Minimum with inequality constraint applied to increasing cubic, logistic and Gomperz or convex quartic and biexponential regressions

Josef Bukac
Bulharska 298, 55102
Jaromer-Josefov, Czech Republic

Keywords:convex quartic, Gomperz, increasing cubic, positive bi-exponential, restricted, starting values, sum of squares.

Abstract: We present a method of minimizing an objective function subject to an inequality constraint. It enables us to minimize the sum of squares of deviations in linear regression under inequality restrictions. We demonstrate how to calculate the coefficients of cubic function under the restriction that it is increasing, we also mention how to fit a convex quartic polynomial.

We use such results for interpolation as a method for calculation of starting values for iterative methods of fitting some specific functions, such as four-parameter logistic, positive bi-exponential, or Gomperz functions. Curvature-driven interpolation enables such calculations for otherwise solutions to interpolation equations may not exist or may not be unique.

We also present examples to illustrate how it works and compare our approach with that of Zhang (2020).

1. Introduction

This paper deals mostly with S-functions, also known as sigmoid functions due to their shape. They are typically nonlinear in parameters. If the data are given, the calculation of optimal parameters typically ends up as an iterative process to minimize the residual sum of squares.

To start iterations, we have to use some initial values. Initial values are essential because, in the case of nonlinear regression, there may be more than one local minimum or, on the other hand, we have to consider a warning that the parameters that would minimize the sum of squares may not even exist, Bukac (2001) or Nievergelt (2013).

Since there might be difficulties in using iterations when applying the least-squares method, we advocate the use of all the available methods of obtaining initial estimates. Some methods of calculating initial values do not work when the number of data points is small or the variability is too big. We present an interpolation approach that may work even for a small number of data points.

There are two ways to do this.

1) It is easy to fit a polynomial function to datapoints and, consequently, interpolate this polynomial function by a nonlinear function.

2) Another way is to apply this approach to the inverse of the nonlinear function. We swap the dependent and independent variables, calculate a polynomial by the least-squares method, and use interpolation as a means to find the parameters of the inverse of the nonlinear function in question.

In some cases, we can try each of the approaches and pick a better one according to the residual sum of squares. Especially in a case like an exponential function, depending on how the parameters are set, the function $y = a + b\exp(cx)$ may be increasing or decreasing, convex or concave.

We suggest that, once some function presents a good fit, we may use interpolation to obtain parameters of another type of function. Obviously, the easiest functions to use in regression are the polynomial functions because they are linear in parameters.

In the following, we present a theorem that allows us to calculate the parameters of a cubic polynomial function so that this function is increasing.

2. Minimization with one minimum subject to one inequality

It is well known that, if the variance-covariance matrix is full rank, it is positive definite, the minimum of the sum of squares is strict and unique. It is the minimum of a strictly convex function. We use this as an assumption in the following theorem 2.1, which is a bit more general.

Theorem 2.1. Let $\mathbf{b} = (\mathrm{b}_1, \mathrm{b}_2, \dots \mathrm{b}_\mathrm{M})'$. We assume $f(\mathbf{b})$ is a function defined on R^M posessing a unique strict global minimum and no other local minima. We assume $g(\mathbf{b})$ is a continuous function on R^M. The value of $\mathbf{b}$ that minimizes $f(\mathbf{b})$ subject to inequality $g(\mathbf{b}) \geq 0$ may

A) either be the value $\mathbf{b_g}$ that yields the global minimum of $f(\mathbf{b})$ and satisfies $g(\mathbf{b_g}) \geq 0$ or

B) if A is not true and if some $\mathbf{b_r}$ that minimizes $f(\mathbf{b})$ restricted by the inequality $g(\mathbf{b_g}) \geq 0$ exists, then this $\mathbf{b_r}$ satisfies the equality $g(\mathbf{b_r}) = 0$.

Proof.

Case A: If $\mathbf{b_g}$ is the value at which $f(\mathbf{b})$ takes on its global minimum and $g(\mathbf{b_g}) \geq 0$, we are done.

Case B: Let $\mathbf{b_g}$ minimize $f(\mathbf{b})$ under no restriction and let $g(\mathbf{b_g}) < 0$. Let d denote the distance in R^M with which the continuity of g is defined. We obtain a contradiction by assuming there is a $\mathbf{b_r}$ with $g(\mathbf{b_r}) > 0$ that minimizes $f(\mathbf{b})$ restricted by $g(\mathbf{b}) \geq 0$. Let $\epsilon = g(\mathbf{b_r})/2$. Since g is continuous, there is a $\delta > 0$ such that for all $\mathbf{b}$ satisfying $d(\mathbf{b}, \mathbf{b_r}) < \delta$ we get $|g(\mathbf{b}) - g(\mathbf{b_r})| < \epsilon$. It means that f has a local minimum at $\mathbf{b_r} \neq \mathbf{b_g}$ contradicting our assumpption about one minimum.

Sometimes we can show that some $\mathbf{b_r}$ minimizes $f(\mathbf{b})$ subject to the constraint $g(\mathbf{b}) = 0$. In this case, slightly different wording of theorem 2.1 may be useful. The proof would be the same.

Theorem 2.1A. Let $\mathbf{b} = (\mathrm{b}_1, \mathrm{b}_2, \dots \mathrm{b}_\mathrm{M})'$. We assume $f(\mathbf{b})$ is a function defined on R^M posessing a unique strict global minimum and no other local minima. We assume $g(\mathbf{b})$ is a continuous function on R^M. The value of $\mathbf{b}$ that minimizes $f(\mathbf{b})$ subject to inequality $g(\mathbf{b}) \geq 0$ may

A) either be the value $\mathbf{b_g}$ that yields the global minimum of $f(\mathbf{b})$ and satisfies $g(\mathbf{b_g}) \geq 0$ or

B) if A is not true and if some $\mathbf{b_r}$ that minimizes $f(\mathbf{b})$ restricted by the equality $g(\mathbf{b}) = 0$ exists, then this $\mathbf{b_r}$ minimizes $f(\mathbf{b})$ subject to the inequality $g(\mathbf{b_r}) \geq 0$.

Note. Here we have used a counting argument in our proof assuming the objective function f has precisely one local minimum. By the same token, if we knew the objective function has no local minimum, we can use the same idea.

Some examples of applications are:

1) We may change a linear inequality restriction an equality restriction.

2) If we want a quadratic function to be a product of two affine functions, we want the discriminant to be nonnegative, $b^2 - 4ac \geq 0$.

3) We may want a cubic function to be increasing. We may write this requirement in the form of an inequality.

4) We may want a quartic polynomial function to be convex. This case may be resolved in a way similar to the case of a monotone cubic function.

5) The theorem may be generalized for metric spaces instead just for R^M. Perhaps such a generalization could be used in the calculus of variations.

An increasing cubic function, in particular, may be used to calculate the initial parameters for the logistic function: Consider the inverse, calculate a monotone cubic fit, use interpolation.

The question that should not be left open-ended is the one about the existence of the minimal solution as a condition for the application of theorem 2.1. Here we show the answer is easy in the case of linear regression. We use the notation that is usual in regression analysis. We assume that $\mathbf{X}$ is a T by n matrix of rank n of independent variables and $\mathbf{y}$ is the T by 1 vector of response variables. Let $\mathbf{b}$ be an n by 1 vector of regression coefficients. The sum of squares to be minimized may be written as $(\mathbf{b}'\mathbf{X}' - \mathbf{y}')(\mathbf{X}\mathbf{b} - \mathbf{y})$.

Definition. The set of regression coefficients for which $(\mathbf{b}'\mathbf{X}' - \mathbf{y}')(\mathbf{X}\mathbf{b} - \mathbf{y}) \leq K$ is called a level set and is denoted by $L(K) = \{\mathbf{b} : (\mathbf{b}'\mathbf{X}' - \mathbf{y}')(\mathbf{X}\mathbf{b} - \mathbf{y}) \leq K\}$.

A level set $L(K)$ is closed because $(b'X' - y')(Xb - y)$ is a continuous function specifically of b and a level set is nothing but an inverse image of $(-\infty, K]$ which is a closed set.

A level set $L(K)$ is bounded if it is a subset of another bounded set. In the following theorem, we will find a bounded set containing a level set and it will mean the level set is bounded.

Theorem 2.2. Given any constant K, the level set of those $\mathbf{b}$ for which the sum of squares $(\mathbf{b}'\mathbf{X}' - \mathbf{y}')(\mathbf{X}\mathbf{b} - \mathbf{y})$ is less than or equal to K is either empty or bounded.

Proof.

It is well known that if the matrix $\mathbf{X}$ is of rank n, the unique least squares solution to the minimization problem is given by $\mathbf{b_{ls}} = (\mathbf{X}'\mathbf{X})^{-\mathbf{1}}\mathbf{X}\mathbf{y}$. Any n by 1 vector $\mathbf{c} \neq \mathbf{b}$ may be written as $\mathbf{c} = \mathbf{b_{ls}} + t\mathbf{d}$, where $\mathbf{d}$ is a unit n by 1 vector and t is a scalar. We write $t\mathbf{d} = (\mathbf{c} - \mathbf{b_{ls}})/||\mathbf{c} - \mathbf{b_{ls}}||$ and take $t = ||d||$.

We get $(\mathbf{c}'\mathbf{X}' - \mathbf{y}')(\mathbf{X}\mathbf{c} - \mathbf{y}) = (\mathbf{b}'_{\mathbf{ls}}\mathbf{X}' + t\mathbf{d}'\mathbf{X}' - \mathbf{y}')(\mathbf{X}\mathbf{b_{ls}} + t\mathbf{X}\mathbf{d} - \mathbf{y}) = S + t^2\mathbf{d}'\mathbf{X}'\mathbf{X}\mathbf{d} + 2t\mathbf{d}'\mathbf{X}'(\mathbf{X}\mathbf{b_{ls}} - \mathbf{y})$ where $S = (\mathbf{b}'_{\mathbf{ls}}\mathbf{X}' - \mathbf{y}')(\mathbf{X}\mathbf{b_{ls}} - \mathbf{y})$ is independent of the choice of $\mathbf{c}$.

Since $\mathbf{d}'\mathbf{X}'\mathbf{X}\mathbf{d}$ is continuous on the compact set given by $||\mathbf{d}|| = 1$, we may define

$$A = \min_{||\mathbf{d}||=1} \mathbf{d}'\mathbf{X}'\mathbf{X}\mathbf{d}.$$

If $\mathbf{d}'\mathbf{X}'\mathbf{X}\mathbf{d}$ is minimal at $\mathbf{d}_1$, with $||\mathbf{d}_1|| = 1$, then $\mathbf{d}'_1\mathbf{X}'\mathbf{X}\mathbf{d}_1 > 0$ because the matrix $\mathbf{X}'\mathbf{X}$ is positive definite. Consequently $A > 0$. If there is another, say $\mathbf{d}_2$, for which $\mathbf{d}'\mathbf{X}'\mathbf{X}\mathbf{d}$ is minimal then obviously $\mathbf{d}'_1\mathbf{X}'\mathbf{X}\mathbf{d}_1 = \mathrm{d}'_2\mathbf{X}'\mathbf{X}\mathbf{d}_2$, therefore A is well defined.

Since the sign of $\mathbf{d}'\mathbf{X}'(\mathbf{X}\mathbf{b_{ls}} - \mathbf{y})$ may vary depending on $\mathbf{d}$, $||\mathbf{d}|| = 1$, we investigate the absolute value of $\mathbf{d}'\mathbf{X}'(\mathbf{X}\mathbf{b_{ls}} - \mathbf{y})$ and define

$$B = \max_{||\mathbf{d}||=1} |\mathbf{d}'\mathbf{X}'(\mathbf{X}\mathbf{b_{ls}} - \mathbf{y})|.$$

It is clear that $B \geq 0$ is finite because $|\mathbf{d}'\mathbf{X}'(\mathbf{X}\mathbf{b_{ls}} - \mathbf{y})|$ is a continuous function of $\mathbf{d}$ defined on a compact set.

Now we can write $S + t^2\mathbf{d}'\mathbf{X}'\mathbf{X}\mathbf{d} + 2t\mathbf{d}'\mathbf{X}'(\mathbf{X}\mathbf{b_{ls}} - \mathbf{y}) \geq t^2A - 2tB + S$ for any $\mathbf{d}$ satisfying $||\mathbf{d}|| = 1$. Since A is positive, there exists a t_0 such that for any $t > t_0$ we have $K < t^2A - 2tB + S \leq S + t^2\mathbf{d}'\mathbf{X}'\mathbf{X}\mathbf{d} + 2t\mathbf{d}'\mathbf{X}'(\mathbf{X}\mathbf{b_{ls}} - \mathbf{y})$.

The closed ball centered at $\mathbf{b_{ls}}$ with a radius t_0 is certainly bounded and contains the level set $L(K)$. Therefore, the level set $L(K)$ is bounded.

Application: We minimize the sum of squares $(\mathbf{b}'\mathbf{X}' - \mathbf{y}')(\mathbf{X}\mathbf{b} - \mathbf{y})$ subject to $g(\mathbf{b}) = 0$ using theorem 2.1 conclusion B. We assume not only the continuity of g but also the existence of some solution $\mathbf{b_t}$, perhaps just temporary, that is, $g(\mathbf{b_t}) = 0$. Since $g(\mathbf{b})$ is continuous, the inverse image of the single point $\{0\}$ is a closed set. Now we set $K = (\mathbf{b_t'}\mathbf{X}' - \mathbf{y}')(\mathbf{X}\mathbf{b_t} - \mathbf{y})$ and due to theorem 2.2 the level set $L(K) = \{\mathbf{b} : (\mathbf{b}'\mathbf{X}' - \mathbf{y}')(\mathbf{X}\mathbf{b} - \mathbf{y}) \leq K\}$ is closed and bounded. The intersection of the two closed nonempty sets, $L(K) \cap \{\mathbf{b} : g(\mathbf{b}) = 0\}$, is bounded, closed and not empty. It follows the minimum of the sum of squares subject to $g(\mathbf{b}) = 0$ exists.

Note: There might be other theorems that characterize precisely what the level sets of $(\mathbf{b}'\mathbf{X}' - \mathbf{y}')(\mathbf{X}\mathbf{b} - \mathbf{y})$ look like. We have presented our theorem only because we need to know that level sets are bounded and since $(\mathbf{b}'\mathbf{X}' - \mathbf{y}')(\mathbf{X}\mathbf{b} - \mathbf{y})$ is continuous as a function of $\mathbf{b}$, the level sets are also closed, therefore compact.

3. Minimization with no local minimum subject to one inequality

We will not use the following theorem 3.1 in our paper except for an example. It is just an example of another application of the counting argument in the case that there is no local minimum.

Theorem 3.1. Let $\mathbf{b} = (\mathrm{b}_1, \mathrm{b}_2, \ldots \mathrm{b}_\mathrm{M})'$. Let $f(\mathbf{b})$ be a function defined on R^M posessing no local minimum. We assume $g(\mathbf{b})$ is a continuous function on R^M. The value of $\mathbf{b}$ that minimizes $f(\mathbf{b})$ subject to the inequality constraint $g(\mathbf{b}) \geq 0$ is the value $\mathbf{b_r}$ that minimizes $f(\mathbf{b})$ subject to the equality constraint $g(\mathbf{b}) = 0$ if such $\mathbf{b_r}$ exists.

Proof.

To obtain a contradiction we may assume that $f(\mathbf{b})$ takes on its minimum value subject to $g(\mathbf{b}) > 0$ at $\mathbf{b_r}$ with $g(\mathbf{b_r}) > 0$.

Let $\epsilon = g(\mathbf{b_r})/2$. Since g is continuous, there exists a $\delta > 0$ such that for all $\mathbf{b}$ satisfying $d(\mathbf{b}, \mathbf{b_r}) < \delta$ we have $|g(\mathbf{b}) - g(\mathbf{b_r})| < \epsilon$. It means that f has a local minimum at $\mathbf{b_r}$, which contradicts our assumpption about no local minimum.

Example. Minimize $S(x_1, \dots, x_N) = \sum_{i=1}^N 1/x_i^2$ on a closed unit ball, that is, subject to $\sum_{i=1}^N x_i^2 \leq 1$. We modify the function S to make it bounded and continuous thus defined on the whole closed ball while not having a local minimum. We pick a small value of M for which $\sum_{i=1}^N M^2 = NM^2 < 1$. We construct a function $\hat{f}$ such that $\hat{f}(x) = M + 1/M^2 - |x|$ for $|x| \leq M$ but $\hat{f}(x) = 1/x^2$ otherwise. We may plot the graph of the function $\hat{f}(x)$ and see why we use the hat notation. Thus $1/x^2$ may be replaced by $\hat{f}(x)$ and we minimize $\hat{S}(x_1, x_2, \dots, x_N) = \sum_{i=1}^N \hat{f}(x_i)$ which would give us the same minimum at the same point but $\hat{S}$ is defined and continuous even if $x_i = 0$ for some i.

Now that we can apply theorem 3.1 and minimize $\hat{S}$ subject to the equality constraint $\sum_{i=1}^N x_i^2 = 1$, we use the substitution $x_1^2 = 1 - \sum_{i=2}^N x_i^2$ and minimize the function

$$f = (1 - \sum_{i=2}^N x_i^2)^{-1} + \sum_{i=2}^N x_i^{-2}$$

by setting the numerators of partial derivatives equal to zero, $\delta f/\delta x_j = 0$, for $j = 2, \dots, N$ to get equations $x_j - (1 - \sum_{i=2}^N x_i^2)^2 x_j^{-3} = 0$. We substitute $x_1^2 = (1 - \sum_{i=2}^2)^2$ and obtain $x_1^2 = x_j^2$ for $j = 2, \dots, N$. We conclude that the desired stationary points are $|x_i| = 1/\sqrt{N}$.

Harmonic mean. We use an example of N capacitors in series with unknown capacities $L_i > 0$. Under the condition that $\sum_{i=1}^N L_i \leq 1$, what values of L_i minimize $\sum_{i=1}^N 1/L_i$ so the resulting total capacity $L_T = \left(\sum_{i=1}^N 1/L_i\right)^{-1}$ is maximal? We use the substitution $x_i = \sqrt{L_i}$ and apply the above example to obtain $L_i = 1/N$ for $i = 1, 2, \dots, N$. An analogous formula could be used for resistors connected in parallel and, generally, in the case of harmonic mean.

Counterexample. Minimize $S(x_1, \ldots, x_N) = \sum_{i=1}^N 1/x_i^2$ outside an open unit ball, that is, subject to $1 \le \sum_{i=1}^N x_i^2$ or $\sum_{i=1}^N x_i^2 - 1 \ge 0$. No local minimum exists at $x_1, x_2, \ldots, x_N$ for which $\sum_{i=1}^N x_i^2 - 1 \ge 0$ because we might consider $2x_1, 2x_2, \ldots, 2x_N$ and obtain a smaller value $\sum_{i=1}^N 1/(2x_i)^2$.

4. Fitting a monotone cubic function

A cubic function has the form $f(x) = ax^3 + bx^2 + cx + d$, the first derivative is $f'(x) = 3ax^2 + 2bx + c$, the second one is $f''(x) = 6ax + 2b$.

To derive a condition under which the cubic function is increasing assuming $a > 0$, we solve for x in $f''(x) = 6ax + 2b = 0$ and obtain the point of inflexion $x_{infl} = -b/(3a)$. The derivative at the point of inflexion is obtained by substituting $-b/(3a)$. We get $f'(x_{infl}) = -b^2/(3a) + c$, which should be nonnegative, $3ac - b^2 \ge 0$.

We use theorem 2.1 and minimize $\sum_{i=1}^T (ax_i^3 + bx_i^2 + cx_i + d - y_i)^2$ under no restrictions and denote the minimal solution as $a_{ls}, b_{ls}, c_{ls}, d_{ls}$. If $3a_{ls}c_{ls} - b_{ls}^2 \ge 0$, we are done.

If $3a_{ls}c_{ls} - b_{ls}^2 < 0$, we could pick any a, b, d, but why not a_{ls}, b_{ls}, d_{ls}, assuming $a_{ls} > 0$. We substitute $c = b_{ls}^2/(3a_{ls})$.

Now we imagine that $K = \sum_{i=1}^T (a_{ls}x_i^3 + b_{ls}x_i^2 + b_{ls}^2 a_{ls}^{-1} x_i/3 + d_{ls} - y_i)^2$. Due to theorem 2.2 we know the level set $L(K)$ of the sum of squares $\sum_{i=1}^T (ax_i^3 + bx_i^2 + cx_i + d - y_i)^2$ is nonempty and compact. From the definition of K it follows that the intersection of the level set $L(K)$ and the preimage of the closed halfline $[0, \infty)$ under a continuous mapping $3ac - b^2$ is not empty, it is closed and bounded, thus compact, and that all means the optimal solution exists. We can now use theorem 1 to help us find it.

We will substitute for $c = b^2/(3a)$ when we minimize the residual sum $\sum_{i=1}^T (ax_i^3 + bx_i^2 + cx_i + d - y_i)^2$ subject to $b^2 = 3ac$ which will enable us to minimize a function of only three variables $S(a, b, d) = \sum_{i=1}^T (ax_i^3 + bx_i^2 + b^2 a^{-1} x_i/3 + d - y_i)^2$ with no restriction.

When we use the following notation

$$M_{x1} = \sum_{i=1}^{T} x_i,\ M_{x2} = \sum_{i=1}^{T} x_i^2,\ \ \ldots, M_{x6} = \sum_{i=1}^{T} x_i^6,\ M_{y1} = \sum_{i=1}^{T} y_i,$$

$$M_{y2} = \sum_{i=1}^{T} y_i^2,\ C_1 = \sum_{i=1}^{T} x_i y_i,\ C_2 = \sum_{i=1}^{T} x_i^2 y_i,\ C_3 = \sum_{i=1}^{T} x_i^3 y_i,$$

the residual sum of squares is

$$S = \sum_{i=1}^{T} (a x_i^3 + b x_i^2 + c x_i + d - y_i)^2 =$$

$$a^2 M_{x6} + b^2 M_{x4} + c^2 M_{x2} + T d^2 + M_{y2} + 2ab M_{x5} + 2ac M_{x4} + 2ad M_{x3}$$

$$-2aC_3 + 2bc M_{x3} + 2bd M_{x2} - 2bC_2 + 2cd M_{x1} - 2cC_1 - 2d M_{y1}.$$

It may be calculated without any further retrieval of the data points once the moments and covariances have been calculated. The formulas for partial derivatives may be simplified in such a way that the original data points are not required either.

We may use the Gauss-Newton method or the gradient method. Unfortunately, we found out that, when we use these methods, overshooting happens slowing down the iterative process.

4. Application to logistic functions

An ordered four-tuple of equidistant points may be written as $x_i = F + Si$, where $i = 0, 1, 2, 3$, $F = x_0$ is the value of the first of them, $S > 0$ is the length of each step. Thus $S = x_1 - x_0 = x_2 - x_1 = x_3 - x_2$.

Let y_0, y_1, y_2, y_3 be four values corresponding to x_0, x_1, x_2, x_3. We are looking for parameters A_0, B_0, C_0, and D_0 of the logistic function for which the equations

$$D_0 + \frac{C_0}{1 + B_0 \exp(A_0 x_i)} = y_i \qquad \text{for} \quad i = 0, 1, 2, 3$$

are satisfied.

We prefer a different notation

$$D_0 + \frac{C_0}{1 + B_0 \exp(A_0 F) \exp(A_0 S i)} = D + \frac{C}{1 + BR^i} = y_i$$

where $B = B_0 \exp(A_0 F)$ and $R = \exp(A_0 S)$.

Theorem 4.1. (Quadratic equation) Let B, C, D, R be given, $R > 0$. The system of equations

$$D + \frac{C}{1 + BR^i} = y_i \qquad \text{for} \quad i = 0, 1, 2, 3$$

for some y_0, y_1, y_2, y_3 has a solution with a positive R if and only if there is a positive solution of the quadratic equation

$$(y_3 - y_2)(y_1 - y_0)R^2 + ((y_2 - y_1)(y_0 - y_3) + (y_3 - y_2)(y_1 - y_0))R + (y_3 - y_2)(y_1 - y_0) = 0$$

Proof. We multiply each equation by the denominator $1 + BR^i$ to obtain

$$D + DBR^i + C = y_i + By_i R^i \qquad \text{for} \quad i = 0, 1, 2, 3.$$

We subtract the equation number zero, $D + DB + C = y_0 + By_0$, from the remaining equations to obtain

$$DB(R^i - 1) = y_i - y_0 + B(y_i R^i - y_0) \qquad \text{for} \quad i = 1, 2, 3.$$

We let $i = 1$ and obtain

$$DB = \frac{y_1 - y_0 + By_1 R - By_0}{R - 1} \quad \text{or} \quad DB(R - 1) = y_1 - y_0 + By_1 R - By_0$$

If we let i=2, the LHS of the equation is $DB(R^2 - 1) = DB(R-1)(R+1)$ we use the equation for $i = 1$ and obtain $DB(R^2 - 1) = (R+1)(y_1 - y_0 + By_1 R - By_0)$

so the equation for $i = 2$ yields

$$(y_1 - y_0 + By_1R - By_0)(R + 1) = y_2 - y_0 + B(y_2R^2 - y_0)$$

and we express B as

$$B = \frac{-(y_1 - y_0)R + y_2 - y_1}{(y_1 - y_2)R^2 + (y_1 - y_0)R}.$$

In the equation for $i = 3$ we substitute for DB using equation for $i = 1$ to obtain

$$\frac{y_1 - y_0 + By_1R - By_0}{R - 1}(R^3 - 1) = (y_3 - y_0 + B(y_3R^3 - y_0))$$

which enables us to write

$$B = \frac{(y_3 - y_0)(R - 1) - (y_1 - y_0)(R^3 - 1)}{(y_1R - y_0)(R^3 - 1) - (y_3R^3 - y_0)(R - 1)}$$

When we use substitution for B we obtained from the equation for $i = 2$, we obtain the following equation

$$\frac{-(y_1 - y_0)R + y_2 - y_1}{(y_1 - y_2)R^2 + (y_1 - y_0)R}\big((y_1R - y_0)(R^3 - 1) - (y_3R^3 - y_0)(R - 1)\big) =$$

$$(y_3 - y_0)(R - 1) - (y_1 - y_0)(R^3 - 1).$$

Writing this equation as a quintic algebraic equation in R is a routine task but finding roots of such an equation is not a routing programming job. That was why we investigated the polynomial a bit more and found out that it is divisible by $R(R - 1)^2$. Once we know it, the equation we are interested in is quadratic.

Note 1: If a quadratic equation has a solution R, we may calculate

$$B = \frac{-(y_1 - y_0)R + y_2 - y_1}{(y_1 - y_2)R^2 + (y_1 - y_0)R},$$

$$D = \frac{y_1 - y_0 + B(y_1 R - y0)}{B(R-1)},$$

$$C = (y_0 - D)(1 + B)$$

To be able to use the formula for B, we have to guarantee that the denominator is not zero. We assume it is equal to zero, $(y_1 - y_2)R + (y_1 - y_0) = 0$, to obtain $R = (y_1 - y_0)/(y_2 - y_1)$. This expression is plugged in the quadratic equation in theorem 4.1. We, of course, want to get rid of division and multiply the expression by $(y_2 - y_1)^2$. Finally, after factorization, we obtain a test of feasibility

$$(y_1 - y_0)(y_2 - y_0)(y_0 y_2 - y_0 y_3 - y_1^2 + y_1 y_2 + y_1 y_3 - y_2^2) = 0.$$

If this equality is true, there is no logistic function satisfiying the interpolation problem.

For the formua for D to be meaningful the numerator in the formula for B has to be nonzero, thus $-(y_1 - y_0)R + y_2 - y_1 = 0$ is not allowed. R may be written as $R = (y_2 - y_1)/(y_1 - y_0)$. Now we plug it in the quadratic equation in theorem 4.1, multiply the equation by $(y_1 - y_0)$ to avoid division and, finally, after factorization we obtain

$$(y_2 - y_0)(y_0 y_2 - y_0 y_3 - y_1^2 + y_1 y_2 + y_1 y_3 - y_2^2) = 0.$$

It is good to notice the coincidence that the left hand side of this equality is contained in the expression for the test of feasibility of the denominator in the formula for B.

When we put together the quadratic equation in theorem 4.1 and the notes following it, we are lead to the following conclusion.

Theorem 4.2. (Logistic Interpolation) Let y_0, y_1, y_2, y_3 be given and let the following hold:

1) $y_0 < y_1 < y_2 < y_3$,

2) $y_0y_2 - y_0y_3 - y_1^2 + y_1y_2 + y_1y_3 - y_2^2 \neq 0$,

3) The discriminant of the quadratic equation

$$(y_3-y_2)(y_1-y_0)R^2+((y_2-y_1)(y_0-y_3)+(y_3-y_2)(y_1-y_0))R+(y_3-y_2)(y_1-y_0) = 0$$

is positive.

Then there is a logistic function $D + C/(1 + BR^x)$ such that

$$D + \frac{C}{1 + BR^i} = y_i \qquad \text{for} \quad i = 0, 1, 2, 3.$$

Note The above theorem 4.1 is oneway by which we mean that the quadratic equation has to be satisfied for any logistic function. It is not true, that for any $y_0, \ldots, y_3$ we get a logistic function. If, for example, $y_0 = y_1$ or $y_2 = y_3$, the leading coefficient is zero and so is the constant term and it follows that the solution of such an equation is $R = 0$ which is useless. We also check the expression for D in note 1 to see that $B = 0$ does not make sense either. One reason is the division by 0, the other reason is that $D + C/(1 + 0 \times R^i)$ cannot be a logistic function. One has to check for such special cases because it would be so easy to get a nonsense value as the output.

Counterexample: Let $y_0 = 0$, $y_1 = 4$, $y_2 = 6$, and $y_3 = 7$. The quadratic equation for R, theorem 4.1, is $4R^2 - 10R + 4 = 0$, its discriminant is 36, thus $R_1 = (10-6)/8 = 0.5$. The numerator of the expression for B is $-(y_1 - y_0)R_1 + y_2 - y_1 = -4 \times 0.5 + 2 = 0$. It means that $y_0, \ldots, y_3$ do not come from any four-parametric logistic function.

When writing and debugging a program, we should be very carefull when using exponential functions because it is so easy to get an overflow but it is much more dangerous to get an unreported underflow. That is why writing the logistic function as

$$d + \frac{c}{1 + b\exp(mx)}$$

is more convenient.

Theorem 4.3. (Uniqueness of logistic function) If a logistic function of x is given, $f(x) = D_1 + C_1/(1 + B_1 R_1^x)$, with $0 < R_1 \neq 1$, then there is presicely one more distintinct set of paramaters $C_2 = -C_1$, $D_2 = D_1 + C_1$, $B_2 = 1/B_1$, and $R_2 = 1/R_1$ such that the two logistic functions are identical as functions,

$$D_1 + \frac{C_1}{1 + B_1 R_1^x} = D_2 + \frac{C_2}{1 + B_2 R_2^x} \quad \text{for all} \quad x.$$

Proof. (Existence) We set $R_2 = 1/R_1$ and write the two expressions as

$$\frac{(D_1 + C_1) + D_1 B_1}{1 + B_1 R_1^x} = \frac{(D_2 + C_2) + D_2 B_2 / R_1^x}{1 + B_2 / R_1^x} = \frac{(D_2 + C_2) R_1^x + D_2 B_2}{R_1^x + B_2},$$

$$\text{thus} \quad \frac{(D_1 + C_1) + D_1 B_1}{1 + B_1 R_1^x} = \frac{(D_2 + C_2) R_1^x / B_2 + D_2}{1 + R_1^x / B_2}.$$

We can see that if we further set $C_2 = -C_1$, $D_2 = D_1 + C_1$, $B_2 = 1/B_1$, the desired equality holds true.

(Uniqueness) Let a logistic function be given with parameters D_1, C_1, B_1, R_1 be given and pick any four equidistant points x_0, x_1, x_2, x_3. Our interpolation theorem guarantees that there are precisely two parameters R_1 and R_2 that allow interpolation at these equidistant points. There is no third option, which finishes the proof.

Interpretation of parameters is the criterion we apply in deciding which of the two ways of presenting the logistic function to use. If we choose $0 < R < 1$, and some $D, C > 0, B > 0$ to define $F(x) = D + C/(1 + BR^x)$, then $\lim F(x) = D$ for $x \to -\infty$, $\lim F(x) = D + C$ for $x \to \infty$, $F(x)$ taking on values between D and $D + C$. This choice is clearly the better one.

The motivation of the following is to determine the sign of the discriminant in the case that the sequence y_0, y_1, y_2, y_3 is increasing and concave. There are α and β such that $y_1 = \alpha + 1\beta$ and $y_2 = \alpha + 2\beta$. We can write $y_0 = \alpha + 0\beta - y$

for some y and $y_3 = \alpha + 3\beta - x$ for some x. Now it is obvious that the sequence of y_i, for $i = 0, \ldots, 3$ is convex if and only if both $0 \leq x$ and $0 \leq y$.

Since y_i appears only in the form of differences $y_i - y_j$, the parameter α is always cancelled. We can write the discriminant as

$$((2\beta-\beta)(-\beta y-\beta(3-x))+(\beta(3-x)-2\beta)(\beta+\beta y))^2-4(\beta(3-x)-2\beta)^2(\beta+\beta y)^2 =$$

$$= \beta^4(2-x)(y+2)(3xy+2x-2y)$$

It is easy to check that under the condition the sequence y_i, $i = 0, \ldots, 3$, is increasing and $x > 0, y > 0$, the factors $(2-x)$ and $(y+2)$ are positive. Thus the sign of the discriminant depends only on the single term $(3xy+2x-2y)$. It is also useful to substitute $y_0 = \alpha - y$, $y_1 = \alpha_\beta$, $y_2 = \alpha + 2\beta$, and $\alpha + 3\beta - x$ in the expression $y_0y_2 - y_0y_3 - y_1^2 - y_2^2 + y_1y_2 + y_1y_3$ obtaining $\beta y - \beta x - xy = 0$ as a condition for feasibility of the formula for B.

We also mention a special case of $y = 0$. Then the discriminant is $\beta^4 4x(2-x)$. It follows that for a positive x the discriminant is positive. The feasibility of the formula for B is checked for $y = 0$ as $-\beta x = 0$ which does not happen if $\beta > 0$ and $x > 0$.

It is now much easier to see that in the practical situations, such as the use of the inverse of the increasing cubic function the nterpolation with the logistic function will sometimes work but sometimes it won't. If we have a set of datapoints, we flip them and calculate the increasing cubic function minimizing the sum of squares. We then take the inverse and try the interpolation by the logistic function using four equidistant points somehow derived from the datapoints. It would look like using the minimum and maximum and two more points in the middle while all the points being equidistant. We call this approach a data-driven interpolation. It may work or or it may not work because the discriminant of the quadratic equation in theorem 4.1 may not be positive or the feasibility of the formula for B may not be satisfied.

If the data-driven interpolation does not work, we use another approach we call a curvature-driven interpolation. This approach is related to the increasing cubic function without any reference to the datapoints it was calculated from. Our first try will be the point of inflection. When the coefficients of a cubic polynomial $ax^3 + bx^2 + cx + d$ are given, we take the second derivative, set it equal to zero and obtain $x_{infl} = -b/(3a)$.

The other point independent of the datapoints directly seems difficult to find but we will see it is not. We checked the behavior of the second derivative of the inverse of the cubic function but the trouble appeared because the denominator could be zero. We concluded that the best choice could be the use of the notion of the radius of curvature

$$R_c = \frac{(1+f'^2)^{3/2}}{|f''|} \quad \text{but we use} \quad \frac{1}{R_c^2} = \frac{f''^2}{(1+f'^2)^3},$$

the denominator of which is always positive, thus the expression is defined correctly. The numerator is zero at the point of inflexion. If we find the point x_{Rc} of a local maximum of $1/R_c^2$, this x_{Rc} is also the point of local minimum of R_c^2.

Such a point will be another point obtained from the shape of the cubic function not dependent on the datapoints directly. If we define an increasing $f(x) = ax^3 + bx^2 + cx + d$, we are interested more in its inverse f^{-1}. In this case the difference $S = |f^{-1}(x_{Rc}) - f^{-1}(x_{inflex})|$ will be used as the length S. As a result, the points at which we interpolate the logistic function may be determined as $x_0 = f^{-1}(x_{inflex}) - S$, $x_1 = f^{-1}(x_{inflex})$, $x_2 = f^{-1}(x_{Rc})$, $x_3 = f^{-1}(x_{Rc}) + S$.

If the interpolation does not work even in this setup, we may try to replace y_0 in such a way that y_0, y_1, y_2 are on a line going through y_1, y_2 which guarantees the existence of logistic interpolation.

We derive the formula for the minimal point of curvature.

$$\frac{1}{R_c^2} = \frac{f''^2}{(1+f'^2)^3} = \frac{(6ax+2b)^2}{(1+(3ax^2+2bx+c)^2)^3} = \frac{4(3ax+b)^2}{(1+(3ax^2+2bx+c)^2)^3}$$

by using the substitution $3ax + b = y$ or $x = (y-b)/(3a)$ making a seemingly hard problem easy

$$\frac{1}{4R_c^2} = \frac{y^2}{(1+(3a\frac{(y-b)^2}{(3a)^2}+2b\frac{y-b}{3a}+c)^2)^3} = \frac{y^2}{(1+\frac{1}{9a^2}(y^2+3ac-b^2)^2)^3}.$$

The second substitution is $y^2 = z$. To simplify the formula we introduce $Q = 3ac - b^2$ so the function to minimize for $z \geq 0$ is

$$\frac{z}{(1+\frac{1}{9a^2}(z+3ac-b^2)^2)^3} = \frac{z}{(1+\frac{1}{9a^2}(z+Q)^2)^3}.$$

We calculate the derivative with respect to z and set its numerator equal to zero to obtain the equation for z

$$5z^2 + 4Qz - (9a^2 + Q^2) = 0.$$

The discriminant is $36(Q^2 + 5a^2) > 0$ which means there are two solutions. It is easy to show that one of the solutions is always negative and the another one is always positive. It makes sense to consider only the positive solution $z = (3\sqrt{(Q^2+5a^2)} - 2Q)/5$, calculate two solutions of $y^2 = z$, and finally calculate x.

5. Fitting positive bi-exponential through convex quartic function

Positive bi-exponential interpolation problem can be solved if and only if the four values defined at four equidistant points are strictly logarithmically convex as was pointed out in Bukac (2013). If some data points are given, we take the logarithm of the dependent variables values and proceed by fitting a strictly convex quartic polynomial function $f(x)$. The bi-exponential function may be obtained by the way of interpolation at four equidistant points and values $y_i = exp(f(x_i))$ because they are obviously strictly logarithmically convex for any four equidistant points x_i.

A quartic function has the form $f(x) = ax^4 + bx^3 + cx^2 + dx + e$, the first derivative is $f'(x) = 4ax^3 + 3bx^2 + cx + d$, and the second one is $f''(x) =$

$12ax^2 + 6bx + c$.

A quadratic function $f''(x) = 12ax^2+6bx+c$ should be nonnegative if $f(x)$ is to be convex. Let us write $g(x) = f''(x) = 12ax^2+6bx+c$ and $g'(x) = 24ax+6b$. The function $g(x)$ takes on its extreme value if $24ax + 6b = 0$ which is at the point $x_0 = -6b/24a = -b/4a$. At this point we have to have $g(x_0) \geq 0$ to make $f(x)$ convex, that is, $12ax_0^2 + 6bx_0 + c \geq 0$ and when we substitute for x_0, we get $12a(-b/4a)^2 + 6b(-b/4a) + c \geq 0$ as a condition for $f(x)$ to be convex. We simplify this condition as $4ac - 3b^2 \geq 0$. Since this condition implies that the point $x_0 = -b/(4a)$ at which $f''(x)$ is zero is unique and $f''(x) > 0$ for $x \neq x_0$, the function $f(x)$ is strictly convex even if $4ac - 3b^2 = 0$.

First we minimize $\sum_{i=1}^{T}(ax_i^4 + bx_i^3 + cx_i^2 + dx_i + e - y_i)^2$ with no restrictions. We denote the optimal solution as $a_{ls}, b_{ls}, c_{ls}, d_{ls}, e_{ls}$. If $4ac - 3b^2 \geq 0$, we are done.

If $4a_{ls}c_{ls} - 3b_{ls}^2 < 0$, we could pick any a, b, d, e but why not $a_{ls}, b_{ls}, d_{ls}, e_{ls}$ assuming $a_{ls} > 0$. We substitute $c_{ls} = 3b_{ls}^2/(4a_{ls})$.

Now we take $K = \sum_{i=1}^{T}(a_{ls}x_i^4 + b_{ls}x_i^3 + 3b_{ls}^2/(4a_{ls})x_i^2 + d_{ls}x_i + e_{ls} - y_i)^2$. Theorem 2.2 says the level set $L(K)$ of the sum of squares $\sum_{i=1}^{T}(ax_i^4 + bx_i^3 + cx_i^2 + dx_i + e - y_i)^2$ is compact. The intersection of the level set $L(K)$ and the preimage of the closed halfline $[0, \infty)$ under a mapping $4ac - 3b^2$ is not empty. It is closed and bounded and it follows it is compact and the optimal solution exists. We may now use teorem 2.1 and proceed in the same way as above in the case of the increasing cubic function.

The interpolation by a positive bi-exponential function $a\exp(bx)+c\exp(dx)$, $a > 0$, $c > 0$ is studied in Bukac (2013). It exists if and only if the four values at equidistant points are logarithmically convex. It means that the condition $4ac - 3b^2 > 0$ is of course sufficient but if $4ac - 3b^2 = 0$, we rely on the fact that if the second derivative is positive except for one point at which it is zero, the function is strictly convex.

6. Application to Gomperz function

An ordered four-tuple of equidistant points may be written as $x_i = F + Si$, where $i = 0, 1, 2, 3$, $F = x_0$ is the value of the first of them, S is the length of each step, $S = x_1 - x_0 = x_2 - x_1 = x_3 - x_2$,

Let y_0, y_1, y_2, y_3 be four values corresponding to x_0, x_1, x_2, x_3. We are looking for parameters D, C, A, and B of the Gomperz function.

Theorem 6.1. (Gomperz Interpolation) If y_0, y_1, y_2, y_3 are given, parameters D, C, A, and B for which $D + CA^{B^i} = y_i$ for $i = 0, 1, 2, 3$ hold true, then

$$\left(\frac{\ln\frac{(y_2-D)}{(y_0-D)}}{\ln\frac{(y_1-D)}{(y_0-D)}}\right)^2 - \frac{\ln\frac{(y_2-D)}{(y_0-D)}}{\ln\frac{(y_1-D)}{(y_0-D)}} - \frac{\ln\frac{(y_3-D)}{(y_0-D)}}{\ln\frac{(y_1-D)}{(y_0-D)}} + 1 = 0$$

Proof. We write down the equations as

$CA = y_0 - D$, $CA^B = y_1 - D$, $CA^{B^2} = y_2 - D$, $CA^{B^3} = y_3 - D$

and take the logarithms

$\ln C + \ln(A) = \ln(y_0 - D)$, $\ln C + B\ln(A) = \ln(y_1 - D)$,

$\ln C + B^2\ln(A) = \ln(y_2 - D)$, $\ln C + B^3\ln(A) = \ln(y_3 - D)$.

We calculate the differences to get rid of C,

$$B\ln(A) - \ln(A) = \ln(y_1 - D) - \ln(y_0 - D) = \ln\frac{(y_1 - D)}{(y_0 - D)}$$

$$B^2\ln(A) - \ln(A) = \ln(y_2 - D) - \ln(y_0 - D) = \ln\frac{(y_2 - D)}{(y_0 - D)}$$

$$B^3\ln(A) - \ln(A) = \ln(y_3 - D) - \ln(y_0 - D) = \ln\frac{(y_3 - D)}{(y_0 - D)}$$

Now we calculate the ratios to eliminate A,

$$\frac{B^2\ln(A) - \ln(A)}{B\ln(A) - \ln(A)} = \frac{\ln\frac{(y_2-D)}{(y_0-D)}}{\ln\frac{(y_1-D)}{(y_0-D)}} \quad \text{and} \quad \frac{B^3\ln(A) - \ln(A)}{B\ln(A) - \ln(A)} = \frac{\ln\frac{(y_3-D)}{(y_0-D)}}{\ln\frac{(y_1-D)}{(y_0-D)}}$$

which may be rewritten as

$$B = \frac{\ln\frac{(y_2-D)}{(y_0-D)}}{\ln\frac{(y_1-D)}{(y_0-D)}} - 1 \quad \text{and} \quad B^2 + B + 1 = \frac{\ln\frac{(y_3-D)}{(y_0-D)}}{\ln\frac{(y_1-D)}{(y_0-D)}}$$

Substitution leads us to

$$\left(\frac{\ln\frac{(y_2-D)}{(y_0-D)}}{\ln\frac{(y_1-D)}{(y_0-D)}}-1\right)^2+\frac{\ln\frac{(y_2-D)}{(y_0-D)}}{\ln\frac{(y_1-D)}{(y_0-D)}}=\frac{\ln\frac{(y_3-D)}{(y_0-D)}}{\ln\frac{(y_1-D)}{(y_0-D)}}.$$

Such a theorem shows that the solution of interpolation equations may be obtained if we can find a point at which a function of one variable is zero but it does not give us any answer as to when the solution exists or not or how many solutions there are. There are examples in which the equation has two solutions but we don't care about such cases leaving such questions open.

We write the equation as

$$\left(\frac{\ln\frac{y_2-y_0+y_0-D}{y_0-D}}{\ln\frac{y_1-y_0+y_0-D}{y_0-D}}\right)^2-\frac{\ln\frac{y_2-y_0+y_0-D}{y_0-D}}{\ln\frac{y_1-y_0+y_0-D}{y_0-D}}-\frac{\ln\frac{y_3-y_0+y_0-D}{y_0-D}}{\ln\frac{y_1-y_0+y_0-D}{y_0-D}}+1=0$$

to make it convenient for a substitution $z_0=0$, $z_1=y_1-y_0$, $z_2=y_2-y_0$, $z_3=y_3-y_0$, $x=y_0-D$ leading to an equivalent equation

$$\left(\frac{\ln\frac{z_2+x}{x}}{\ln\frac{z_1+x}{x}}\right)^2-\frac{\ln\frac{z_2+x}{x}}{\ln\frac{z_1+x}{x}}-\frac{\ln\frac{z_3+x}{x}}{\ln\frac{z_1+x}{x}}+1=0.$$

Finding roots of such an equation seems to be beyond our ability and, as a consequence, we try to study a case in which the values of z_i are increasing and convex and the first three values, z_0, z_1, z_2 are on a line, z_3 is below that line. It is the same as setting $z_0=0$, $z_1=b$, $z_2=2b$, $z_3=3b-q$ and solve for x. Our assumption is that $b>0$ and $z_3=3b-q>2b=z_2$.

We can imagine an s-function, such as a four-parametric logistic function, for which z_1 corresponds to its value at an inflection point, $z_2>z_1$ may correspond to the point at which the third derivative of the logistic function is zero. The point of maximal curvature would be difficult to calculate. z_0 is equal to $z_1-(z_2-z_1)$, and z_3 is the value that makes the sequence increasing and convex. The assumption about $z_0=z_1-(z_2-z_1)$ may be satisfied by simply defining z_0 that way. It obviously means some kind of symmetry that may also be achieved when using the four-parametric logistic function.

We can now write the equation as

$$\left(\frac{\ln\frac{2b+x}{x}}{\ln\frac{b+x}{x}}\right)^2 - \frac{\ln\frac{2b+x}{x}}{\ln\frac{b+x}{x}} - \frac{\ln\frac{3b-q+x}{x}}{\ln\frac{b+x}{x}} + 1 = 0,$$

$$\left(\frac{\ln\frac{2+x/b}{x/b}}{\ln\frac{1+x/b}{x/b}}\right)^2 - \frac{\ln\frac{2+x/b}{x/b}}{\ln\frac{1+x/b}{x/b}} - \frac{\ln\frac{3-q/b+x/b}{x/b}}{\ln\frac{1+x/b}{x/b}} + 1 = 0.$$

We substitute $R = x/b$ and $Q = q/b$ to obtain a formula for Q.

$$\left(\frac{\ln\frac{2+R}{R}}{\ln\frac{1+R}{R}}\right)^2 - \frac{\ln\frac{2+R}{R}}{\ln\frac{1+R}{R}} - \frac{\ln\frac{3-Q+R}{R}}{\ln\frac{1+R}{R}} + 1 = 0,$$

$$Q = 3 + R - R\exp(\frac{(\ln\frac{2+R}{R})^2}{\ln\frac{1+R}{R}} - \ln\frac{2+R}{R} + \ln\frac{1+R}{R}),$$

$$Q = 3 + R - \frac{1+R}{2+R}R\exp\left(\frac{\ln^2(1+2/R)}{\ln(1+1/R)}\right).$$

It is not our assignment to calculate Q as a function $Q(R)$ of R, because we want to calculate the inverse of $Q(R)$, that is, some $Q_0 \in (0,1)$ is given and we want to determine which R_0, if any, satisfies the equation above.

To show that for any $Q \in (0,1)$ an $R \in (0,\infty)$ exists satisfying the above equations we calculate two limits. One for $R \to 0+$ and one for $R \to \infty$.

Theorem 6.2.

$$\lim_{R\to 0+} Q(R) = \lim_{R\to 0+} 3 + R - \frac{1+R}{2+R}R\exp\left(\frac{\ln^2(1+2/R)}{\ln(1+1/R)}\right) = 1.$$

Proof. Substitution $S = 1/R$ and the continuity of exponential function imply

$$\lim_{S\to\infty} \exp\left(\frac{(\ln(1+2S))^2}{\ln(1+S)} - \ln(S)\right)$$

$$\exp\left(\lim_{S\to\infty}\left(\frac{(\ln(1+2S))^2 - \ln(S)\ln(1+S)}{\ln(1+S)}\right)\right.$$

To show that the limit of the expression in the big parentheses is finite as S goes to ∞ we use the formula $ab - cd = a(b - d) + d(a - c)$

$$\frac{(\ln(1+2S))^2 - \ln(S)\ln(1+S)}{\ln(1+S)} =$$

$$\frac{\ln(1+2S)(\ln(1+2S) - \ln(1+S)) + \ln(1+S)(\ln(1+2S) - \ln(S))}{\ln(1+S)} =$$

$$\frac{\ln(1+2S)}{\ln(1+S)} \ln \frac{1+2S}{1+S} + \frac{\ln(1+S)}{\ln(1+S)} \ln \frac{1+2S}{S} \to \ln 4$$

Thus

$$\lim_{R\to 0+} Q(R) = 3 + \lim_{R\to 0+} \left(R - \frac{1+R}{2+R} \exp(\ln 4) \right) = 3 - \frac{1}{2} \times 4 = 1.$$

This result coincides with the fact that the values of Q have to be less than zero. The next step is to show that the limit of $Q(R)$ is zero as $R \to \infty$.

Theorem 6.3.

$$\lim_{R\to\infty} Q(R) = \lim_{R\to\infty} \left(3 + R - \frac{1+R}{2+R} R \exp\left(\frac{\ln^2(1+2/R)}{\ln(1+1/R)} \right) \right) = 0.$$

Proof. The calculation of this limit is more tedious. First we apply the substitution $S = 1/R$ to be able to use a power series representation of the functions involved.

$$\lim_{R\to\infty} \left(3 + R - \frac{1+R}{2+R} R \exp\left(\frac{\ln^2(1+2/R)}{\ln(1+1/R)} \right) \right) =$$

$$\lim_{S\to 0+} \left(3 + \frac{1}{S} - \frac{1+S}{S(2S+1)} \exp\left(\frac{\ln^2(1+2S)}{\ln(1+S)} \right) \right) =$$

We calculate the Taylor series

$$\frac{1+S}{(2S+1)} \exp\left(\frac{\ln^2(1+2S)}{\ln(1+S)} \right) = 1 + 3S - S^3 + (5S^4)/2 + \dots,$$

divide it by S and subtract from $3 + 1/S$ to obtain

$$S^2 - 5S^3/2 + 55S^4/12 + \dots$$

The calculations would be tedious if it were not for symbolic computations. We would have to use the power series representation of $\ln(1 + S)$ and several theorems about products of series, e.g. the Cauchy product definition and his theorem on the product convergence, the theorem on composition of power series which includes the division of series.

Theorem 6.2 together with theorem 6.3 together not only imply that for any $Q_0 \in (0, 1)$ there exists a solution of the equation $Q(R) = 0$, they can be used to calculate it. Theorem 6.2 says that for $R_0 = 0$ $Q(R_0) > Q_0$. Now, due to theorem 6.3, we can find an R_1 for which $Q_0 > Q(R_1)$ numerically. This can be done by taking just the first term in the series representation in Theorem 6.3 and a reasonable upper bound is obtained as $S_L = \sqrt{Q_0}$ or $R_u = 1/\sqrt{Q_0}$. We may continue by using the method of bisection starting with the interval $(0, R_u)$.

7. Two examples

One example is from Kennedy (2020), figure 2, where the horizontal axis indicates the time, vertical axis indiates the number of infected. The time starts at zero and increases by one, the number of infected is 4 times 1, 7 times 2, 4, 5, 6, 6, 7, 7, 8, 8, 8, 9, 10, 10, 10, 11, 12, 13, 14, 14, 15, 16, 17, 15 times 18, 19 times 19, and 13 times 20. In the very beginning we consider the inverse and fit the cubic function. The parameters are $a = 0.0468$, $b = -1.293$, $c = 11.223$, $d = -9.815$, yelding the sum of squares of deviation $SS = 2072$. When we minimize the cubic function under the restriction $c = b^2/(3a)$, the starting parameters are $a = 0.0468$, $b = -1.293$, $c = 11.918$, $d = -9.815$ yielding $SS = 11413$. After several iterations we obtain $a = 0.0377$, $b = -1.0185$, $c = 9.169$, $d = -7.6195$, $SS = 2208$. This is an increasing cubic function and we can define its inverse. We use the inflection point and a point at which the curvature is maximal to define the four equidistant nodes needed for interpolation. $x_0 = 10.522$, $x_1 = 19.895$, $x_2 = 29.267$, and $x_3 = 38.639$. We now calculate the inverse of the increasing cubic funtion to give us the values at those nodes $y_0 = 2.715$, $y_1 = 9.002$, $y_2 = 15.289$, and $y_3 = 16.924$. The discriminant of the quadratic equation in theorem 4.1 is $D = 5827$, therefore the interpolation problem has a solution $D = 0.7990$, $C = 16.4065$, $B = 73.3015$, and $A = -0.21587$, $SS = 231.8$. for parameters of the interpolating logistic function $D + C/(1 + B\exp(Ax))$. After several iterations we obtain the minimal sum of square $SS = 28.8$ for $D = 0.1271$, $C = 19.3340$, $B = 27.2096$, and $A = -0.14542$.

We proceed to calculate the parameters of the Gomperz function by way of interpolation. We take the inflection point $x_1 = 22.7176$, add the points at which the third derivative is zero, that is, $x_0 = 13.6613$ and $x_2 = 31.7738$. We also get $x_3 = x_2 + (x_2 - x_1) = 40.8301$. The values of the minimizing logistic function at these points are respectively $y_0 = 4.213$, $y_1 = 9.794$, $y_2 = 15.375$, and $y_3 = 18.166$. The requirements for the equation in theorems 6.1, 6.2, 6.3 are satisfied and its solution yields $D = 3.101$, $C = 16.724$, $B = 0.887$, and $A = 8.87e - 7$, with $SS = 63.2$. After several iterations we get parameters $D = 1.8711$, $C = 17.6756$ $B = 0.8871$, and $A = 2.67e - 6$ of the function $D + CA^(B^x)$, $SS = 42.4$.

This second example is about heart rate depending on exercize. The time as an independent variable starts from one, increases by one and ends at fifteen. The corresponding heart rates are 70, 70, 70, 71, 85, 105, 115, 120, 125, 127, 130, 133, 135, 137, 136. We formally swap the dependent and independent variables and use the least squares method to calculate the best fitting cubic function. The resulting cubic function is increasing and its inverse is well defined. The inflection point is $x_1 = 5.766$, but the point of maximal curavature is at -156.24. This is way lower than the minimum $x_{min} = 1$ of all the values of independent variable. Practicioners know that polynomials are very flexible when we use them for approximations but at the price of being no good for extrapolation. That is why we prefer to use a value within the interval (x_{min}, x_{max}). This way we set the distance between the interpolation nodes to be $d = 3(x_1 - x_{min})/4$, thus $x_0 = x_1 - d$, $x_2 = x_1 + d$, and $x_3 = x_1 + 2d$. In our case those are $x_0 = 2.1914$, $x_1 = 5.7657$, $x_2 = 9.3400$, and $x_3 = 12.9143$. The corresponding values of the inverse cubic function are $y_0 = 69.350$, $y_1 = 97.451$, $y_2 = 125.552$, and $y_3 = 134.152$. We are now ready to calculate the parameters of the interpolating logistic function $D = 58.901$, $C = 77.101$, $B = 19.866$, and $A = -0.5184$, giving $SS = 239.4$ But after several iterations we get $D = 65.904$, $C = 68.101$, $B = 90.772$, and $A = -0.7608$ as parameters of $D + C\exp(\exp(x\ln(B))\ln(A))$ giving $SS = 158.4$.

The reader may be encouraged to plot the graphs of all these functions to see the data points and compare them with their approximations.

8. On a method of Zhang

We will discuss the application of the method of Zhang (2020) to finding initial parameters of the logistic function. We will use theorem 4.1 and the remarks that follow it. The basic idea suggests picking all the possible quadruples of the independent variable, but theorem 4.1 provides us with a method to facilitate solving the interpolation problem only for equally spaced nodes, not for arbitrary nodes.

In the first example, we generated all 1008 quadruples. Each quadruple was tested for feasibility, unfeasible quadruple was discarded. In the 260 cases of feasibility, we calculated the required parameters. When this was done, we calculated the means as $\bar{D} = 0.2678$, $\bar{C} = 18.6812$, $\bar{B} = 92.006e + 9$, $\bar{A} = -0,20679$. One can easily see that $\bar{B}$ would not be the right choice as an initial parameter because we can say that now that we know what the approximate values of such initial estimates should look like. The reason for what happened is that in some cases the values of B were extremely high, which makes the value of $\bar{B}$ very high too. Even though the method of Zhang is appreciated, this is generally a serious drawback.

We avoid this kind of trouble by using the median because it is less sensitive to outliers, $\tilde{D} = 0.7789$, $\tilde{C} = 18.1423$, $\tilde{B} = 47.086$, $\tilde{A} = -0.1655$. Not only do such initial values look reasonable, but these values give the sum of squares equal to 40.0, less than $SS = 231.8$ which is what our initial values based on the inverse of the increasing cubic yield.

In the second example, we generated 32 quadruples but only 17 of them were feasible. We got the means $\bar{D} = 104.48$, $\bar{C} = 27.078$, $\bar{B} = 695785$, $\bar{A} = -1.07$ giving us $SS = 7399$. It is obvius that such parameters are way off. The medians are $\tilde{D} = 69.991$, $\tilde{C} = 50.202$, $\tilde{B} = 733.7$, $\tilde{A} = -0.9624$ giving us $SS = 2176$. Initial values obtained with the inverse of inreasing cubic give $SS = 158.4$ which happens to be lower than the sum of squares with initial values obtained by the Zhang method.

The method of Zhang is general in the sense that we can try to apply it to any type of nonlinear regression. Unfortunately, our ability to solve the equations defined by the interpolation problem is very limited. We have to be able to decide if the solution exists or not and how many solutions we have. If the unique solution does exist, it may be, in some cases, very far from the initial value we are looking for and may affect the resulting mean.

We believe that our approach is more stable and visually pleasing because we can easily see how the approximation by the inverse of the increasing cubic function works in the case that something perhaps went wrong.

Our approach is based on moving from one S-function to another one or moving from one convex function to another convex function. It is us who chooses the nodes for interpolation in such a way that the equations we obtain have precisely one solution. The use of this idea is limited in this sense.

9. Conclusion

An interpolation approach serves only the purpose of finding initial values of parameters in nonlinear regression. Various approaches are sometimes used, but other times no other method is available. The cost of extra calculations of coefficients of polynomials is negligible with the exception of an iterative process when we want to use an increasing cubic function or convex quartic function but the least squares method alone does not suffice. We have presented the four-parameter logistic, positive bi-exponential, and Gomperz functions just because we have shown how to handle such situations.

The days when textbooks offered guessing the initial values of parameters by a fluke belong to the past. Especially when measurements are fully automated and guessing the parameters would be prohibitive.

There are, of course, methods of random search that are able to deliver optimal solutions, but they have to start somewhere anyway.

We have presented only several types of functions. Of course, there could be many more types of functions for which a polynomial regression and interpolation could be used to estimate initial values of parameters but we do not discuss those because they do not require the use of our minimization method. Those could be, as an example, Michaelis-Menten function $bx/(1+ax)$, generalized as $c + bx/(1+ax)$, sum of linear and exponential functions $c + b\exp(ax)$ or $d + cx + b\exp(ax)$, and many other types of functions for which the solution of interpolation equations is not straightforward.

References

Bukac, J., (2001), Polynomials associated with exponential regression, Applicationes Mathematicae, Volume 28, Issue 3, pp 247-255.

Bukac, J., (2013), Positive bi-exponential interpolation, Journal of Interpolation and Approximation in Scientific Computing, (2013), 1-6.

Kennedy, G., (2020), Flattening the curve, The College Mathematics Journal, 51:4, p.254-259.

Nievergelt, Y., On the existence of best Mitscherlich, Verhulst, and West growth curves for generalized least-squares regression, Journal of Computational and Applied Mathematics, (2013), Volume 248, pp 3146.

Zhang, G., Allaire, D., Cagan, J., (2020) Taking the guess work out of the initial guess: a solution interval method for least-squares parameter estimation in nonlinear models, Journal of Computing and Information Science in Engineering, 21 (2), p 21011-1.