Interpretation of nonlinear curve parameters

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1. Introduction

Within the hierarchical data context, polynomial functions have frequently been used to describe, for example, the growth of respondents over time. Polynomial functions are functions that are linear in terms of the model parameters. This familiar model can be expressed as

$$y_{ij} = b_0 + b_1 x_{ij} + b_2 x_{ij}^2 + e_{ij}$$

and at level-2

$$b_0 = \beta_0 + u_{i0}$$
$$b_1 = \beta_1 + u_{i1}$$
$$b_2 = \beta_2 + u_{i2}$$

While the coefficient b_0 representing the intercept is interpretable, the same cannot be said for the other parameters, making it more difficult to connect the results obtained to the actual behavior being studied. Another drawback of this model is that it does not allow for inflection points and thus models that have this capability may offer a better description of the data. In contrast, many nonlinear functions have the advantage that parameters are directly related to the change process being studied.

1.1 Definition of models

In particular, the Richards (1959) family of curves offer the opportunity to use flexible response functions with directly interpretable parameters. The Richards curve can be defined as

$$f(\boldsymbol{\alpha},\lambda,t_i)=\alpha(1+s\beta_s\rho^{t_i})^{\lambda}$$
$$\boldsymbol{\alpha}'=(\alpha,\beta_s,\rho) \qquad (1)$$

and *s* denotes the sign of the term $\beta_s\rho^t$. If the response function increases monotonically in t_i, then *s* = -1 for $\lambda\geq 0$ and *s* = 1 for $\lambda<0$. Opposite signs are allocated when the response function decreases monotonically in t_i. The following linear inequality constraints are imposed on the elements of $\boldsymbol{\alpha}$:

$$\alpha\geq 0$$
$$\beta_1\geq 0;\quad 0\leq\beta_{-1}\leq 1$$
$$0\leq\rho\leq 1.$$

The constraint $0\leq\beta_{-1}\leq 1$ is imposed to avoid the occurrence of complex roots in the expression $\left(1-\beta_{-1}\rho^{t_i}\right)^{\lambda}$.

Three well-known growth functions can be obtained as special cases of (1):

the monomolecular ($\lambda=1$)

$$f(\boldsymbol{\alpha};1,t_i)=\alpha(1-\beta\rho^{t_i}) \qquad (2)$$

the Gompertz function ($\lambda\to\infty$)

$$f(\boldsymbol{\alpha};1,t_i)=\alpha\exp(\beta^{*\rho^{t_i}})$$
$$\beta^{*}=s\beta_s\lambda \qquad (3)$$

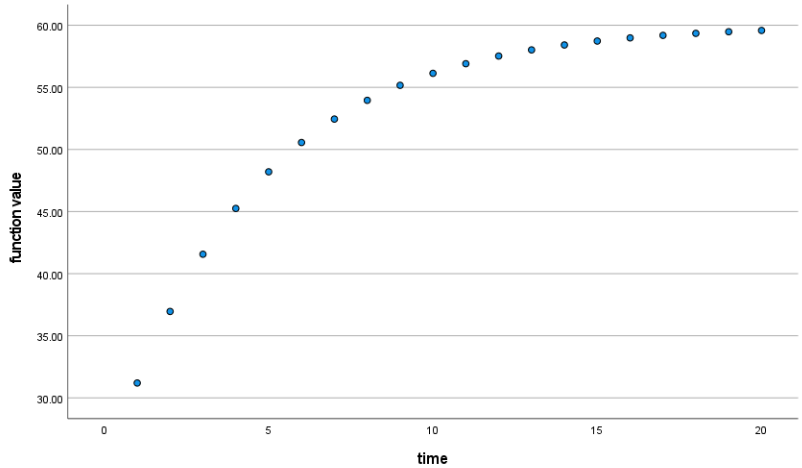
and the logistic function ($\lambda=-1$)

$$f(\boldsymbol{\alpha};1,t_i)=\frac{\alpha}{1+\beta\rho^{t_i}} \qquad (4)$$

The monomolecular curve (2) has no point of inflection, the logistic (4) is symmetric around its point of inflection and the Gompertz curve is asymmetric, inflecting at $e^{-1}\alpha$. A Gompertz curve can be approximated with considerable accuracy if a value of, say, 1 000 or -1 000 is chosen for λ.

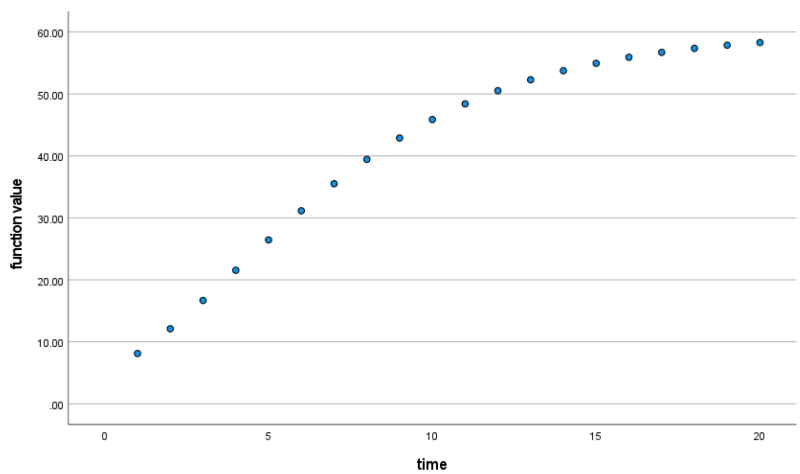
The parameter α represents the time-asymptotic value of the measured characteristic. β represents the potential increase or decrease in the value of the function $f\left(\boldsymbol{\alpha},\lambda,t_i\right)$ during the course of time t_1 to t_p. The parameter ρ characterizes the rate of growth. Apart from their degree of compression, the differing shapes of the curves are due solely to differences in the parameter λ. Examples of these curves are shown below.

Monomolecular curve: $f(\boldsymbol{\alpha};1,t_i) = 60(1-0.6(0.8)^{t_i})$

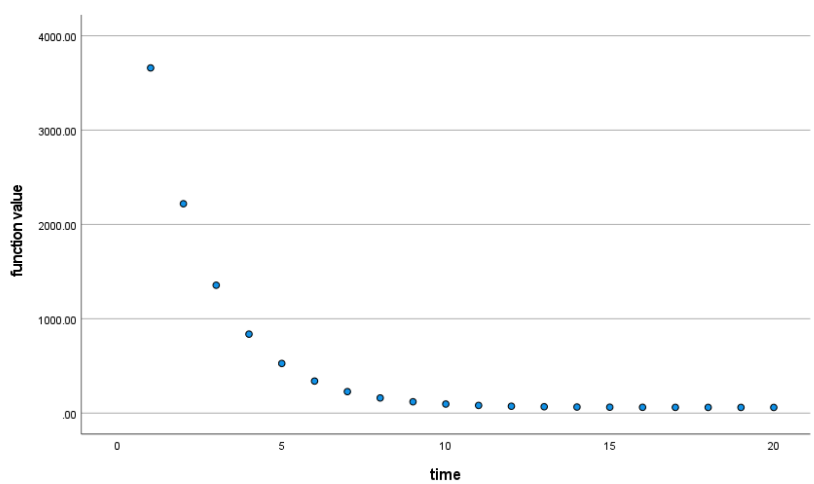


Gompertz curve:

$f(\boldsymbol{\alpha};1,t_i) = 60\exp(-2.5(0.8)^{t_i})$



Logistic curve: $f(\boldsymbol{\alpha};1,t_i) = \dfrac{60}{1+100(0.6)^{t_i}}$



1.2 Distributional assumptions

Let y_{ij} denote the observed value for level-2 unit *i* at occasion t_{ij} where $j = 1, 2, ..., n_i$ and let $f\left(\mathbf{b}', t_{ij}\right)$ denote one of the nonlinear functions, for example

$$f_{ij}(\mathbf{b}', t_{ij}) = b_1(1 + \exp(b_2 + b_3 t_{ij}).$$

We assume the following model

$$\mathbf{y}_i = \mathbf{f}_i + \mathbf{e}_i, \quad i = 1, 2, ..., n_i$$

where y_{ij} and f_{ij} are typical elements of $\mathbf{y}_i$ and $\mathbf{f}_i$. To obtain the log-likelihood function it is further assumed that $\mathbf{b} \sim N(\mathbf{0}, \Theta)$ and $\mathbf{e}_i \sim N(\mathbf{0}, \sigma^2 \mathbf{I})$. To evaluate the log-likelihood, use is made of the adaptive gaussian quadrature procedure.

2. Interpretation of parameters

We now consider the three curves identified in the previous section individually and take a closer look at the interpretation of the parameters and the effect of changes in the value of these parameters. We use the parameterization of these models as used in the LISREL Multilevel module. Finally, we also take a look at the other two functions currently available in LISREL: the exponential and the power function.

2.1 Monomolecular curve

In LISREL, the model specified and estimated is

$$\begin{aligned}
y_{ij} &= b_1 / [1 + s * \exp(b_2 - b_3 * t_{ij})] + e_{ij} \\
b_1 &= \beta_1 + u_1 \\
b_2 &= \beta_2 + u_2 \\
b_3 &= \beta_3 + u_3
\end{aligned}$$

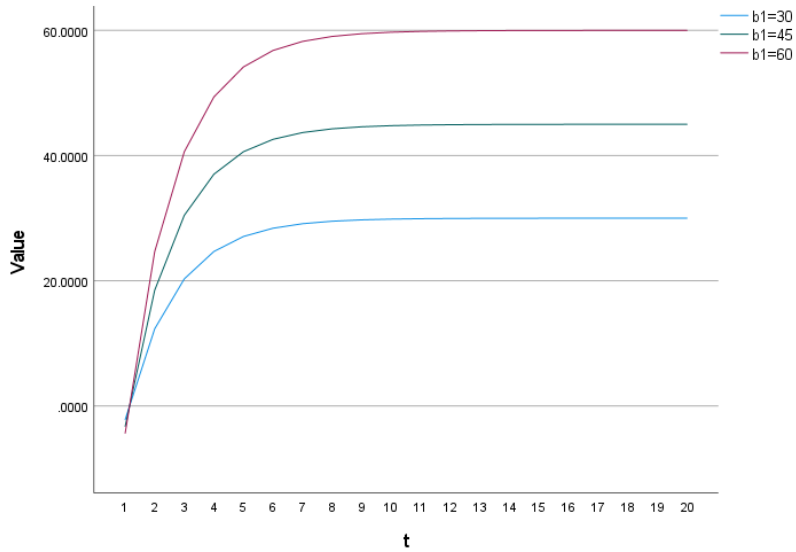
where t_{ij} indicates the variable representing the change in time over measurements and *s* and *s* has a value of 1 when the function values decrease with a monotonic increase in time and -1 if it increases.

For the Vonesh and Carter (1992) data, for example, the ultrafiltration rates measured at different pressures can be described using a model such as

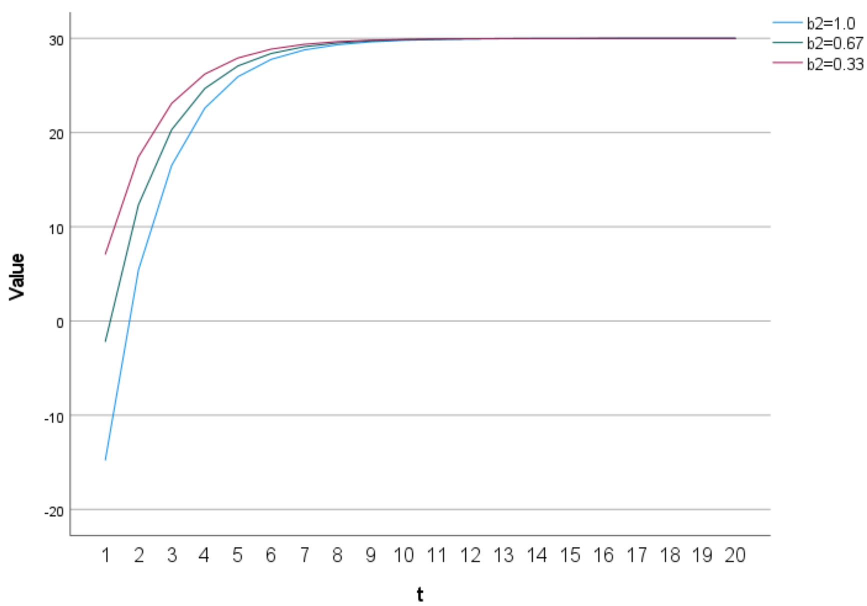
$$\begin{aligned}
y &= b_1 / [1 + \exp(b_2 - b_3 * Pressure) + e \\
b_1 &= \beta_1 + u_1 \\
b_2 &= \beta_2 + u_2 \\
b_3 &= \beta_3 + u_3
\end{aligned}$$

LISREL also allows for the inclusion of covariates in the model but, for simplicity sake, we consider models without covariates in the present case.

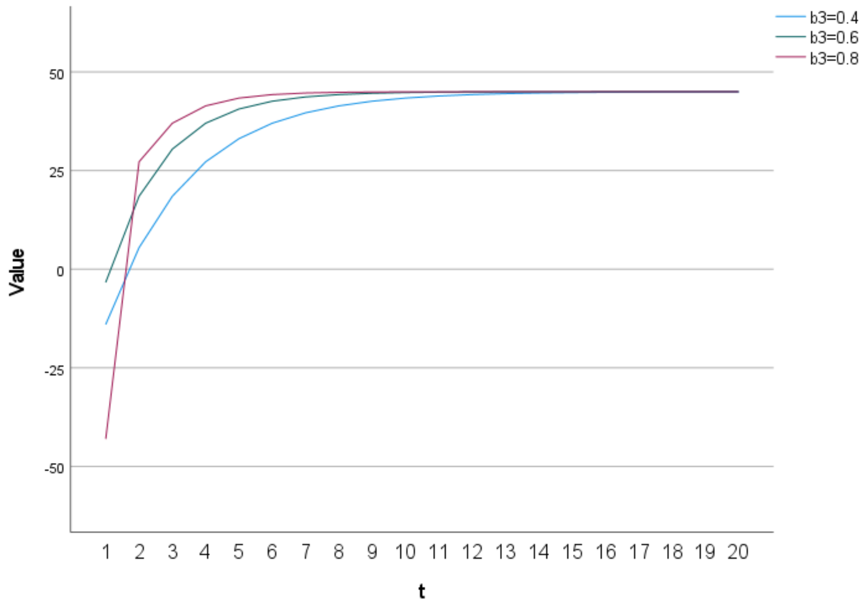
In the first of the graphs shown below, values of the first parameter b_1 assumed three different values, while b_2 was held constant at a value of 0.67 and b_2 was held constant at a value of 0.6. An increase in the value of b_1, holding the other two parameters constant, results in an increase in time-asymptotic value of y. Basically, b_1 reflects the final height of the curve.



When the parameter b_2 varies while b_1 was held constant at a value of 45 and b_3 was held constant at a value of 0.6, an increase in the value of b_2, holding the other two parameters constant, leads to the potential increase or decrease in the value of the function $f(\boldsymbol{\alpha}, \lambda, t_i)$ during the course of time t_1 to t_p.



Finally, we consider the effect of an increase in b_3, holding b_1 constant at a value of 45 and b_2 at of 0.67. It is clear from the graph that the rate of increase in y is higher with larger values of b_3. This parameter characterizes the rate of growth over time.



2.2 Gompertz curve

We repeated the same process as described for the monomolecular curve for the Gompertz curve. The Gompertz model is well known and widely used in many aspects of biology for example the growth of animals and plants. It is also used in the estimation of the number or volume of bacteria and cancer cells.

The parameterization for this function as implemented in LISREL is

The model is defined as

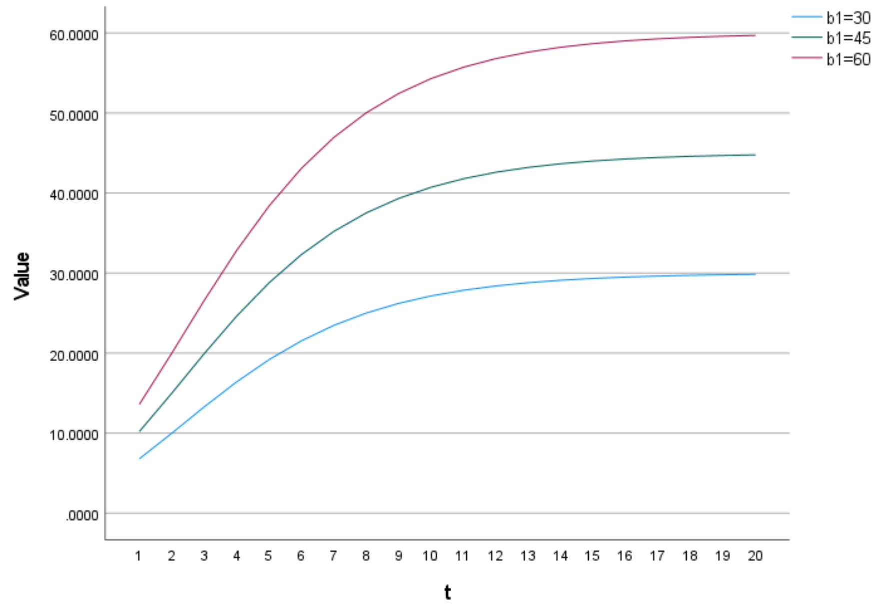
$$y = b_1 * \exp(-b_2 \exp(s * b_3 * Time)) + e$$

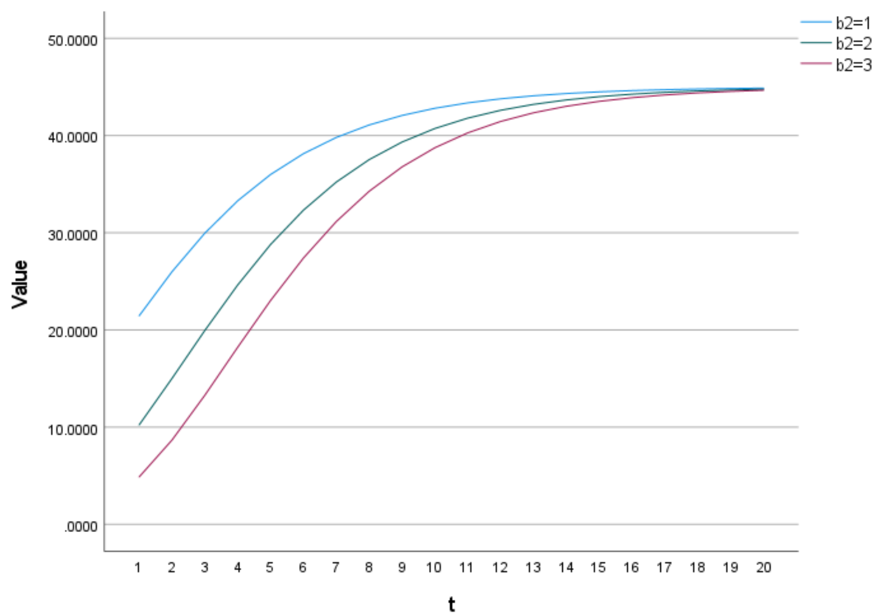
where

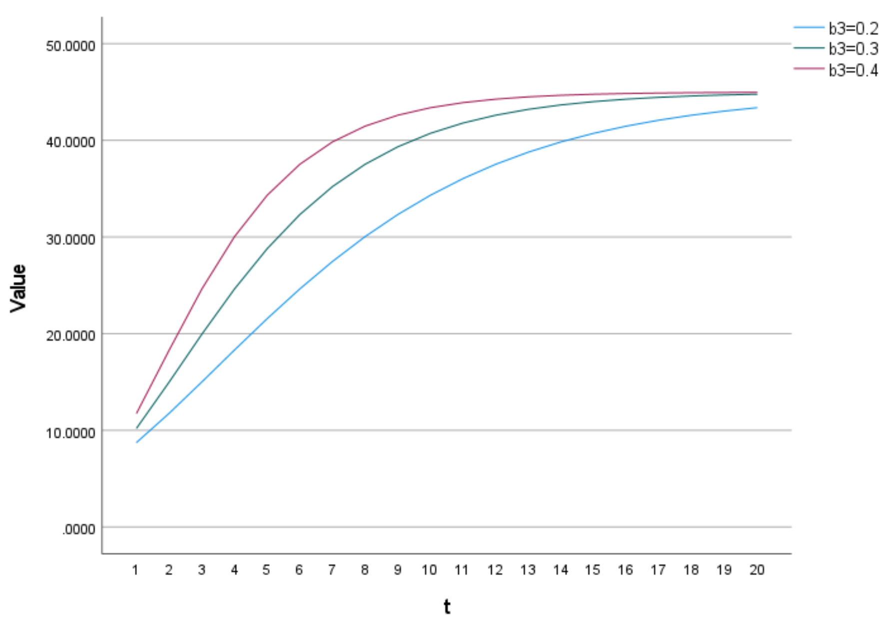
$$b_1 = \beta_1 + u_1$$
$$b_2 = \beta_2 + u_2$$
$$b_3 = \beta_3 + u_3$$

and s has a value of 1 when the function values increase with a monotonic increase in time and -1 if it decreases.

The graphs representing changes in y with changes in individual parameters, holding the other parameters constant, are given below. We note that the same interpretation of parameters given for the monomolecular model also holds in the case of the Gompertz curve.


b1=30
b1=45
b1=60
60.0000
50.0000
40.0000
30.0000
20.0000
10.0000
.0000
Value
1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20
t


b2=1
b2=2
b2=3
50.0000
40.0000
30.0000
20.0000
10.0000
.0000
Value
1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20
t


b3=0.2
b3=0.3
b3=0.4
50.0000
40.0000
30.0000
20.0000
10.0000
.0000
Value
1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20
t

2.3 Logistic curve

The parameterization for this function as implemented in LISREL is

The model is defined as

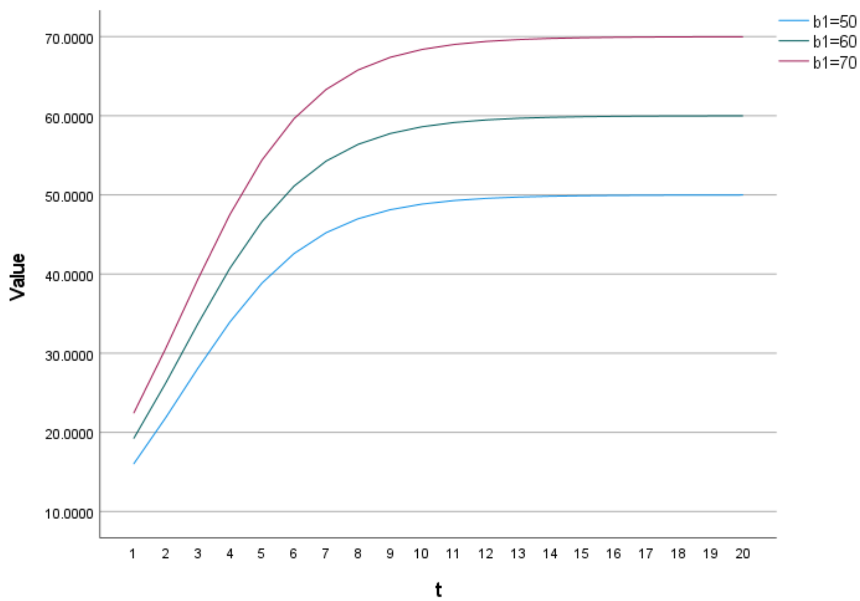
$$y = b_1 / (1 + s * \exp(b_2 - b_3 * Time)) + e$$

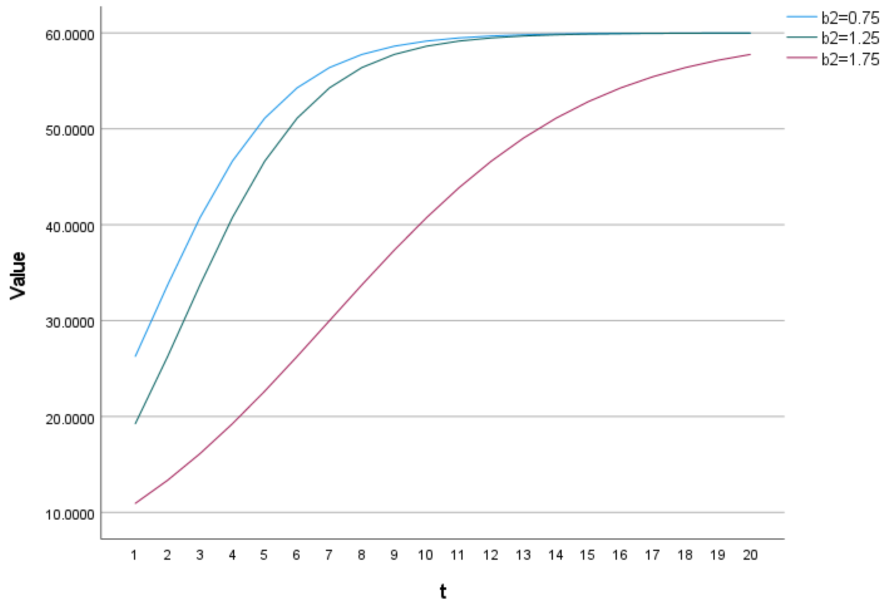
where

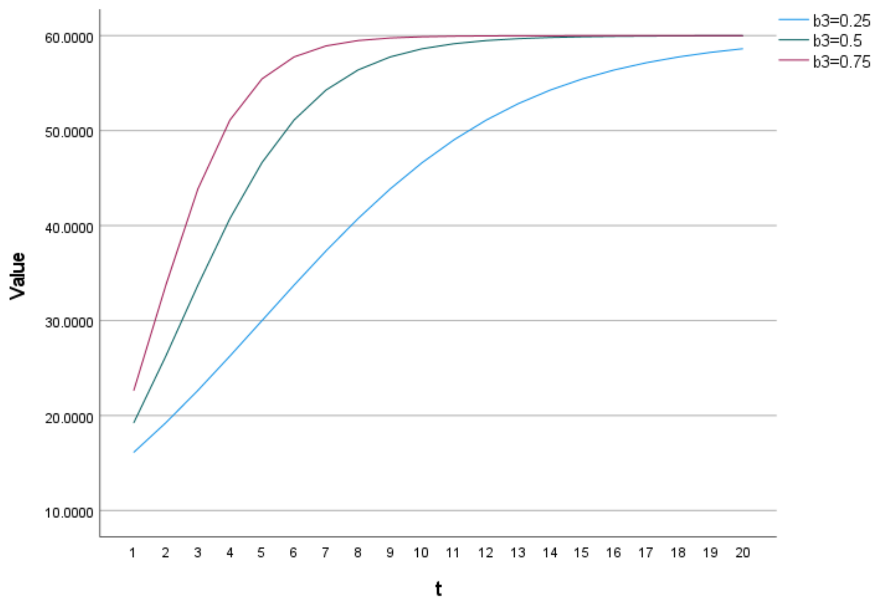
$$b_1 = \beta_1 + u_1$$
$$b_2 = \beta_2 + u_2$$
$$b_3 = \beta_3 + u_3$$

and s has a value of 1 when the function values increase with a monotonic increase in time and -1 if it decreases.

The graphs representing changes in y with changes in individual parameters, holding the other parameters constant, are given below. We note that the same interpretation of parameters given for the monomolecular model also holds in the case of the previous two curves. The potential increase/decrease in function value for a higher value of b_2 is more apparent here.







2.4 Exponential curve

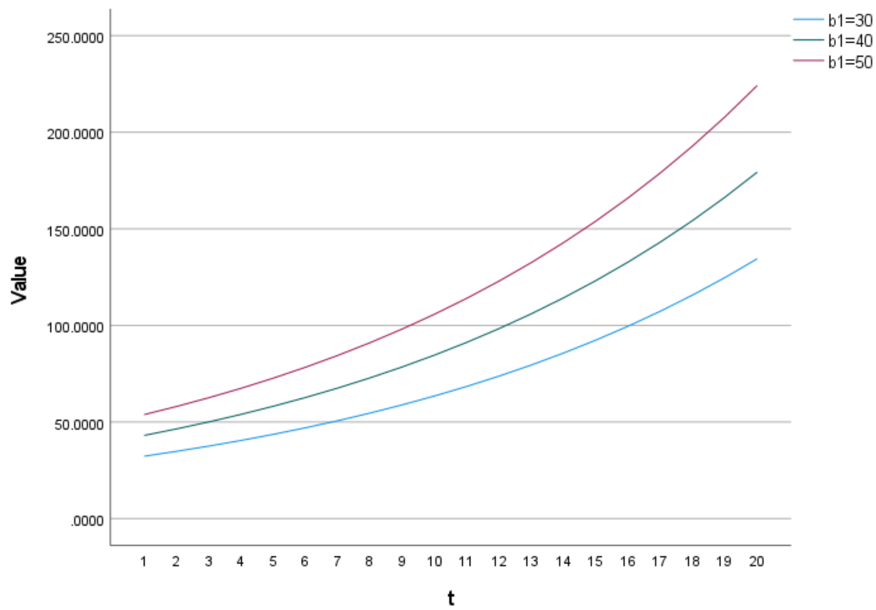
While this nonlinear function falls outside the family of Richards curves considered up to this point, it is another nonlinear function that is often used. The parameterization as implemented in LISREL is

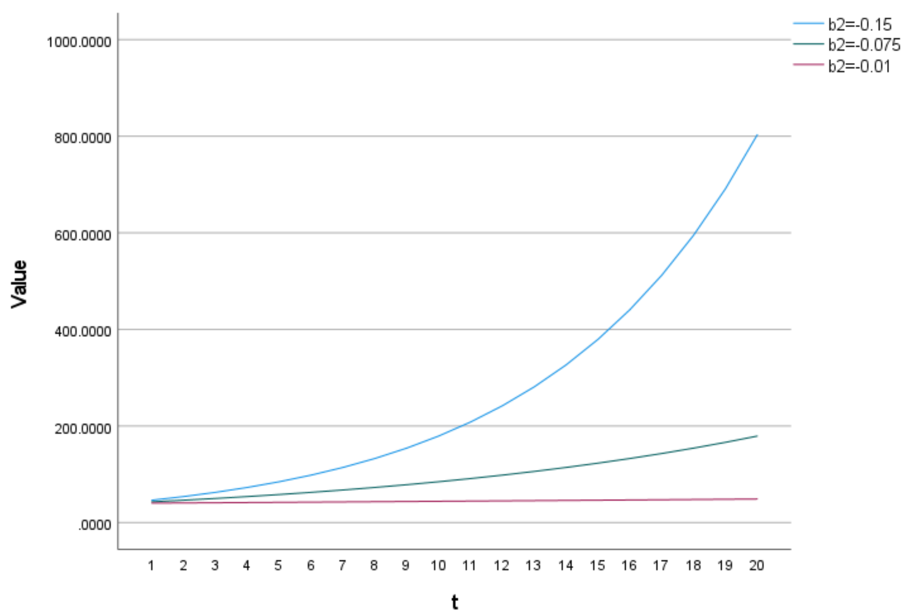
$$y = b_1 \exp(-b_2 * Time)) + e$$

where

$$b_1 = \beta_1 + u_1$$
$$b_2 = \beta_2 + u_2$$

An increase in the value of b_1, while holding the value of b_2 constant, results in an increase of the function value over time. However, when we inspect the graph for varying values of b_2 (holding b_1 constant at 40) we note that higher b_2 not only controls the rate of growth over time but also seems to results in an increase in the function value over time. We conclude that the interpretation of the two parameters in this model is not as straightforward as in the case of the previous three models considered.





2.5 Power curve

The parameterization for this function as implemented in LISREL is

The model is defined as

$$y = b_1(b_2^{\,t}) + e$$

where

$$b_1 = \beta_1 + u_1$$
$$b_2 = \beta_2 + u_2$$

Graphically, power functions can resemble exponential or logarithmic functions depending on the values of b_2. Large increases in b_2 will, however, lead to divergence between these three functions. An exponentially growing function will overtake a growing power function for large values of b_2. On the other hand, growing power functions will overtake logarithmic functions for large values of b_2. A good example is the example published by Max Kleiber in 1932. He published an equation describing the metabolic rate of an animal as a function of its mass.

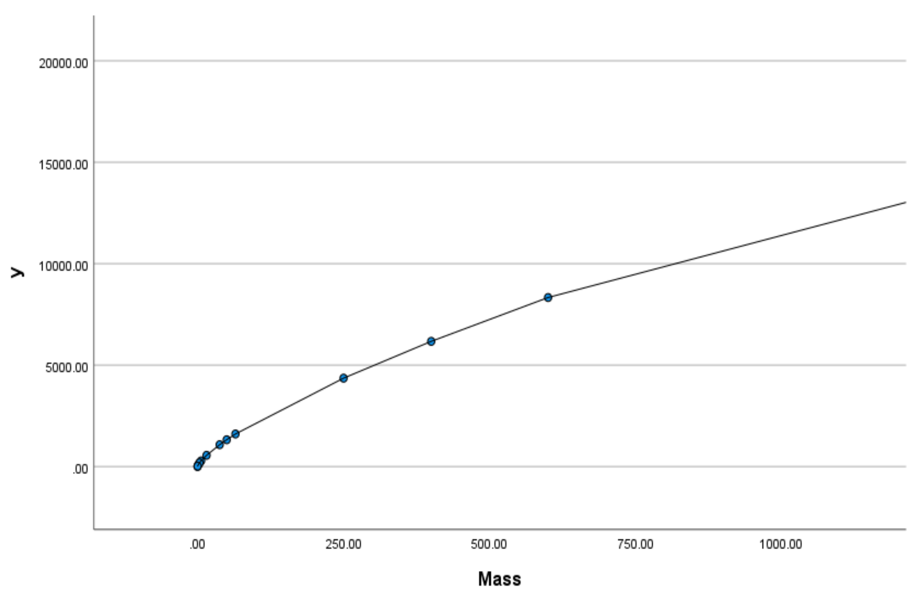
The simple data set he used is given in the table below.

Animal	**Mass (kg)**	**Metabolic rate (kcal/day)**
Baboon	6.2	300
Cat	3.0	150
Chimpanzee	38	1110
Cow	400	6080
Dog	15.5	520
Elephant	3670	48,800
Guinea pig	0.8	48
Human	65	1660
Mouse	0.02	3.4
Pig	250	4350
Polar bear	600	8340
Rabbit	3.5	165
Rat	0.2	28
Sheep	50	1300

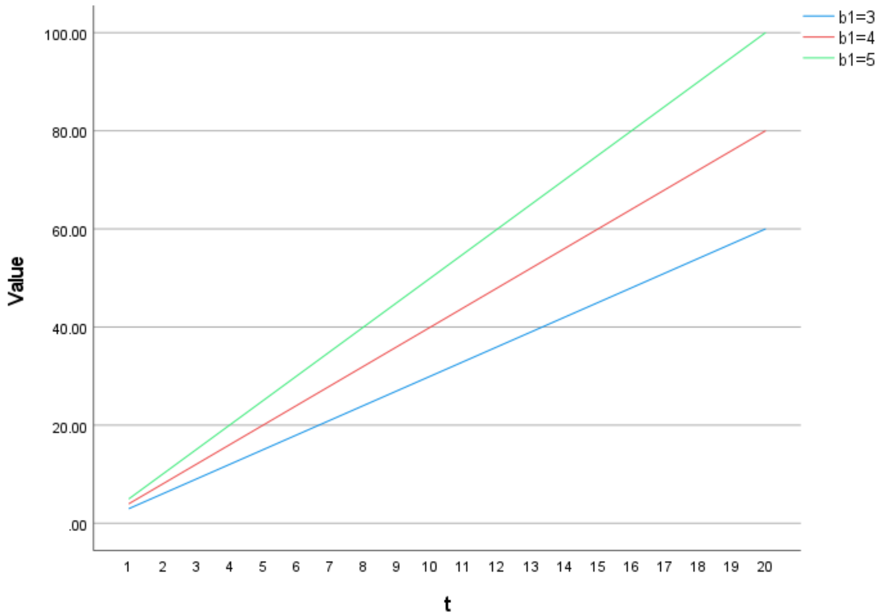
Plotting these data using the power function

$$y = 73.3 * mass^{0.74}$$

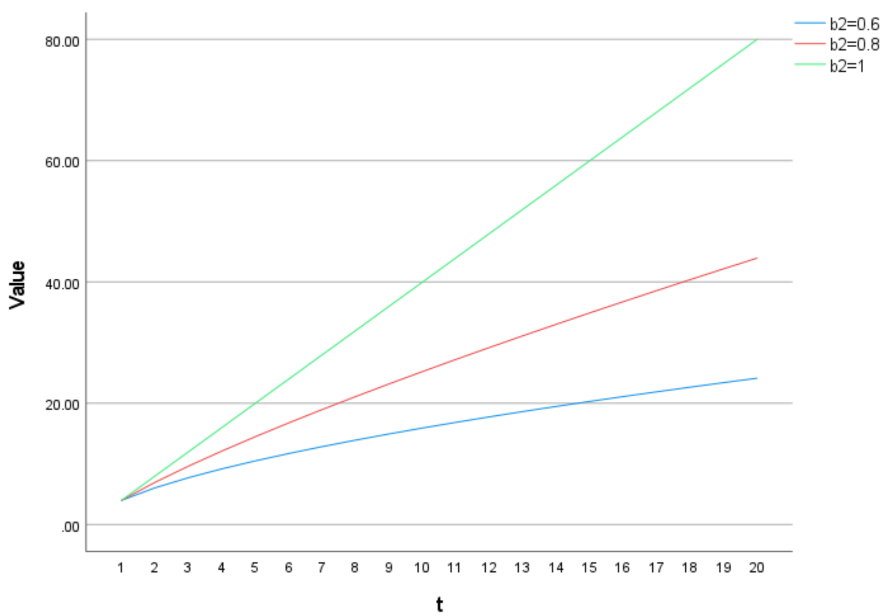
produced the famous mouse-to-elephant curve shown in the figure below.



In the next graph we plotted the function value for 3 values of b_1 while holding the value of b_2 constant at 0.6. An increase in b_1 is associated with an increase in the function value over time. The rate of change of the three curves increases with larger values of b_1.



Turning to function value for various values of b_2 (holding b_1 constant at 4) we see an increase in rate of change and function value associated with larger values of b_2.



Finally, note that when the value of b_2 is negative as in the graph below, the function value approaches the limit value of 0.0 over time.