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On the existence of best Mitscherlich, Verhulst, and West growth curves for generalized least-squares regression

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ABSTRACT

Practical difficulties arise in fitting Mitscherlich, Verhulst, or West growth curves to data. Obstacles include divergent iterations, negative values for theoretically positive parameters, or the absence of any best-fitting curve. An analysis reveals that such obstacles occur near removable singularities of the objective function to be minimized for the regression. Such singularities lie at the transition to different types of curves, including exponentials, hyperbolae, lines, and step functions. Removing the singularities fits all such curves into a connected compactified topological space, which guarantees the existence of a global minimum for the continuous objective function, and which also provides a smooth and transparent transition from one type of curve to another.

0. Introduction

This article determines the existence, or the absence, of "best" shifted exponential curves (1), called *Mitscherlich's laws*, relative to weighted or generalized (correlated) least squares. Also called *asymptotic regression* [1–3], the problem consists in fitting to data points $(t_1, q_1), \ldots, (t_N, q_N)$ the parameters A, B, and C in Eq. (1):

$$q = A \cdot e^{C \cdot t} + B. \tag{1}$$

Eq. (1) describes all phenomena modeled by the first-order linear differential equation

$$\frac{dq}{dt} = C \cdot (q - B) \tag{2}$$

with constant coefficients B and $C \neq 0$, and hence also by Bernoulli equations [4, pp. 58–59]. For instance, West's recent model of ontogenetic growth of organisms [5],

$$\frac{dm}{dt} = a \cdot (m^{3/4} - m/M^{1/4}), \tag{3}$$

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is a Bernoulli equation, which reduces to Eq. (2) for $q := m^{1/4}$:

$$\frac{d}{dt}(m^{1/4}) = \frac{-a}{4 \cdot M^{1/4}} \cdot (m^{1/4} - M^{1/4}), \tag{4}$$

with $B = M^{1/4}$ and $C = -a/(4 \cdot M^{1/4})$, or $M = B^4$ and $a = -4 \cdot B \cdot C$. The solution

$$m^{1/4}(t) = M^{1/4} + (m_0^{1/4} - M^{1/4}) \cdot e^{a \cdot (t_0 - t)/(4 \cdot M^{1/4})} \tag{5}$$

is Mitscherlich's law (1) with $A = (m_0^{1/4} - M^{1/4}) \cdot e^{a \cdot t_0/(4 \cdot M^{1/4})}$, or $m_0^{1/4} = A \cdot e^{-C \cdot t_0} + B$. If $A, B, q > 0$, then $K := 1/B$, $D := \ln(A/B)$, and $y := 1/q$ give a *Verhulst* curve (6):

$$y = \frac{K}{1 + e^{D + C \cdot t}}. \tag{6}$$

Applications of Mitscherlich, West, and Verhulst curves (1), (5) and (6) include, for instance,

1. agronomy, to evaluate and optimize the efficiency of fertilizers [2,3];
2. chemical kinetics [6, p. 20, Eq. (29)], [7, p. 993], [8, p. 65], [9,10], [11, p. 393, Eq. (1)], to identify the type of chemical reaction occuring in experiments;
3. population growth [12–23];
4. physiology, to model the growth over time of plants and animals [24,5], or individual organs, for example, wing span [25, p. 808];
5. rheology [26].

Hence arises the need to estimate the parameters A, C, and B or K, that fit the data best relative to generalized (ordinary, weighted, or correlated) least squares [27]. General theorems already provide sufficient conditions on the monotonicity and convexity of the data for the existence of a weighted least-squares Mitscherlich curve [28] or necessary and sufficient conditions for a weighted least-squares Verhulst curve [29]. Examples show that there are data that fail to satisfy the hypothesis of such theorems and for which no best-fitting curves exist [30–32,28]. Alternatively, computed solutions yield negative values for theoretically positive parameters:

> A successful fit results in positive values for $[K]$ and $[-C]$ but data which deviate too far from the model result in either a fit to a curve with a negative $[K]$ or negative $[-C]$ [18, p. 94, Section 2].

The present analysis . shows that such situations reflect features of the modeled phenomenon. For instance, replacing the Verhulst equation (6) by the modeling differential equation

$$\frac{dy}{dt} = \frac{C}{K} \cdot y \cdot (K - y). \tag{7}$$

L. J. Reed and J. Berkson [20, p. 765] had already pointed out that the solution curve y becomes a hyperbola if $A \cdot B < 0$ and C/K remains constant while K tends to 0, though they did not mention the possibility that the solution becomes a Malthusian [33, II.7] exponential growth curve as K diverges to $+\infty$. In either case C/K need not remain constant but need only converge to a limit. A similar situation occurs as A tends to 0. Neither did Reed and Berkson [20] mention why or how parameters would diverge, converge to anything, or change in the first place. Indeed, they selected the type of curve to be fitted *before* starting the regression, which never failed for their examples [20, pp. 769–779]. The present analysis shows that the limits happen to lie exactly at a removable singularity of the objective function for the generalized least-squares regression.

Specifically, the present work first extends the literature from weighted to potentially correlated least squares with potentially non-invertible covariance matrices, second reveals that the correlated least-squares objective function extends analytically to the special case of straight lines and continuously to step functions, and third extends such results to West's ontogenetic growth curves.

The strategy adopted here consists of fixing one parameter, C for Mitscherlich's law (1), and in analyzing the explicit formulas for the solutions of the generalized *linear* least-squares regression with the other two parameters, A and B, in terms of the fixed parameter C.

To this end, Sections 1 and 2 are akin to [34, Ch. 4] but extended to generalized least squares with semi scalar-products. Section 1 summarizes *motivations* for generalized least squares from probability or statistics. Section 2 summarizes *solutions* for generalized least squares using only linear algebra, without probability or statistics. Section 3 applies the previous sections to regressions for Mitscherlich's law (1) parametrized by C. Using [35], Section 4 generalizes the previous sections further to handle singular covariance matrices. Section 5 establishes sufficient criteria for a best-fitting Mitscherlich's law (1) to be the reciprocal of a Verhulst curve (6). Section 6 presents examples with real data.

1. Notation for generalized least-squares

Though the numerical solution of least-squares problems proceeds more accurately with other algorithms [36–38], the present analysis and resolution of singularities use explicit formulas for the solutions. Moreover, examples from Section 6