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Applications of the Discrete Least Squares 3-Convex Fit To Sigmoid Data

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***Abstract*—Let data of a univariate process be given. If the data are related by a sigmoid curve, but the sigmoid property has been lost due to the errors of the measuring process, then the least sum of squares change to the data that provides nonnegative third divided differences may be required. It is a structured quadratic programming calculation, which is solved very efficiently by a special least squares algorithm that takes into account the form of the constraints. The algorithm is outlined and two examples on real economic data are considered. The first is an application to the U.S.A. renewable energy consumption data during the period 1980-2010, which exhibit a sigmoid pattern. The second is an application to technological substitutions among the PDP computers to the VAX computers between the years 1984 and 1991. The results are briefly analyzed and the modeling capability of the method is demonstrated.**

***Index Terms*—3-convex sigmoid, divided difference, renewable energy consumption, least squares data fitting, technological substitution**

I. Introduction

Applications of sigmoid curves are common in science, technology, economics and medicine [1, 7, 14, 17, 25]. For, example, a biological growth follows a sigmoid curve or logistic curve, which best models growth and decline over time [16]. Since the adoption of technology and technology-based products is similar to biological growth, many growth curve models have been developed to forecast the penetration of these products with the logistic curve and the Gompertz curve the most frequently referenced [20, 21]. Other examples with the sigmoid assumption come from economic substitution [22], from production and distribution cost data for analysis of operations of a firm [9], from decision making [13] and from image processing [11], for instance.

We consider the general problem where measurements from a sigmoid process are to provide estimation to an underlying sigmoid function $f(x)$, but the measurements include random errors. If it is known that the data can be modeled by growth curves or sigmoid curves or that they allow a certain sigmoid form that depends on a few parameters rather than having to estimate unknown function values, then the analysis is usually simplified by existing parametric methods [6, 15, 27]. In this paper we outline an algorithm for estimating points on a sigmoid curve *of unspecified parametric form, when the process is subject to increasing marginal returns or subject to diminishing marginal returns*. The algorithm may be applied to a variety of situations, where the analyst takes the view that the "sigmoid" property of the (unknown) underlying function has been lost due to errors in the data.

Let $\{\phi_i : i = 1, 2, \ldots, n\}$ be a sequence of measurements (data) of smooth function values $\{f(x_i) : i = 1, 2, \ldots, n\}$, where the abscissae $\{x_i : i = 1, 2, ..., n\}$ are in strictly ascending order, and let $\phi[x_{i-1}, x_i, x_{i+1}, x_{i+2}]$ designate the third divided difference relative to the four abscissae x_{i-1}, x_i, x_{i+1} and x_{i+2}:

$$\begin{aligned}\phi[x_{i-1}, x_i, x_{i+1}, x_{i+2}] &= \\ &\frac{\phi_{i-1}}{(x_{i-1}-x_i)(x_{i-1}-x_{i+1})(x_{i-1}-x_{i+2})} \\ &+\frac{\phi_i}{(x_i-x_{i-1})(x_i-x_{i+1})(x_i-x_{i+2})} \\ &+\frac{\phi_{i+1}}{(x_{i+1}-x_{i-1})(x_{i+1}-x_i)(x_{i+1}-x_{i+2})} \\ &+\frac{\phi_{i+2}}{(x_{i+2}-x_{i-1})(x_{i+2}-x_i)(x_{i+2}-x_{i+1})}, \\ &i = 2, 3, ..., n-2. \qquad (1)\end{aligned}$$

The sequence of the third differences $\{\phi[x_{i-1}, x_i, x_{i+1}, x_{i+2}],\ i = 2, 3, \ldots, n-2\}$ is an appropriate description of the third derivative of $f(x)$ and if the data are error free, then the number of sign changes in (1) is no greater than the number of sign changes in the third derivative of $f(x)$. However, due to errors of measurement it is possible that the sequence $\{\phi[x_{i-1}, x_i, x_{i+1}, x_{i+2}],\ i = 2, 3, \ldots, n-2\}$ contains far more sign changes than the sequence $\{f[x_{i-1}, x_i, x_{i+1}, x_{i+2}],\ i = 2, 3, \ldots, n-2\}$.

We assume that no sign changes occur in the third derivative of the underlying function. Thus, if the third divided differences of the data show sign irregularities, we take the view of [5] that some smoothing should be possible in order to recover the missing property. Specifically, we address the problem of making least changes to the data subject to nonnegative third divided differences. We define "least change" with respect to the L_2 norm, which means that we seek a vector $\underline{y}$ that minimizes the sum of the squares

$$\Phi(\underline{y}) = \sum_{i=1}^{n}(y_i - \phi_i)^2 \qquad (2)$$

subject to the constraints

$$y[x_{i-1}, x_i, x_{i+1}, x_{i+2}] \geq 0,\ i = 2, 3, \ldots, n-2, \qquad (3)$$

where we regard the data $\{\phi_i :\ i = 1, 2, \ldots, n\}$ and the best fit $\{y_i :\ i = 1, 2, \ldots, n\}$ as components of the $n-$vectors $\underline{\phi}$ and $\underline{y}$, respectively. Notice that in the title of the paper we use the term "discrete 3-convex fit" for the best fit, because of its association with the third divided differences

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(cf. [12]:p.23, [26]). In order to simplify our notation, we denote the constraint normals with respect to $\underline{y}$ by $\{\underline{a}_i : i = 2, 3, \ldots, n-2\}$ and we set $y[x_{i-1}, x_i, x_{i+1}, x_{i+2}] = \underline{y}^T \underline{a}_i$, for $i = 2, 3, \ldots, n-2$. It is important to note that the constraints on $\underline{y}$ are linear and have linearly independent normals. Also, the second derivative matrix with respect to $\underline{y}$ of the objective function (2) is twice the unit matrix. Thus, the problem of minimizing (2) subject to (3) is a strictly convex quadratic programming problem that has a unique solution. There exist several general algorithms (see, for example, [8], [19]) and two special algorithms [2], [4] that may be applied to this problem after appropriate modifications.

Since the ith third divided difference can be expressed as the difference of two consecutive second divided differences divided by the difference between those arguments which are not in common (see, for example, [23])

$$y[x_{i-1}, x_i, x_{i+1}, x_{i+2}] = \frac{1}{(x_{i+2} - x_{i+1})} \left(y[x_i, x_{i+1}, x_{i+2}] - y[x_{i-1}, x_i, x_{i+1}] \right) \quad (4)$$

the constraints (3) imply the inequalities

$$y[x_i, x_{i+1}, x_{i+2}] \geq y[x_{i-1}, x_i, x_{i+1}], \; i = 2, 3, \ldots, n-2. \quad (5)$$

The essential concept in restrictions (5) is process subject to non-decreasing marginal returns, marginal return being the term used for the change in return due to an increase in x. Criterion (3) or the equivalent criterion (5) provides a property that allows a sigmoid shape for the underlying function, as we explain next. Indeed, without loss of generality we assume that there is an index k inside the interval $[2, n-2]$ such that $\{y[x_i, x_{i+1}, x_{i+2}] \leq 0, \; i = 1, 2, \ldots, k-2\}$ and $\{y[x_i, x_{i+1}, x_{i+2}] \geq 0, \; i = k-1, k, \ldots, n-2\}$. It follows that there is a concave region of the fit on $[x_1, x_k]$ and a convex region on $[x_{k-1}, x_n]$. In the concave region, the fit exhibits non-increasing returns

$$y[x_i, x_{i+1}] \geq y[x_{i+1}, x_{i+2}], \; i = 1, 2, \ldots, k-2$$

and in the convex region exhibits non-decreasing returns

$$y[x_i, x_{i+1}] \leq y[x_{i+1}, x_{i+2}], \; i = k-1, k, \ldots, n-2,$$

where $y[x_i, x_{i+1}] = (y_{i+1} - y_i)/(x_{i+1} - x_i)$ is the fist divided difference relative to x_i and x_{i+1}. It follows that our assumption on non-decreasing second divided differences seems suitable for applications to sigmoid data fitting. Further, it is interesting to note that if we replace the third differences (3) by the analogous second or first differences, we obtain the best convex fit [5], or the best monotonic fit [24] to the data, the latter problem especially having found numerous applications in various subjects during the last 60 years.

The paper is organized as follows. In Section II we outline a quadratic programming method for this optimization calculation. In Section III we consider two examples on real economic data and reveal important properties of the process. The first is an application to the U.S.A. renewable energy consumption data during the period 1980-2010. The second is an application to technological substitutions among the PDP computers to the VAX computers between the years 1984 and 1991. The results are briefly analyzed and the modeling capability of the method is demonstrated. In Section IV we present some concluding remarks and discuss on the possibility of future directions of this research.

The method may also be applied to the problem where inequalities (3) are replaced by the reversed ones, in which case we obtain a convex / concave fit. The latter problem may be treated computationally as the former one after an overall change of sign of $\underline{\phi}$.

II. An Outline of the Method of Calculation

It is straightforward to calculate the solution of the problem of Section I by standard quadratic programming methods. However, because each of the constraint functions $y[x_{i-1}, x_i, x_{i+1}, x_{i+2}]$, for $i = 2, 3, \ldots, n-2$, depends on only four adjacent components of $\underline{y}$ and because of the tractability of the least squares objective function, we have developed a special version of the quadratic programming algorithm of [4] that is faster than general algorithms.

Our algorithm generates a finite sequence of subsets $\{A_k : k = 1, 2, \ldots\}$ of the constraint indices $\{2, 3, \ldots, n-2\}$ with the property

$$\underline{y}^T \underline{a}_i = 0, \; i \in A_k. \quad (6)$$

For each k, we denote by $\underline{y}^{(k)}$ the vector that minimizes (2) subject to the equations (6) and we call each constraint in (6) an active constraint. All the active constraints constitute the active set. Since the constraint normals are linearly independent, unique Lagrange multipliers $\{\lambda_i^{(k)} : i \in A_k\}$ are defined by the first order optimality condition

$$2(\underline{y}^{(k)} - \underline{\phi}) = \sum_{i \in A_k} \lambda_i{}^{(k)} \underline{a}_i, \quad (7)$$

while, by strict complementarity, $\lambda_i^{(k)} = 0, \; i \notin A_k$. The method chooses A_k so that each $\lambda_i^{(k)}$ satisfies the conditions

$$\lambda_i^{(k)} \geq 0, \; i \notin A_k. \quad (8)$$

If A_k is not the final set of the mentioned sequence, A^* say, then the quadratic programming algorithm makes adjustments to A_k until the solution is reached. The Karush-Kuhn-Tucker conditions [8]:p.200 provide necessary and sufficient conditions for optimality. They state that $\underline{y}$ is optimal if and only if the constraints (3) are satisfied and there exist nonnegative Lagrange multipliers $\lambda_i \geq 0, \; i \in A^*$ such that (7) holds, after we replace $\underline{y}^{(k)}$ by $\underline{y}$, $\lambda_i^{(k)}$ by λ_i and A_k by A^*.

The calculation begins from any vector $\underline{y}^{(1)}$ such that $\lambda_i^{(1)} \geq 0$, for $i \in A_1$, where a suitable choice for A_1 is provided by [4]. If the constraints (3) hold at $\underline{y} = \underline{y}^{(1)}$, then the calculation terminates because the Karush-Kuhn-Tucker conditions are satisfied. We assume that at the kth iteration, A_k, $\underline{y}^{(k)}$ and $\underline{\lambda}^{(k)}$ are available, but $\underline{y}^{(k)}$ violates some of the constraints (3). Then, the index of the most violated constraint, ℓ say, is added to A_k and new values of the Lagrange multipliers are calculated. Now, if there are negative multipliers indexed in A_k, then an index, κ say, that is always different from ℓ, is picked from A_k, the κth constraint is dropped from the active set and A_k is set to $A_k \setminus \{\kappa\}$. The algorithm continues iteratively dropping constraints from the active set until it eventually recovers the

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inequalities (8). Then a new iteration starts, while current A_k is distinct from all its previous instances at this step and, in exact arithmetic, the value of (2) moves strictly upwards. Since there is only a finite number of sets A_k, the algorithm cannot cycle indefinitely between its steps. This approach is well suited to our problem, while a particular advantage is that only $O(n)$ computer operations are needed for updating the matrices associated with the calculation of $\underline{y}^{(k)}$ and $\underline{\lambda}^{(k)}$. Matrix updating techniques may be found in [10]. An implementation of this method in FORTRAN is provided by a version of [3].

III. Applications

Substitution in economics is the process at which one product supplants another as it enters the market [22]:p. 273. In competitive strategy several important questions are raised on how to best defend against a substitute, or how to promote substitution. Although the rate of penetration of substitutes differs from product to product, the path of substitution for successful substitutes looks like an S-curve, where demand is plotted against time.

In this section we present two applications of our method to real data from economic substitutions. First, the set of annual data of renewable energy consumption in quadrillion Btu (a unit of energy equal to about 1055 joules) in the U.S.A. for the period 1980-2010 (Release Date Report: March 2010 by the Energy Information Administration [28]) is used to illustrate the modeling performance of our method in calculating the best fit. The data are presented in the first two columns of Table I. For purposes of analysis we are not interested in the physical details of the process, but only in what they imply for the shape of the relationship over time. Since we have to estimate values for an unknown consumption function, initially we make an attempt to distinguish any trends by a primary analysis of the scaled first, second and third differences of the data. These differences are presented in columns 3, 4 and 5, respectively, of Table I, rounded to four decimal places. The first differences show a slight convex trend, but the second and third differences appear to fluctuate irregularly around zero, as it is shown in Fig. 1. Furthermore, as the trend indicates, the data first seem to increase less than proportionately, then to decrease and then to increase more than proportionately. Therefore we take the view that the underlying consumption function follows the shape of a concave / convex curve.

The method of Section II was applied to these data (columns 1 and 2 in Table I). Without any preliminary analysis the data were fed to the computer program and within 17 active set changes the solution was reached. The best fit is presented in the sixth column of Table I and the corresponding Lagrange multipliers are presented in the seventh column. Fig. 2 shows the data and the fit. Furthermore, the scaled sequences of first, second and third divided differences of the best fit are presented in the last three columns of Table I. We can immediately notice the non-decreasing property of the sequence of the second divided differences and the correspondence between the zero Lagrange multipliers and the non-zero third divided differences. The zero Lagrange multipliers show that all the constraints, but those corresponding to the years 1983, 1999 and 2000, are active. As points with zero third divided differences lie on

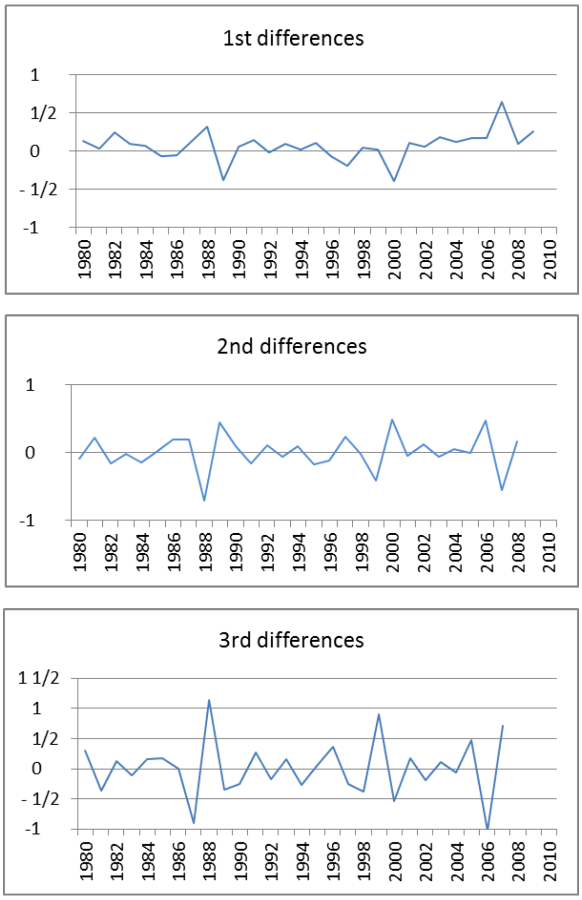

Fig. 1. First, second and third divided differences of the data given in Table I (columns 3, 4 and 5 respectively). The continuous line is only for illustration.

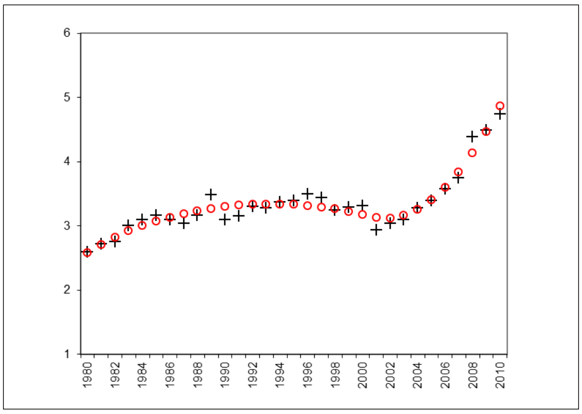

Fig. 2. Graphical representation of the data given in Table I. The data of column 1 annotate the x-axis. The data of column 2 are denoted by (+) and the best fit of column 6 by (o).

a parabola, it follows that the calculated consumption curve consists of three overlapping parabolae. A sensitivity analysis would conclude that the best fit is strongly dependent upon the placement of all active constraints on [1984,1998] and on [2001,2007], because the associated Lagrange multipliers are away from zero. In addition, the inactive constraints allowed for the best fit to follow the data trends.

The piecewise monotonicity of the first differences (column 8) and the sign change of the second differences (column 9) may lead one's search for estimating the inflection point of the consumption curve. Indeed, the first differences

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TABLE I
LEAST SQUARES FIT BY NONNEGATIVE THIRD DIVIDED DIFFERENCES TO U.S.A. RENEWABLE ENERGY CONSUMPTION DATA (IN BTU) PER YEAR

Data					Best fit				
Year x_i	Consumption φ_i	1st differences	2nd differences	3rd differences	Best fit y_i	Lagrange multiplier	1st differences	2nd differences	3rd differences
1980	2.5853	0.1273	-0.0902	0.3029	2.5742	0.0667	0.1328	-0.0165	0.0000
1981	2.7126	0.0371	0.2127	-0.3679	2.7070	0.2336	0.1163	-0.0165	0.0000
1982	2.7496	0.2498	-0.1552	0.1305	2.8233	0.0587	0.0998	-0.0165	0.0000
1983	2.9994	0.0945	-0.0247	-0.1162	2.9231	0.0000	0.0833	-0.0165	0.0091
1984	3.0940	0.0699	-0.1409	0.1559	3.0064	0.5830	0.0667	-0.0075	0.0000
1985	3.1638	-0.0711	0.0150	0.1694	3.0731	2.3521	0.0593	-0.0075	0.0000
1986	3.0927	-0.0561	0.1844	0.0068	3.1323	5.0696	0.0518	-0.0075	0.0000
1987	3.0367	0.1283	0.1912	-0.8971	3.1841	7.8506	0.0443	-0.0075	0.0000
1988	3.1650	0.3196	-0.7058	1.1444	3.2284	10.3146	0.0368	-0.0075	0.0000
1989	3.4846	-0.3863	0.4385	-0.3471	3.2653	13.7771	0.0294	-0.0075	0.0000
1990	3.0983	0.0523	0.0914	-0.2543	3.2947	17.0604	0.0219	-0.0075	0.0000
1991	3.1506	0.1437	-0.1628	0.2715	3.3165	19.1687	0.0144	-0.0075	0.0000
1992	3.2943	-0.0191	0.1087	-0.1777	3.3310	19.8823	0.0069	-0.0075	0.0000
1993	3.2752	0.0896	-0.0690	0.1596	3.3379	18.8250	-0.0005	-0.0075	0.0000
1994	3.3648	0.0206	0.0906	-0.2650	3.3374	16.1612	-0.0080	-0.0075	0.0000
1995	3.3853	0.1111	-0.1744	0.0498	3.3294	12.2266	-0.0155	-0.0075	0.0000
1996	3.4965	-0.0633	-0.1246	0.3601	3.3139	8.1166	-0.0230	-0.0075	0.0000
1997	3.4331	-0.1879	0.2355	-0.2604	3.2909	4.6843	-0.0304	-0.0075	0.0000
1998	3.2453	0.0476	-0.0249	-0.3846	3.2605	1.8382	-0.0379	-0.0075	0.0000
1999	3.2929	0.0227	-0.4095	0.8993	3.2226	0.0000	-0.0454	-0.0075	0.0556
2000	3.3156	-0.3868	0.4898	-0.5334	3.1772	0.0000	-0.0528	0.0482	0.0012
2001	2.9289	0.1030	-0.0436	0.1679	3.1244	0.6650	-0.0047	0.0494	0.0000
2002	3.0319	0.0594	0.1243	-0.1878	3.1197	1.4678	0.0447	0.0494	0.0000
2003	3.0913	0.1837	-0.0635	0.1176	3.1644	1.9700	0.0941	0.0494	0.0000
2004	3.2750	0.1202	0.0541	-0.0572	3.2584	2.2709	0.1434	0.0494	0.0000
2005	3.3953	0.1743	-0.0031	0.4806	3.4019	2.3309	0.1928	0.0494	0.0000
2006	3.5696	0.1712	0.4774	-1.0293	3.5947	1.9994	0.2422	0.0494	0.0000
2007	3.7408	0.6487	-0.5518	0.7116	3.8369	0.7004	0.2916	0.0494	0.0000
2008	4.3895	0.0968	0.1598	-	4.1284	-	0.3409	0.0494	-
2009	4.4863	0.2566	-	-	4.4694	-	0.3903	-	-
2010	4.7430	-	-	-	4.8597	-	-	-	-

decrease monotonically until 2001 and increase monotonically subsequently, indicating a lower turning point of the marginal consumption curve in the interval [2000,2001]. The essential feature for the consumption curve is that its secant-slope (cf. first differences), though decreasing until 2001 starts increasing afterwards. Moreover, it is positive up to 1992, then negative up to 2001 and positive afterwards. A rationalization of this is the idea that after 2001, the intensity of the use of renewable energy is increased annually, either because of increased energy demands or because other energy types are been replaced by renewable ones leading to larger and larger consumption increments of renewable energy. The size of the Lagrange multipliers shows that the strongest resistance of the energy market to the renewable energy entering is during [1991,1994]. Moreover, since the first twenty second differences are negative and the last nine are positive the best fit consists of one concave section on the interval [1980,2001] and one convex section on the interval [2000,2010]. Hence the inflection point of the consumption curve lies in the interval [2000,2001]. Furthermore, the analysis suggests that any estimation of the upper limit in the maximum possible value of energy market penetration rate, which is highly desirable in estimating substitution processes [21], is rather immature at this stage of the renewable energy consumption process.

The second application is a fit to data provided by Modis [18]. Modis analyzes technological substitutions among computer products of Digital Equipment Corporation^{TM} in Europe and discusses on the limitations of Fisher and Pry's model [7] on these data. The transitions are from the PDP computers to the VAX computers between the years 1984 and 1991, and the data have been derived on 31 trimesters. The first column of Table II displays the trimesters and the second column presents the percentage of substitution of PDP by VAX products. The data were fed to our computer program and the best fit subject to non-positive third divided differences is presented in the sixth column of Table II. All the other columns are explained in Table I. Especially for the differences presented in columns 3, 4 and 5, we notice that the first and second differences show concave trends, while the third differences exhibit deviations along their range that need investigation. Further, Fig. 3 displays the data and the fit. The computer program terminated at the optimum within 33 active set changes. Without entering a theoretical justification of the results, we note that our method provides an informative description of the substitution process. Indeed, in view of the active constraints, it reveals the ranges of convexity and concavity as well as the rates of marginal change, and, where a Lagrange multiplier is large, the problem is particularly dependent upon the associated constraint.

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TABLE II
LEAST SQUARES FIT BY NON-POSITIVE THIRD DIVIDED DIFFERENCES TO TRANSITIONS FROM THE PDP COMPUTERS TO THE VAX COMPUTERS BETWEEN THE YEARS 1984 AND 1991

Data					Best fit				
Trimester x_i	%Substitution φ_i	1st differences	2nd differences	3rd differences	Best fit y_i	Lagrange multiplier	1st differences	2nd differences	3rd differences
1	3.55	6.750	-9.910	13.670	12.690	54.840	-4.534	1.231	0.000
2	10.30	-3.160	3.760	-5.200	8.156	151.652	-3.303	1.231	0.000
3	7.14	0.600	-1.440	-1.450	4.852	276.710	-2.072	1.231	0.000
4	7.74	-0.840	-2.890	16.830	2.780	400.252	-0.841	1.231	0.000
5	6.90	-3.730	13.940	-33.810	1.938	492.508	0.390	1.231	0.000
6	3.17	10.210	-19.870	31.750	2.328	548.425	1.621	1.231	0.000
7	13.38	-9.660	11.880	-11.650	3.949	511.415	2.852	1.231	0.000
8	3.72	2.220	0.230	1.230	6.800	399.958	4.083	1.231	0.000
9	5.94	2.450	1.460	8.710	10.883	243.711	5.314	1.231	0.000
10	8.39	3.910	10.170	-17.460	16.196	89.510	6.545	1.231	0.000
11	12.30	14.080	-7.290	21.560	22.741	0.000	7.776	1.231	-1.014
12	26.38	6.790	14.270	-23.930	30.516	0.000	9.007	0.217	-1.079
13	33.17	21.060	-9.660	-0.280	39.523	127.627	9.224	-0.862	0.000
14	54.23	11.400	-9.940	24.340	48.747	349.983	8.362	-0.862	0.000
15	65.63	1.460	14.400	-33.100	57.109	615.940	7.500	-0.862	0.000
16	67.09	15.860	-18.700	32.140	64.609	910.613	6.638	-0.862	0.000
17	82.95	-2.840	13.440	-31.840	71.247	1163.785	5.776	-0.862	0.000
18	80.11	10.600	-18.400	28.330	77.024	1356.937	4.914	-0.862	0.000
19	90.71	-7.800	9.930	-5.850	81.938	1437.439	4.053	-0.862	0.000
20	82.91	2.130	4.080	-10.510	85.991	1423.772	3.191	-0.862	0.000
21	85.04	6.210	-6.430	3.930	89.181	1340.785	2.329	-0.862	0.000
22	91.25	-0.220	-2.500	6.200	91.510	1190.039	1.467	-0.862	0.000
23	91.030	-2.720	3.700	-4.340	92.977	983.214	0.605	-0.862	0.000
24	88.310	0.980	-0.640	-2.480	93.582	751.943	-0.257	-0.862	0.000
25	89.290	0.340	-3.120	-2.030	93.325	520.435	-1.119	-0.862	0.000
26	89.630	-2.780	-5.150	21.250	92.206	304.149	-1.981	-0.862	0.000
27	86.850	-7.930	16.100	-26.080	90.226	123.336	-2.843	-0.862	0.000
28	78.920	8.170	-9.980	4.990	87.383	28.776	-3.704	-0.862	0.000
29	87.090	-1.810	-4.990	-	83.679	-	-4.566	-0.862	-
30	85.280	-6.800	-	-	79.112	-	-5.428	-	-
31	78.480	-	-	-	73.684	-	-	-	-

There exist 26 active constraints, the non-active ones being the 11th and 12th associated with zero Lagrange multipliers. It follows that the calculated substitution curve consists of two overlapping parabolae, one on the interval [1,13] and one on the interval [13,31]. The first differences increase monotonically until the 13th trimester and decrease monotonically subsequently, indicating an upper turning point of the marginal substitution curve in the interval [12,13]. Moreover, they are negative on the first four trimesters, positive up to the 23rd trimester and negative afterwards, which is indicative of the penetration rates on these ranges. Also, we see that the PDP to VAX transition took 16 trimesters to go from about 4% to 90%. The sequence of the second differences is non-increasing, where the first twelve second differences are positive and the last sixteen are negative. It follows that the best fit consists of one convex section on the interval [1,14] and one concave section on the interval [13,31]. Hence, the inflection point of the substitution curve lies in the interval [12,13]. The discussion suggests that our method is able to describe the substitution process everywhere except possibly at the beginning of the data, where substitution is still quite immature.

IV. CONCLUDING REMARKS

We have proposed a quadratic programming calculation that gives the best least squares fit to data values contaminated by random errors subject to nonnegative third divided differences. The method is suitable when the data exhibit a sigmoid trend, where a concave region is followed by a convex one. The method is also suitable when it would be better to employ non-positive instead of nonnegative divided differences, in which case a convex region precedes a concave one. The fit consists of a certain number of overlapping parabolae, which not only provides flexibility in data fitting, but also helps managing further operations with the data fit like interpolation, extrapolation, differentiation and integration. Moreover, the interval of the inflection point of the fit is provided automatically by the calculation.

This data fitting procedure may be used in many situations, when analyzing processes that are subject to diminishing marginal returns, as for example in modeling product life-cycles. Analogously, for increasing marginal returns, as for example in estimating cost and production functions. The accompanying FORTRAN program is suitable for calculations that involve several thousand data points and it would be most useful for real problem applications. Numerical

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experiments in order to test the efficiency of the method are on the way. Moreover, it would be very helpful to try to solve particular problems of sigmoid character, in order to receive guidance from numerical results and from modeling practices. In addition, there is nothing to prevent combining certain features of our method with the logistic curve or the Gompertz curve and other parametric sigmoid forms if there exists an opportunity for improved practical analyses.

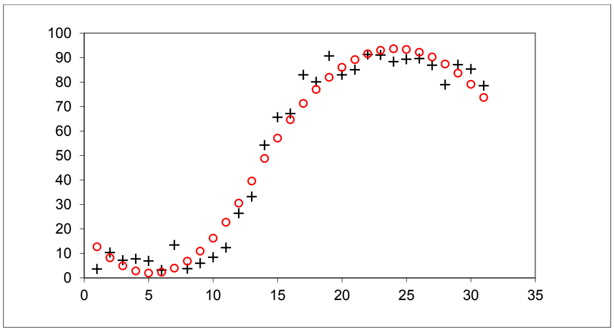

Fig. 3. Graphical representation of the data given in Table II, with the notation of Fig. 2.

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