2011). When models are *nested* (one model is a special case of another), the above criteria are applicable (Fig. 1). When models are *non-nested* (models having different structures, e.g., Eq. [2.1] vs. Eq. [2.5]), typically the AIC and the BIC criteria are used

(Fig. 1). However, from a practical point of view, one model might be preferred over another based on interpretability and specific objectives. There needs to be a balance between statistical model performance and how effectively the model answers research questions.

For two nested models, one with two parameters (reduced, e.g., Eq. [3.9] in Table 3) and one with four parameters (full, Eq. [3.8] in Table 3) to check whether the addition of the two extra parameters has a statistically significant contribution on the model performance, we can use the following F test:

$$F = \frac{\left(\mathrm{SS}_{\mathrm{full}} - \mathrm{SS}_{\mathrm{reduced}}\right) / \left(\mathrm{df}_{\mathrm{full}} - \mathrm{df}_{\mathrm{reduced}}\right)}{\mathrm{SS}_{\mathrm{full}} / \mathrm{df}_{\mathrm{full}}}$$

where $\mathrm{SS}_{\mathrm{full}}$ and $\mathrm{SS}_{\mathrm{reduced}}$ are the regression model sum of squares for the full and reduced model, respectively, and $\mathrm{df}_{\mathrm{full}}$ and $\mathrm{df}_{\mathrm{reduced}}$ are the degrees of freedom for the full and the reduced model, respectively. The p value can be calculated at $\mathrm{df}_{\mathrm{full}} - \mathrm{df}_{\mathrm{reduced}}$ (numerator), $n - p$ (denominator), where p is the number of parameters for the full model and n is the number of observations, and a decision can be made. This test is sometimes referred to as extra-sum-of-squares or multiple partial F test (Hoffmann, 2005; Ritz and Streibig, 2008), and it is computed when the least squares method is used to fit the data (see section on fitting nonlinear models). When the maximum likelihood method is used to fit the data, then the likelihood ratio test (LRT) statistic is computed to compare nested models:

$$\mathrm{LRT} = 2\log\left(L_{\mathrm{full}} / L_{\mathrm{reduced}}\right) = 2\left(\log L_{\mathrm{full}} - \log L_{\mathrm{reduced}}\right)$$

$$Q = 2\log\left(L_{\mathrm{full}} / L_{\mathrm{reduced}}\right) = 2\left(\log L_{\mathrm{full}} - \log L_{\mathrm{reduced}}\right)$$

where L_{full} and L_{reduced} are the likelihood functions for the full and reduced model, respectively. These functions are closely related to the residual sum of squares (see Eq. [2.4] in Ritz and Streibig, 2008). It is assumed that the LRT statistic is approximately χ^2–distributed with $\mathrm{df}_{\mathrm{full}} - \mathrm{df}_{\mathrm{reduced}}$ degrees of freedom (for details, see Ritz and Streibig, 2008). Another approach for model selection involves calculating the AIC and BIC values for each model (i) separately:

$$\mathrm{AIC}_i = -2\log L_i + 2p_i$$

$$\mathrm{BIC}_i = -2\log L_i + p_i \log n$$

where L_i and p_i are the likelihood and the number of parameters for each model, and n is the number of observations. For both statistical criteria, a smaller value indicates a preferable model. The BIC criteria differs from the AIC only in the second term which depends on n. As n increases, the BIC favors simpler models (fewer parameters). This explains why sometimes the decision made on the basis of AIC and BIC indexes disagree. More information about these indexes is provided in Burnham and Anderson (2002). Note that LRT, AIC, and BIC are all designed to compare the performance of models that have been fitted to data via maximum likelihood estimation.

Goodness of Fit

To assess the goodness of fit, there are many different graphical methods and numerical indexes that highlight different features of the data and the model. Graphical comparisons provide a quick visual assessment of the goodness of fit (see examples below, Fig. 4). Numerical statistical indexes such as R^2, bias, mean squared error, root mean square error (RMSE), modeling efficiency, concordance correlation, and others (Wallach, 2006) can be used as quantitative summaries to assess the goodness of fit. Some indexes measure the absolute error (includes units), and some others measure the relative error (unitless). Depending on the data type, a combination of these indexes can be used. For example, the relative term is more meaningful than the absolute when comparing errors from different data sets such as biomass, yield, phenology, and nitrate leaching. The following equations are commonly used in model evaluation (for a comprehensive review of those we refer to Wallach, 2006):

$$\text{Bias} = \frac{1}{n}\sum_{i=1}^{n}\left(Y_i - \hat{Y}_i\right)$$

$$R^2 = 1 - \frac{\text{SS}_{\text{residual}}}{\text{SS}_{\text{total}}} = 1 - \frac{\sum_{i=1}^{n}(Y_i - \hat{Y}_i)^2}{\sum_{i=1}^{n}(Y_i - \hat{Y}_i)^2 + \sum_{i=1}^{n}(\hat{Y}_i - \overline{Y})^2}$$

$$\text{RMSE} = \sqrt{\frac{\text{SS}_{\text{residual}}}{n-p}}$$

$$\text{ME} = 1 - \frac{\text{SS}_{\text{residual}}}{\text{SS}_{\text{model}}} = 1 - \frac{\sum_{i=1}^{n}(Y_i - \hat{Y}_i)^2}{\sum_{i=1}^{n}(\hat{Y}_i - \overline{Y})^2}$$

where bias, R^2, RMSE, and ME (modeling efficiency) are numerical statistical indexes; n is the number of data points; Y_i and $\hat{Y}_i$ are the observed and predicted values; $\overline{Y}$ is

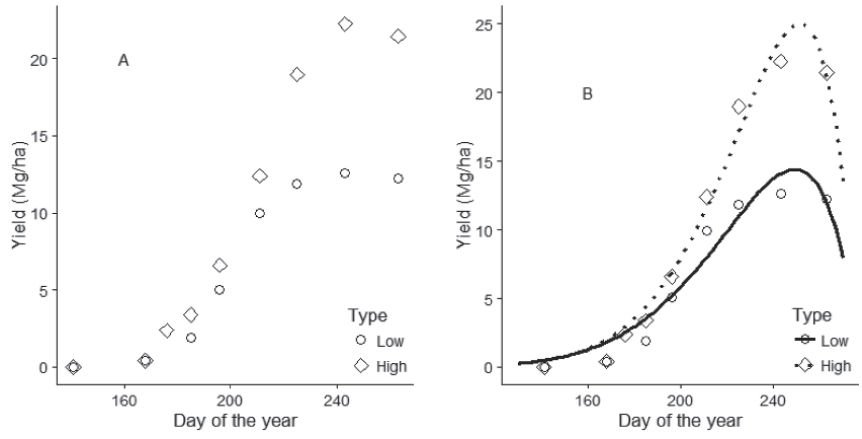


FIG. 4. (A) Observed yield during the growth season. (B) Predicted yield (line) versus observed (point) for both agricultural inputs

the mean observed value; p is the number of model parameters; $SS_{residual}$, SS_{model}, and SS_{total} are the sum of squares for the residual, regression model and the total, respectively.

Although often used, R^2 does not represent a good metric of model performance for nonlinear models. It has several limitations (e.g., it does not account for the number of parameters); therefore, we recommend that other measures of agreement (or combinations) should be used (Wallach, 2006). For nonlinear models, specifically, the main limitation of R^2 is that the full model does not necessarily include the simpler model with one single parameter, as is the case with linear models (see Exercise 2).

The numerical statistical descriptors indicate the average performance of the model across the sample. When the variability is not constant throughout the sample (e.g., biomass increase over time), then statistical indexes do not capture the fact that the uncertainty is not the same at different magnitudes of the response variables (see the extended example below). We should often be concerned with the predictive ability of the model. For this, cross-validation techniques can be used, and the mean squared error of prediction is an appropriate measure for goodness of fit (Wallach, 2006).

To illustrate the principles presented so far, we will now discuss examples of applications of nonlinear models with increasing level of complexity.

Example 1: Maize Biomass Accumulation

Goal: Investigate the effect of agricultural input level on maximum yield of maize using the beta growth function.

Fitting Procedure

The dataset used in this example contains plant biomass (Mg ha^{-1}) for different days of the year during the growing season and for different levels of agricultural inputs. The dataset is called "sm" and it is also part of the "nlraa" R package [available in R-forge and can be install through R command line by: install.packages("nlraa", repos = "http://RForge.R-project.org")]. As a first step we plot the observed data and confirm, visually, that the pattern is well represented by the function of choice. According to Fig. 4, the observed biomass for both low and high agricultural inputs follow a sigmoidal pattern (i.e., S-shape), making the Beta function a suitable choice. One of its main characteristics is that it allows for a decline in growth at later stages.

In the R command line this dataset can be loaded (the "nlraa" package is needed).

```
data(sm)
```

In the beta growth function (Eq. [2.5] in Table 1) there is one predictor (time or t) and one response variable (Y) while there are three coefficients that need to be estimated. In this example, Y is the response variable which stands for plant biomass or yield, while t represents time measured as day of the year (DOY).

Using the "nls" function, we can estimate the parameters of a nonlinear model using the least-squares method. The first argument to the "nls" function is the "formula" with the response variable on the left-hand side and the function on the right-hand side, separated by "~": Response~f(*predictor*).

The following is an example of how this function can be used:

```
data(sm)
# filtering the dataset for Maize, different agricultural inputs and
one specific block
# Maize-Block1-Low and high inputs
Maize.B1.low<-sm[(sm$Block==1 & sm$Crop=='M' & sm$Input==1),]
Maize.B1.high<-sm[(sm$Block==1 & sm$Crop=='M' & sm$Input==2),]
# Taking the day of year as the x value and the Yield as the Y value
# Low input
X.low<-Maize.B1.low$DOY
Y.low<-Maize.B1.low$Yield
#High inputs
X.high<-Maize.B1.high$DOY
Y.high<-Maize.B1.high$Yield
# Non linear regression for the low input data - B1=Block 1
reg.low<-nls(Y.low ~ bgf(X.low, w.max, t.e, t.m),data=Maize.B1.low,
start=list(w.max=13,t.e=230,t.m=180))

# Non linear regression for the High input data - B1=Block 1
reg.high<-nls(Y.high ~ bgf(X.high, w.max, t.e, t.m),data=Maize.
B1.high, start=list(w.max=20,t.e=240,t.m=210))
```

From visual inspection we can determine that the highest value for "high input" is about 20 to 25 Mg ha^{-1}, and the highest value for "low input" is about 13 Mg ha^{-1} (Fig. 4). These would be sensible starting values for Y.max parameter. Again, visually, we can estimate the time at which half of the maximum yield is achieved as approximately DOY 220 for both treatments. Similarly, the time at which maximum biomass is attained is about DOY 240.

Input	Y_{max}	t_e	t_m
Low	14.4	249.12	220.35
High	25	251.26	225.78

By using the "summary" function, we can obtain more detailed information about the standard error and *p* value for each coefficient. These *p* values are not typically informative, as they are a test of the null hypothesis that the parameter is equal to zero (strictly, the probability of observing the data that was observed given that the null hypothesis is true). This is almost always true in this type of single curve fitting, but it can be more informative as we evaluate treatment effects.

```
summary(reg.low)
##
## Formula: Y.low ~ bgf(X.low, Y.max, t.e, t.m)
##
## Parameters:
## Estimate Std. Error t value Pr(>|t|)
## Y.max 14.40 2.21 6.5 0.0013 **
## t.e 249.12 3.27 76.1 7.4e-09 ***
## t.m 220.35 4.75 46.4 8.8e-08 ***
## ---
## Signif. codes: 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 1.5 on 5 degrees of freedom
##
## Number of iterations to convergence: 12
## Achieved convergence tolerance: 3.74e-06
```

The fitted model is shown in Fig. 4 B.

Checking Model Assumptions

The first assumption that should be evaluated is whether the regression function is reasonable. This is best done visually by confirming that the function follows the data to a reasonable level. Although linear models have a mean for residuals numerically close to zero, this is not always the case in nonlinear models and checking that the mean of the residuals is "close" to zero is a good first step. This deviation, called bias, is slightly higher than we would like, which suggests that the regression function is not adequately predicting the data.

```
##Mean of the residual
mean(resid(reg.high))
mean(resid(reg.low))
```

Input	Low	High
Mean of residual	−0.23	−0.27

Residual Analysis

Analyzing the residuals of a fitted model can provide additional insight. Is there any clear pattern? Are deviations increasing as the fitted values increase? Do the residuals appear normal? The skill of visual analysis of residuals is not always intuitive, and it is developed through practice.

At first glance, Fig. 5 does not show any major issues with the residuals, but looking more closely, there seems to be a pattern in which model predictions of low yields are overestimated, and predictions of high yields are underestimated. One exception is that the highest predicted yield was overestimated. The deviations are not substantial, so there are no clear "outliers." Residuals are also not increasing with the fitted values (a common issue), suggesting that the assumption of equal variance is reasonable. With these few data points the assumption of normality is difficult to test, but the plot of residuals shows a similar spread in terms of negative and positive residuals, again, not showing a sign of concern.

A normal quantile–quantile (QQ) plot (Fig. 6) helps us evaluate whether the assumption of normality has been met to a reasonable degree. The closer the points are to the straight line, the more normal is their distribution. The QQ plots in this example show a more right skewed distribution for both low and high agricultural

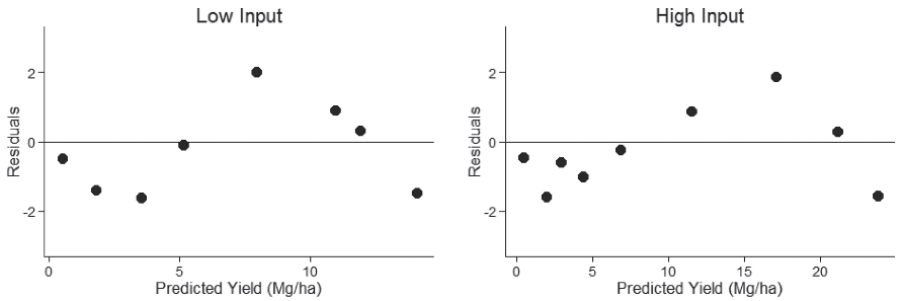


FIG. 5. Standardized residuals against predicted yield for high and low agricultural input fits.

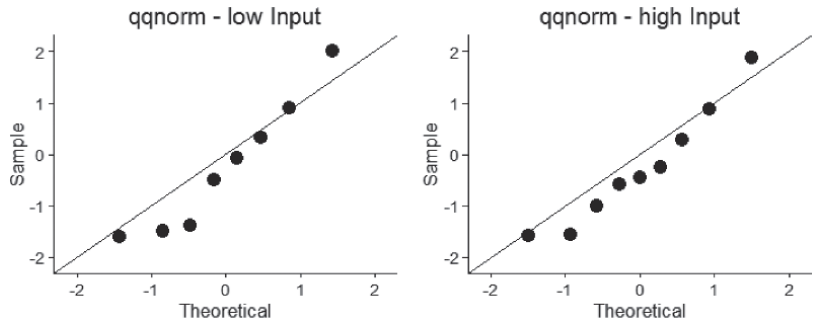


FIG. 6. Normal quantile–quantile (QQ) plot of residuals resulted from fitting process for both agricultural inputs.

inputs. It is also worthwhile to mention that the normality of the residuals also can be tested using more quantitative methods like the Shapiro–Wilk normality test.

Statistical Descriptors

Statistical indexes of model agreement can be calculated using equations in the goodness of fit section above. The first one is the RMSE, which gives an idea of the average deviation in the same units as the response variable. The normalized version of RMSE (NRMSE) shows the overall error relative to the mean of the observed response variable in percent. The bias is included here for completeness, but it was previously addressed. The last index (R^2) suggest a good agreement between the model and the data, but in this specific instance are not very useful. In general they do not provide diagnostic information, unless their values are extremely low.

Input	RMSE	NRMSE(%)	Bias	R^2
Low	1.22	18.05	−0.23	0.95
High	1.1	11.29	−0.27	0.99

The beta growth function was not able to fully capture the initial phase of growth and this was more clearly presented in the graph of residuals. This can be addressed by modifying the function by delaying the growth in the model at the cost of two extra parameters. The modified version of the Beta function (Eq. [3.11] in Table 3) allows for two offsets in both the x and y axes, and they are called t_b and Y_b, respectively. These two parameters (t_b and Y_b) can represent the planting date and the biomass at sowing date, respectively (Yin et al., 2003b). These parameters might not need to be estimated, since they are typically known and can be treated as fixed for a given application. These additional parameters are not necessary if the time scale is redefined as days since planting, but it might be preferred if planting date is an imposed treatment in a given study.

Comparing Alternative Models

GOAL: Compare S-shaped growth patterns models for the dataset introduced in the example for the maize, first block, and high agricultural input.

Answer

As was previously stated, the first step in fitting a nonlinear model is to visually inspect the data (Fig. 7). In the previous example, we found that by using the original beta growth function, some of the assumptions appeared to be not valid. In this exercise, we fit different sigmoid functions, including the modified version of Beta to find the model that best represents the observed yield.

Using the "data" function, we import the data set from the "nlraa" package and subsequently extract the desired predictor (DOY) and response variable (yield in Mg/ha) for the Maize and the first block. In the previous example, we explained how to use the "nls" function to fit our nonlinear model to data. The following block of code makes other uses of the nls function.

```
data(sm)
Maize.B1<-sm[(sm$Block==1 & sm$Crop=='M' & sm$Input==2),]
#Taking the day of year as the x value and yield as the Y value
X<-Maize.B1$DOY
Y<-Maize.B1$Yield
############### Nonlinear Regression for Gompertz function
reg.Gompertz=nls(Y~(Y.asim)*exp(-exp(-k*(X-t.m))),data=Maize.B1.low,
start=list(Y.asim=12.1,k=0.08,t.m=240.5))
############### Nonlinear Regression for Logistic function
reg.Logistic=nls(Y~(Y.asim)/(1+exp(-k*(X-t.m))),data=Maize.B1.low,
start=list(Y.asim=12.1,k=0.08,t.m=240.5))
############### Nonlinear Regression for Richards function
reg.Richards=nls(Y~rich(X, t.m, k, v, Y.asim),data=Maize.B1.low,
start=list(Y.asim=14.1,k=0.07,t.m=200,v=0.6))
############### Nonlinear Regression for Beta function
reg.Beta=nls(Y~SSbgf(X, Y.asim, t.e, t.m),data=Maize.B1.low,
start=list(Y.asim =10.1,t.e=250,t.m=220.1))
############### Nonlinear Regression for Beta function 2
reg.Beta2=nls(Y~bgf2(X, w.max, w.b, t.e, t.m, t.b),data = Maize.
B1.low, start=list(w.max=24,t.e=252,t.m = 215,w.b = 0,t.b = 141))
############### Nonlinear Regression for Weibull function
reg.Weibull=nls(Y~weibull((X-140),a = a, b = b, Yo=Y.asim),data=Maize.
B1.low, start=list(Y.asim=21.0,a=0.0000009,b = 3.3))
```

In the above code, the last four "nls" functions used predefined functions which produced cleaner code.

As a result of fitting different nonlinear growth models (Fig. 8), the following coefficients were obtained. Each model produced different values for their respective parameters but the mean of the residuals (bias) is more revealing in terms of how

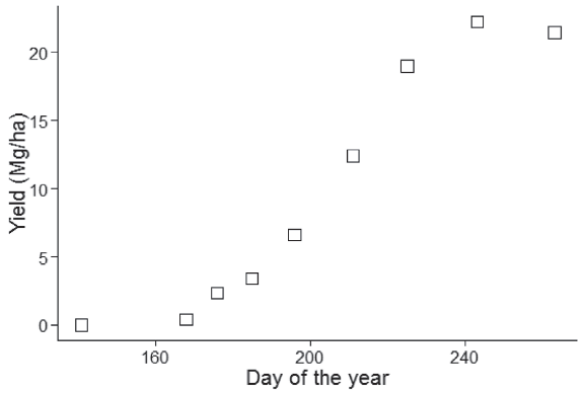


FIG. 7. Observed maize yield during the growth season for the first block and high agricultural input.

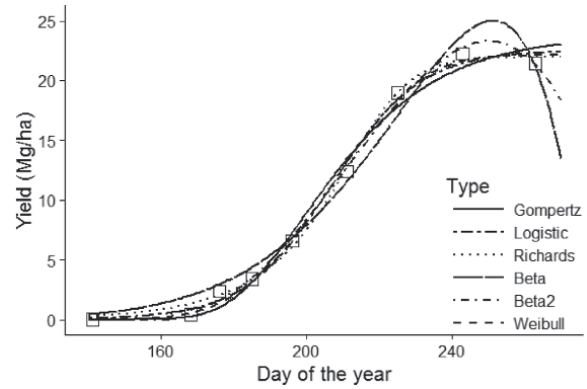


FIG. 8. Simulated yield versus observed for different models and high agricultural inputs

well each model fits the data. The parameter Y.asim presented in the table below is the equivalent to Y.max in beta growth functions.

Model	Y.asim	k	t.m	Mean of residuals
Gompertz	23.78	0.04	199.49	0.12
Logistic	22.52	0.08	206.87	0.02
Richards	21.98	0.13	212.10	−0.06
Beta	25.00	–	225.78	−0.27
Beta2	23.27	–	210.77	-1.265×10^{-8}
Weibull	22.12	–	–	0.08

Checking Model Assumptions

Residuals Mean

The mean of residuals is presented in the last column of the above table. The closest value to zero is given by the Beta and Logistic functions while the original Beta function has the largest absolute value.

Homogeneous Variance

The homogeneity of the variance assumption is investigated using a scatter plot (Fig. 9) between the residual and predicted response variable (Yield). An even distribution of points around the zero line is desirable and typical patterns that deviate from this might appear as a funnel shape (i.e., increasing scatter as the predicted response variable increases).

Normality

The normality of the residuals is more difficult to assess given the small sample size. The QQ plot of residuals for the different models shows a reasonable agreement with a normal distribution (Fig. 10), and, as it was stated earlier, the residuals are considered to follow a normal distribution the closer they are to the 1:1 line.

Based on the figures and interpretation presented above, among all the models, the modified Beta, Logistic, Richards, and Weibull show the least bias, and they meet standard assumptions. On the other hand, the Gompertz and the original

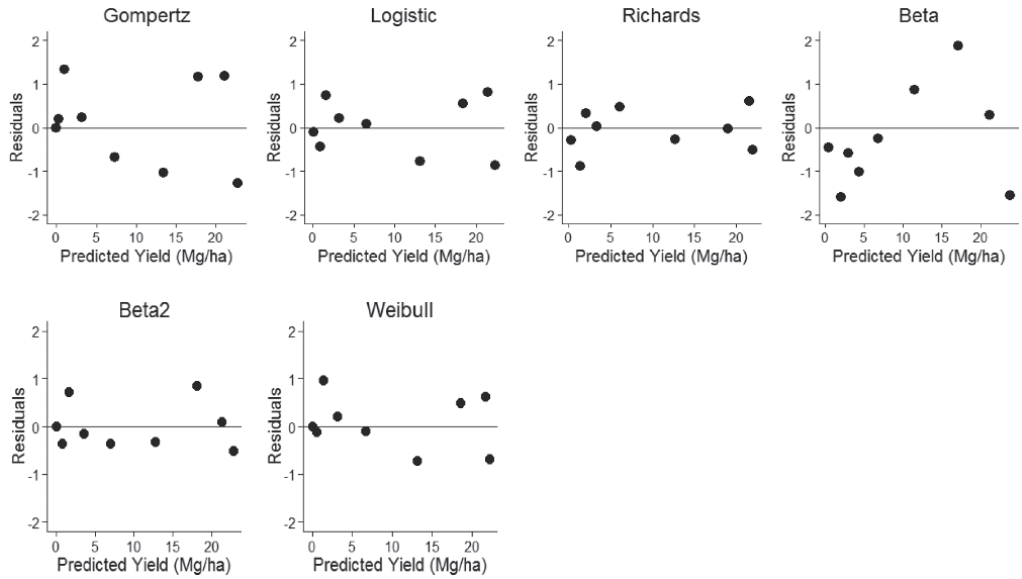


FIG. 9. Standardized residuals against predicted yield for all candidate models.

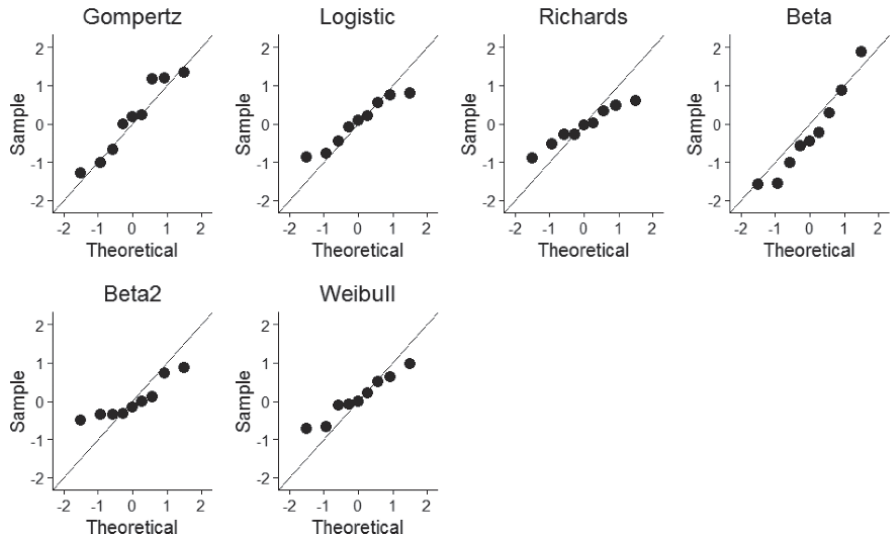


FIG. 10. Normal quantile–quantile (QQ) plot of residuals resulted from fitting process for all candidate models.

Beta function had higher mean of residuals, which are an indication of the pattern in the residuals.

Statistical Descriptors

The statistical descriptors are presented for the Logistic, Richards, Beta2, and Weibull models. From these models the Beta2 and Richards performed better than the Logistic and Weibull. For example, based on the bias, the Logistic and Weibull

models underestimated the observed values, while the other two models tended to overestimate.

Model	RMSE	NRMSE (%)	Bias	R^2	AIC	BIC
Logistic	0.59	6.06	−0.024	0.99	32.23	33.02
Richards	0.46	4.69	0.064	0.99	21.62	22.60
Beta2	0.46	4.74	1.265×10^{-8}	0.99	23.70	24.88
Weibull	0.54	5.60	−0.081	0.99	22.52	23.31

This example illustrates that the original Beta function was modified to capture maize growth more effectively at the cost of having two extra parameters. There is commonly a tradeoff between the complexity of the models and their performance, but ultimately the goals of the analysis should dictate the choice of the model.

Example 2: Extended Application

The following extended example builds on the previous simpler examples, but with the emphasis shifted to the comparison among treatments. The example follows the workflow illustrated in Fig. 1.

DATA: We use data from Danalatos et al. (2009), which represent destructive measurements, taken in 2008 of aboveground biomass accumulation over time for three crops: fiber sorghum (*F*), sweet sorghum (*S*), and maize (*M*) growing in a deep fertile loamy soil of central Greece under two management practices: high and low input conditions. High refers to weekly irrigation (to match 100% of maximum evapotranspiration) and application of 200 kg N ha^{-1}, and low input refers to biweekly irrigation (∼50% of maximum evapotranspiration) and application of 50 kg N ha^{-1}. The experiment was a 2 × 3 factorial completely randomized in four blocks. For more details, see Danalatos et al. (2009). With such data, many questions are possible. Here we will concentrate on three: (i) What is the maximum biomass accumulated by these crops? (ii) At what point in time was this biomass achieved? and (iii) Are there significant treatment effects and/or interactions? This requires us to statistically determine the effects of crop type on the function parameters and also the effect of input level (i.e., high or low). These questions are approachable through the use of a nonlinear model that captures the regression function and the structure of the data.

GRAPHS: Visually (Fig. 11), we can see that the sorghums have higher biomass and that the maximum biomass occurs later in the season. No outliers have been detected at this point. However, without a statistical analysis it is difficult to make sound statements based solely on data visualization.

CHOOSE CANDIDATE MODEL: Danalatos et al. (2009) analyzed the data using the beta growth function (Yin et al., 2003b; Eq. [2.5] in Table 1). That model was selected because it captures the decline of biomass toward the end of the growing season (Fig. 11). Also the parameters have clear meaning and are suitable to answer the research questions.

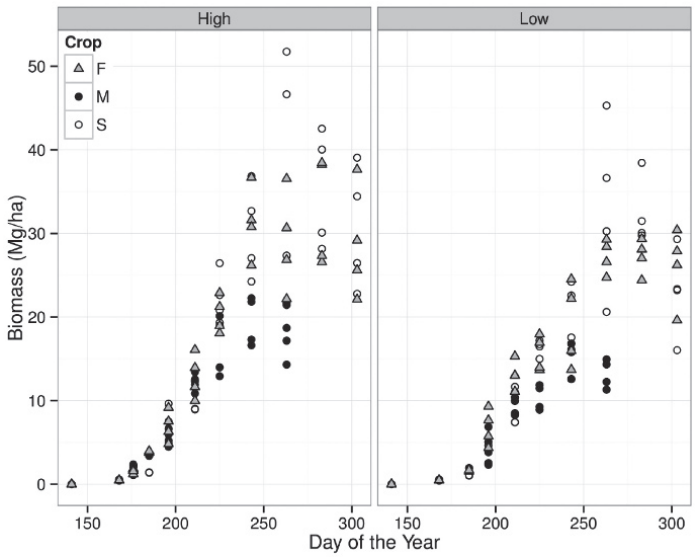


FIG. 11. Biomass accumulation with time for three crops: maize (*M*), fiber sorghum (*F*), and sweet sorghum (*S*) collected in Greece in 2008. The two panels represent the level of agricultural input: high and low.

STARTING VALUES: Since for this function parameters have straightforward interpretations, starting values can be found by visual inspection of Fig. 11. However, in this example, we used a prespecified algorithm that chooses the initial starting values automatically.

FIT MODEL AND CONVERGENCE: Model fit was conducted in the R package using the nonlinear least squares method (nls function, see the "nlraa" R package for details). There are three crops, two levels of agronomic input, and four blocks, which results in 24 possible combinations (experimental units). The model was fit to every experimental unit and apparent convergence was obtained for only 10 experiment units. This suggests that some modifications are needed (see section below on revising the regression model). Checking model assumptions can be useful for diagnosing the problem.

REVISING THE REGRESSION MODEL: This can be addressed in part by using a modified beta growth function (see Eq. [3.11] in Table 3), which is designed to capture more efficiently the initial phase of growth at the cost of two extra parameters. Equation [3.11] allows for an offset in the x axis (t_b) orientation and an offset in the y axis orientation (y_b). We do not fit these parameters, but rather keep them fixed; t_b is the planting date at 141 DOY, and y_b is the biomass weight at sowing, which is zero. As a first step, the fitting process was repeated as above with starting values determined visually as 30 for w.max (same as Y.max), 280 for t.e and 240 for t.m. Apparent convergence was obtained for all the experiment units. The final revised model was fitted to the entire dataset, but at this step the model included the effect of crop type, agronomic input level, and the interaction for each parameter. Full details are available in the vignette of the "nlraa" package.

CHECK MODEL ASSUMPTIONS: Visual inspection of the standardized residuals (Fig. 12) was used to evaluate the assumptions of appropriate regression function and normally distributed errors with homogeneous variance. In this case, a concentration of

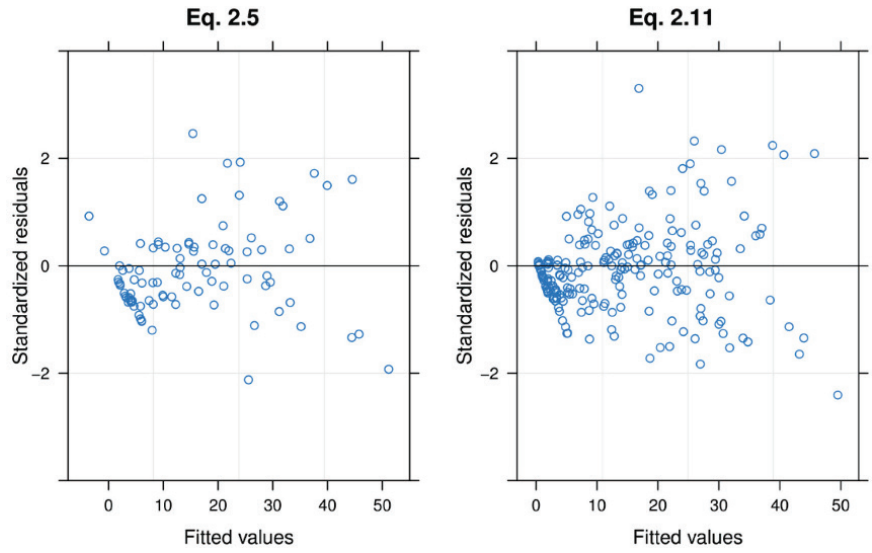


FIG. 12. Standardized residuals from individually fits to all experimental units. Left panel: Eq. [2.5] in Table 1; and right panel: Eq. [2.11] in Table 2. During the fitting procedure, Eq. [2.5] converged in only 10 out of the 24 experimental units, thus the fewer points in the left panel.

points stand out at low fitted values, which indicates overprediction (i.e., bias) at low values. Equation [3.11] (modified beta growth function) alleviated the overprediction at low values, but the bias did not disappear completely. A major argument for choosing Eq. [3.11] over Eq. [2.5] is that convergence was achieved for all experimental units (24 for Eq. [3.11] vs. only 10 for Eq. [2.5]).

VARIANCE HOMOGENEITY: The residual variance was modeled with a power function, and different power parameters were used for the three crops. This function is: $s^2(v) = s^2 * |v|^{2*\theta}$, where v is the covariate (the fitted values in this case), and θ depends on the crop (0.7, 0.86, and 0.89 for maize, fiber, and sweet sorghum respectively).

PARAMETER ESTIMATES AND STANDARD ERRORS: Table 8 illustrates the estimates of the model, the corresponding standard errors, and the p values. These values are final and account for modeling the residual variance. The interaction between agronomic input and crop species was significant for the maximum biomass weight (Y_{max}) and the final growth time point (t_e) (Table 8). The model could be further simplified by dropping the interaction and the effect of the input level on time of maximum biomass (t_m) (Table 9). The final model, which takes into account the interaction between crop level and management input level, has 18 parameters, which are used to describe the regression function and four parameters that describe the variance function (see the vignette in the "nlraa" package for details).

CALCULATE STATISTICAL DESCRIPTORS: Regarding the numerical summaries described in the section "Goodness of Fit," biomass has small initial values and high values at the end of the season (Fig. 13). In this case, use of the average RMSE of 4.1 Mg ha^{-1} might be misleading because it overestimates the error at the initial stages (biomass of 0–10 Mg ha^{-1}) and underestimates the error at advanced stages (biomass of 30–40 Mg ha^{-1}).

TABLE 8. Estimates with standard errors in parenthesis of the beta growth model (Eq. [3.11] in Table 3) used to fit the biomass data reported by Danalatos et al. (2009). Y_{max} is the maximum biomass (Mg ha^{-1}); t_m is the day of the year when the crop growth rate is maximized; and t_e is the day of the year when biomass is maximized. *P* values < 0.05 indicate significant effect of input levels (high or low) for every crop species and parameter.†

Maize			Fiber sorghum			Sweet sorghum		
High	Low	*p*	High	Low	*p*	High	Low	*p*
21.2 (0.99)	15.4 (2.27)	<0.001	38.6 (2.24)	31.8 (5.18)	0.02	43.2 (2.83)	33.9 (6.48)	0.01
215.7 (1.30)	217.1 (3.33)	0.5	234.5 (1.61)	235.8 (4.11)	0.61	239.4 (1.53)	240.0 (3.81)	0.79
248.0 (1.79)	248.8 (4.51)	0.76	277.2 (2.03)	279.4 (5.38)	0.5	278.6 (1.99)	279.0 (4.87)	0.89

† Note: in Eq. [3.11] the parameters Y_b, biomass weight at sowing and t_b, sowing date, were fixed at 0 Mg ha^{-1} and 141 d of the year, respectively.

TABLE 9. Test of fixed effects for the parameters in the model which include the effect of Crop, Management Input, and the interaction using the modified beta growth function. See Table 1, Eq. [2.5] for details.

Term	*F* value	*P* value
Y_{max}	11601	< 0.0001
Y_{max}.Crop	902	< 0.0001
Y_{max}.Input	441	< 0.0001
Y_{max}. (Input × Crop)	34	< 0.0001
t_e	23863	< 0.0001
t_e.Crop	90	< 0.0001
t_e.Input	33	< 0.0001
t_e. (Input × Crop)	59	< 0.0001
t_m	127944	< 0.0001
t_m.Crop	139	< 0.0001
t_m.Input	1	0.4017
t_m.(Input × Crop)	0	0.9667

INTERPRET RESULTS AND DRAW CONCLUSIONS: According to model predictions, the maximum estimated biomass was obtained for sweet sorghum under high inputs and this crop reached a total of 43 Mg ha^{-1} on DOY 279 (Fig. 14; Table 8). On the other extreme, maize reached its maximum biomass under high input of 21 Mg ha^{-1} on DOY 248. The maximum biomass and the time when it was reached were significantly affected by the Crop and Input interaction. In practice, the specific objectives can guide the additional analysis to be conducted such as treatment differences, their significance level (*p* value) and/or having a model capable of producing robust predictions within the range of observed values.

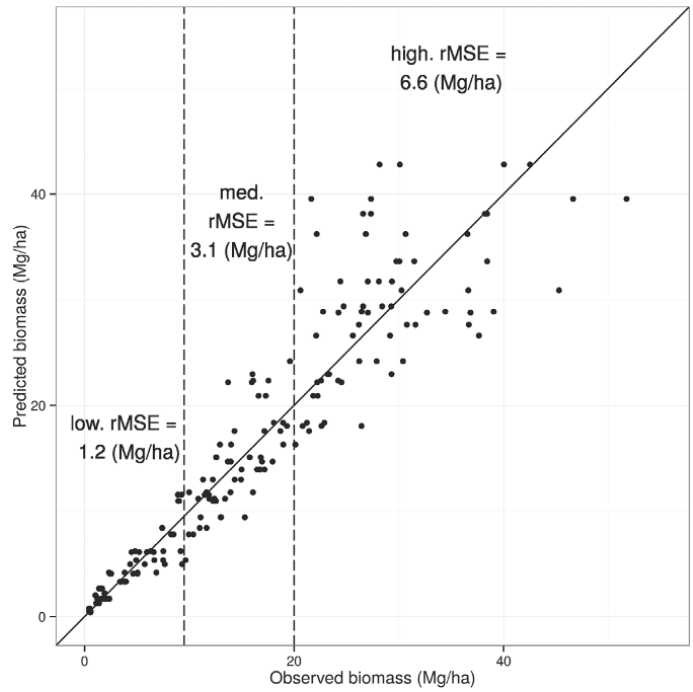


FIG. 13. Observed versus predicted biomass values. The RMSE was used as a measure of goodness of fit, but given that the variability is increasing along with the biomass weight, three RMSE values were calculated for ranges indicated by vertical dashed lines (0–10 10–20, and >20 Mg ha^{-1}).

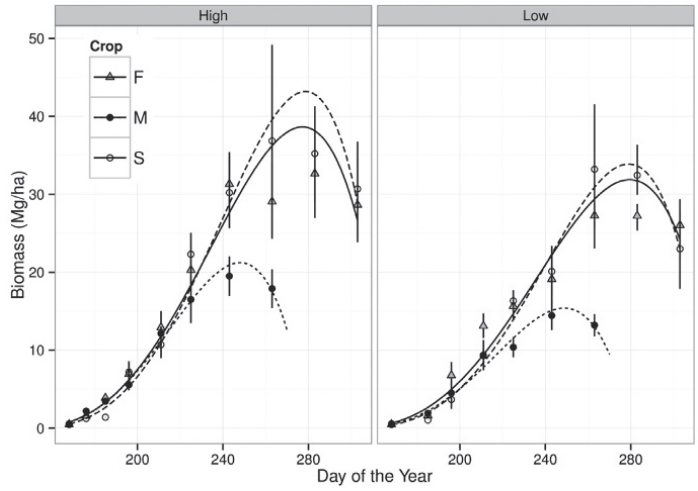


FIG. 14. Observed data and fit for the final model. Vertical bars indicate confidence interval of observations.

Summary

The most critical step which distinguishes nonlinear models from linear models is that the choice of the main function is critical and this can be difficult without appropriate guidance. Here, we present an extensive library of nonlinear functions (77 equations with the associated parameter meaning) and the typical applications, which, we hope, will make the task of choosing candidate models easier. Our review of nonlinear equations is incomplete, as there are countless numbers of potential functions (Ratkowsky, 1990) and their ad hoc modifications. We also contribute a suggested workflow (Fig. 1) that should provide the necessary structure to avoid common errors in the use of nonlinear regression models.

Key Learning Points

- Nonlinear models have the advantages of having meaningful parameters and being parsimonious (few parameters are needed).
- Choosing an appropriate model for a given application is crucial, and both statistical arguments and application specific interpretability should be considered.
- Nonlinear models do not have analytical solutions, and iterative algorithms should be used.
- Model convergence is highly improved by appropriate choice of starting values.
- Graphical analyses are important to evaluate whether the model is correct on average.
- As with linear models the assumptions of the residuals should be evaluated: independence, homogeneity of variance and normality.

Review Questions

1. Which of these functions is not used for data that follows a sigmoidal (S-shape) pattern?

   (a) Logistic
   (b) Gompertz
   (c) Richards
   (d) Weibull
   (e) Arrhenius

2. Which of these functions is typically used for temperature response data?

   (a) Logistic
   (b) Rectangular hyperbola
   (c) Gompertz
   (d) Arrhenius
   (e) Weibull

3. In the beta growth function as described by Yin et. al. (2003b), the parameter tm represents:

   (a) Maximum biomass attained
   (b) Time at which maximum biomass is attained
   (c) Time at which maximum growth rate is attained
   (d) Time at which growth starts
   (e) Time at which growth ends

4. In most photosynthesis functions the parameter Rd

   (a) Maximum rate of photosynthesis
   (b) Dark respiration
   (c) Curvature
   (d) Irradiance level
   (e) Quantum efficiency

5. In the exponential decay function the parameter k cannot be greater than 1.

(a) True
(b) False

Exercises

Exercise 1: Example of Derivatives of Linear Models

The first derivative of a quadratic model can be used to calculate the slope at that point

$$y = \beta_0 + \beta_1 x + \beta_2 x^2$$

where y is the response variable, β_0 is the intercept, β_1 is the slope associated with the independent variable x, and β_2 is the parameter associated with the quadratic term (x^2). The derivative of this function with respect to x is

$$\frac{dy}{dx} = \beta_1 + 2\beta_2 x$$

However, if we calculate the partial derivative with respect to each parameter we have

$$\frac{dy}{d\beta_1} = x$$

and

$$\frac{dy}{d\beta_2} = x^2$$

The second partial derivatives for both of these equations will be exactly zero. Therefore, this is considered a linear model.

1.A. Show that the second derivative of a simple exponential decay function with respect to its parameter is not zero.

1.B. Identify the linear and nonlinear parameters in the following model. Show your work and justify.

$$y = \beta_0 + \beta_1 \exp\left(-\frac{x}{\theta}\right)$$

Exercise 2: Full and Reduced Models

It is common to compare a full model to a simpler model. With linear models, it is common to compare a full model to a reduced model with one single parameter (intercept). This is the basis for the R^2

$$R^2 = \frac{\mathrm{SSE}(\mathrm{reduced}) - \mathrm{SSE}(\mathrm{full})}{\mathrm{SSE}(\mathrm{reduced})}$$

where SSE is the sum of squares of the error. For a simple linear regression:
Full model:

$$y_i = \beta_0 + \beta_1 x_i$$

Reduced model:

$$y_i = \beta_0$$

It is important to recognize that we can obtain the reduced model by setting β_1 equal to zero. For a model with just one parameter (intercept) the least-square estimate is imply the mean ($\overline{y}$). The R^2 for this model is

$$R^2 = 1 - \frac{\sum_i \left[y_i - \left(\hat{\beta}_0 + \hat{\beta}_1 x_i \right) \right]^2}{\sum_i \left(y_i - \overline{y} \right)^2}$$

where $\hat{\beta}_0$ and $\hat{\beta}_1$ are the least-square estimates for β_0 and β_1.

For nonlinear models, the *reduced* model with one single parameter (intercept) is not always a subset of the *full* model. For this to be true, the intercept only model should be a result of setting one or more of the parameters of the full model to a fixed value (typically zero). This is why the R^2 is often not appropriate for nonlinear models.

2.A. Provide examples of nonlinear models which can be reduced to a single parameter (intercept). Show your work.

2.B. Provide examples of nonlinear models which cannot be reduced to a single parameter. Show your work.

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