

Supplemental Materials for

Nonlinear Regression Models and Applications in Agricultural Research

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Supplemental tables with nonlinear equations and the associate parameter meaning

Table S1 – Group I (exponential)

Table S2 – Group II (sigmoid)

Table S3 – Group III (photosynthesis)

Table S4 – Group IV (temperature dependencies)

Table S5 – Group V (bell shape or peak functions)

Table S6 – Group VI (others)

Table S.1 – Equations derived from the exponential equation. Numbering continues from Group I of the Table 1. Placing the parameters and variables together always indicates multiplication (e.g. $kt = k \times t$). $e = \exp$.

(#)	Name and/or Reference	Form	Parameter meaning
1.3	Parallel or double first order	$Y = fY_0e^{-k_1t} + (1 - f)Y_0e^{-k_2t}$	<p>Y is the response variable, t is the explanatory variable (e.g. time), Y_0 is the initial or maximum Y value, k, k_1 and k_2 are rate constants that determine 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 $\frac{3}{4}$ maximum (units: time)</p>
1.4	Triple first order	$Y = f_1Y_0e^{-k_1t} + f_2Y_0e^{-k_2t} + (1 - f_1 - f_2)Y_0e^{-k_3t}$	
1.5	Consecutive first order (Andren and Paustian 1987)	$Y = fY_0e^{-k_1t} + (1 - f)Y_0 \left[e^{-k_2t} + \frac{k_2}{k_1 - k_2} (e^{-k_2t} - e^{-k_1t}) \right]$	
1.6	First order plus linear (Gills and Price 2011)	$Y = Y_0(1 - e^{-kt}) + bt$	
1.7	First order plus logistic (Gills and Price 2011)	$Y = Y_0f(1 - e^{-kt}) + \frac{Y_0(1 - f)}{1 + e^{-\frac{t-t_i}{t_d}}}$	
1.8	Leaf area index nitrogen limited equation Yin et al (2000, 2003a)	$Y_{LAI} = \frac{1}{k_n} \ln \left(1 + \frac{k_n X_N}{n_b} \right)$	<p>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 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_0 is the initial or maximum Y value, c is a dimensionless coefficient</p>
1.9	Protein or nitrogen distribution within plant canopies (Johnson et al., 2010)	$Y_N = Y_0 - (Y_0 - n_b)(1 - e^{-k_n X_{LAI}})^c$	
1.10	Photoperiodic sensitivity (Wang and Engel, 1998)	$Y = e^{-P_{sen}(X - P_c)}$	<p>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 hours for long days</p>
1.11	Horton (1940) model for water infiltration	$Y = Y_c + (Y_0 - Y_c)e^{-kt}$	<p>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,</p>

			Y_c indicates a final or equilibrium capacity (mm/h) Y_o indicates the initial infiltration capacity (mm/h)
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Table S.2 – Additional sigmoid type functions. Numbering continues from Group II of the Table 1. Placing the parameters and variables together always indicates multiplication (e.g. $kt = k \times t$). $e = \exp$.

(#)	Name and/or Reference	Form	Parameter meaning & application
Different version of the logistic equation ^a			
2.7	5-parameter	$Y = Y_{low} + \frac{Y_{asym}}{[1 + e^{-k(t-t_m)}]^c}$	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 the growth rate is maximum, k determines the steepness of the curve, c is a shape parameter
2.8	4-parameter	$Y = Y_{low} + \frac{Y_{asym}}{1 + e^{-k(t-t_m)}}$	
2.9	2-parameter	$Y = \frac{1}{1 + e^{-k(t-t_m)}}$	
2.10	1-parameter	$Y = \frac{1}{1 + e^{-(t-t_m)}}$	
Different versions of the beta function ^b			
2.11	5-parameter; for cases when initial phase is important; Yin et al., 2003	$Y = Y_b + (Y_{max} - Y_b) \left(1 + \frac{t_e - t}{t_e - t_m} \right) \left(\frac{t - t_b}{t_e - t_b} \right)^{\frac{t_e - t_b}{t_e - t_m}}$	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
2.12	2-parameter; for cases when maximum growth rate achieved at the beginning of growth; Yin et al., 2003	$Y = Y_{max}(2t_e - t) \frac{t}{t_e^2}$	
2.13	2-parameter; for cases when maximum growth achieved towards the end of growth period; Yin et al., 2003	$Y = Y_{max}(3t_e - 2t) \frac{t^2}{t_e^3}$	
2.14	3-parameter; Applied to describe leaf senescence; Yin et al., 2009	$Y = Y_{max} \left[1 - \left(1 + \frac{t_e - t}{t_e - t_m} \right) \left(\frac{t}{t_e} \right)^{\frac{t_e}{t_e - t_m}} \right]$	

Exponential functions for plant growth analysis			
2.15	Expolinear (Goudriaan and Monteith 1990)	$Y = \frac{c_m}{r_m} \ln[1 + e^{r_m(t-t_o)}]$	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
2.16	Symmetrical Expolinear (Goudriaan 1994)	$Y = \frac{c_m}{r_m} \ln \left[\frac{1+e^{r_m(t-t_o)}}{1+e^{r_m(t-t_o-\frac{Y_{max}}{c_m})}} \right]$	
Additional generic sigmoid functions			
2.17	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,
2.18	Korf (cited in Zeide, 1993)	$Y = Y_{asym} e^{-\beta t^{-c}}$	
2.19	Special Von Bertalanffy, 1938 ^c	$Y = Y_{asym} (1 - e^{-k(t-t_o)})$	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 = ½ 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)
2.20	Generalized Von Bertalanffy, 1938 ^c	$Y = Y_{asym} (1 - e^{-k(t-t_o)})^v$	
2.21	Log-logistic distribution (Ritz et al., 2013)	$Y = \frac{Y_{asym}}{1+\exp[k\{\log(t)-\log(t_{50})\}]} = \frac{Y_{asym}}{1+\left(\frac{t}{t_{50}}\right)^k}$	
Inverse sigmoid functions used to quantify water retention curves ^d			
2.22	Van Genuchten (1980)	$\theta_h = \theta_r + \frac{\theta_s - \theta_r}{[1 + (ah)^n]^{1-\frac{1}{n}}}$	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 pore-size distribution (n>1)
2.23	Gardner (1958)	$\theta_h = \theta_r + \frac{\theta_s - \theta_r}{1 + (ah)^n}$	
2.24	Brooks and Corey (1964)	$\theta_h = \theta_r + \frac{\theta_s - \theta_r}{(ah)^n}$	
2.25	Campbell (1974)	$\theta_h = \theta_s (ah)^n$	
^a : the 3-parameter logistic equation is given in Table 1 (see equation 2.1)			
^b : For additional versions of the beta growth function see Yin et al (2003b)			
^c : for a comparison of the two Von Bertalanffy (1938) models see Urban, 2002			
^d : The R-package ‘HydroMe’ includes the listed water retention equations (see Omuto and Gumbe, 2009)			

Table S.3 – Additional equations for photosynthesis. Numbering continues from Group III of the Table 1. Placing the parameters and variables together always indicates multiplication (e.g. $kt = k \times t$). e = exp.			
(#)	Name and/or Reference	Form	Parameter meaning & application
3.7	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
3.8	Modified hyperbola used to describe light saturated photosynthesis response to nitrogen (del Pozo & Dennett 1999)	$Y = Y_{asym} \frac{N - N_{min}}{N + k}$	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 $Y=0$
3.9	Weibull type sigmoid function used to assess water stress effects on photosynthesis (Vico and Porporato, 2008)	$Y = Y_{asym} e^{\left[-\left(\frac{-\psi_L}{d} \right)^b \right]}$	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 S.4 – Additional equations for temperature dependencies. Numbering continues from Group IV of the Table 1. Placing the parameters and variables together always indicates multiplication (e.g. $kt = k \times t$). $e = \exp$.			
(#)	Name and/or Reference	Form	Parameter meaning & application
4.6	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
4.7	Logarithmic (e.g. Foereid et al., 2011)	$Y = a + b \ln(T)$	
4.8	Exponential (e.g. Shibu et al., 2006)	$Y = ae^{bT}$	
4.9 ^a	Modified exponential (O'Connell 1990)	$Y = e^{[a+bT(1-0.5\frac{T}{T_o})]}$	
4.10	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
^a : Eq. 4.9 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.			

(#)	Name and/or Reference	Form	Parameter meaning & application
5.4 ^a	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)
5.5 ^a	Lorentzian 4-parameter	$Y = Y_o + \frac{a}{1 + \left(\frac{X - X_o}{b}\right)^2}$	
5.6 ^b	Log Normal 3-parameter	$Y = ae^{-0.5\left(\frac{\ln\left(\frac{X}{X_o}\right)}{b}\right)^2}$	
5.7	Pseudo-Voigt 4-parameters	$Y = a \left[\frac{c}{1 + \left(\frac{X - X_o}{b}\right)^2} + (1 - c)e^{-0.5\left(\frac{X - X_o}{b}\right)^2} \right]$	

Table S.6 – Additional equations. Numbering continues from Group VI of the Table 1. Placing the parameters and variables together always indicates multiplication (e.g. $kt = k \times t$).

(#)	Name and/or Reference	Form	Parameter meaning & application
6.6 ^a	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
6.7 ^b	Shepherd (e.g. Bolker 2008)	$Y = \frac{Y_{asym} X}{b + X^c}$	
6.8 ^b	Hassell (e.g. Bolker 2008)	$Y = \frac{Y_{asym} X}{(b + X)^c}$	
6.9 ^c	2 parameter exponent (e.g. Ratkowsky 1993)	$Y = Y_o b^X$	
6.10	Monod kinetics	$Y = \frac{\mu X}{X + C_{sat}} B$	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
^a : 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) ^b : if $c > 0$ then equation takes a peak form ^c : if $b > 1$ then Y increases; if $b < 1$ then Y decreases.			

References

- Andren, O., and K. Oaustian. 1987. Barley straw decomposition in the field: a comparison of models. *Ecology* 68: 1190–1200.
- Bolker, B.M. 2008. *Ecological models and data in R*. Princeton University Press.
- Brooks, R.H., and A.T. Corey. 1964. Hydraulic properties of porous medium. *Hydrology Paper 3*, Colorado State University, USA, 27pp
- del Pozo, A. and M.D. Dennett. 1990. Analysis of the distribution of light, leaf nitrogen, and photosynthesis within the canopy of *Vicia faba* L. at two contrasting plant densities. *Australian Journal of Agricultural Research* 50: 183–189.
- Campbell, G.S. 1974. A simple method for determining unsaturated conductivity from moisture retention data. *Soil Science* 117: 311–314.
- Gardner, W. 1958. Some steady state solutions of the unsaturated moisture flow equation with application to evaporation from a water table. *Soil Science* 85: 228–232.
- Gills, J.D., and G.W. Price. 2011. Comparison of a novel model to three conventional models describing carbon mineralization from soil amended with organic residues. *Geoderma* 160: 304–310.
- Goudriaan, J., and J.L. Monteith. 1990. A mathematical function for crop growth based on light interception and leaf area expansion. *Annals of Botany* 66: 695–701.
- Goudriaan, J., 1994. Using the expolinear growth equation to analyze resource capture. In: Monteith, J.L., R.K. Scott, and M.H. Unsworth. Eds. *Resource capture by crops*. Nottingham: Nottingham University Press, 99–110.
- Horton, R.E. 1940. An approach towards a physical interpretation of infiltration capacity. *Soil Science Society of America Proceedings* 5: 227–237.
- Johnson, I.R., J.H.M. Thornley, J.M. Frantz, and B. Bugbee. 2010. A model of canopy photosynthesis incorporating protein turnover distribution through the canopy and its acclimation to light, temperature and CO₂. *Annals of Botany* 106: 735–749.
- Kirschbaum, M.U.F. 1995. The temperature dependence of soil organic matter decomposition, and the effect on global warming on soil organic science. *Soil Biology and Biochemistry* 27: 753–760.
- O’Connell, A.M., 1990. Microbial decomposition (respiration) of litter in eucalypt forests of south-western Australia: An empirical model based on laboratory incubations. *Soil Biol. Biochem.* 22: 153–160.
- Omuto, C.T., and L.O. Gumbe. 2009. Estimating water infiltration and retention characteristics using a computer program in R. *Computers and Geosciences* 35: 579–585.

- Ratkowsky, D.A. 1993. Principles of nonlinear regression modeling. *Journal of Industrial Microbiology* 12: 195–199.
- Ritz, C., C.B. Phipper, and J.C. Streibig. 013. Analysis of germination data from agricultural experiments. *European Journal of Agronomy* 45: 1–6.
- Shibu, M.E., P.A. Leffelaar, H. van Keulen, and P.K. Aggarwal. 2006. Quantitative description of soil organic matter dynamics—A review of approaches with reference to rice-based cropping systems. *Geoderma* 137: 1–18.
- Urban, J.H. 2002. Modeling growth of different development stages in bivalves. *Marine ecology progress series* 238: 109–114.
- Van Genuchten, M.T., 1980. A closed-form equation for predicting the hydraulic conductivity of unsaturated soils. *Soil Science Society of America Journal* 44: 892–898.
- Vico, G., and A. Porporato. 2008. Modelling C3 and C4 photosynthesis under water-stressed conditions. *Plant and Soil* 313: 187–203.
- Von Bertalanffy, L. 1938. A quantitative theory of organic growth (Inquires on growth laws II). *Human Biol.* 10: 181–213.
- Wang, E., and T. Engel. 1998. Simulation of phenological development of wheat crops. *Agricultural Systems*: 58: 1–24.
- Ye, Z., and Z. Zhao. 2010. A modified rectangular hyperbola to describe the light-response curve of photosynthesis of *Bidens pilosa* L. grown under low and high light conditions. *Front. Agric. China* 4: 50–55
- Yin, X., A.D.H.C.M. Schapendonk, M. Kroff, M. van Oijen, and P.S. Bindraban. 2000. A Generic equation for nitrogen-limited leaf area index and its application in crop growth models for predicting leaf senescence. *Annals of Botany* 85: 579–585.
- Yin, X., E.A. Lantinga, A.D.H.C.M. Schapendonk, and X. Zhong. 2003a. Some quantitative relationships between leaf area index and canopy nitrogen content and distribution. *Annals of Botany* 91: 893–903.
- Yin, X., J. Goudriaan, E.A. Lantinga, J. Vos, and J.H.J. Spiertz. 2003b. A flexible sigmoid function of determinate growth. *Annals of Botany* 91: 361–371. (with erratum in *Annals of Botany* 91: 753, 2003).
- Yin, X., W. Guo. and J.H. Spiertz. 2009. A quantitative approach to characterize sink–source relationships during grain filling in contrasting wheat genotypes. *Field Crops Research* 114: 119–126.
- Zeide, B. 1993. Analysis of growth equations. *Forest Science* 39: 594–616.