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Necessary and Sufficient Conditions for Best $L1$ Estimates of Ordinates of Convex Functions

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Abstract— **If plotted values of measurements of function values show some gross errors and away from them the function seems to be convex, then it is suitable to make the least sum of absolute change to the data subject to the condition that the second divided differences of the smoothed data are nonnegative. It is a highly structured constrained $L1$ approximation problem, which can be expressed as a linear programming calculation. The constraints enter by the assumption of non-decreasing returns of the underlying function, which implies convexity. Necessary and sufficient conditions for a solution to this $L1$ problem are presented.**

Keywords: convexity, data fitting, divided difference, L1 approximation, linear programming

1 Problem definition

We present characterization conditions for the problem of calculating a best ℓ_1 convex approximation to measured values of a function $f(x)$. The data are the pairs (x_i, ϕ_i), $i = 1, 2, \dots, n$, where the abscissae x_i, $i = 1, 2, \dots, n$, satisfy the inequalities $x_1 < x_2 < \cdots < x_n$, and ϕ_i is the measurement $f(x_i)$. We assume that $\phi_i = f(x_i) + \varepsilon_i$, where ε_i is a random number. We also assume that there are some gross errors in the data due to blunders. As an error consequence the convexity property of the (unknown) underlying function has been lost. We address the problem of calculating numbers y_i, $i = 1, 2, ..., n$, from the measurements that are smooth and closer than the measurements to the true function values. We regard the original data and the smoothed values as n-vectors, $\underline{\phi}$ and $\underline{y}$ respectively, and consider the problem of minimizing the sum of the moduli of the errors

$$\left\|\underline{\phi} - \underline{y}\right\|_1 = \sum_{i=1}^{n} |\phi_i - y_i|, \ \underline{y} \in \mathbb{R}^n, \tag{1}$$

subject to the convexity constraints

$$y[x_{i-1}, x_i, x_{i+1}] \geq 0, \ i = 2, 3, ..., n-1, \tag{2}$$

where

$$y\left[x_{i-1}, x_i, x_{i+1}\right] = \frac{y_{i-1}}{(x_{i-1} - x_i)(x_{i-1} - x_{i+1})} + \frac{y_i}{(x_i - x_{i-1})(x_i - x_{i+1})} + \frac{y_{i+1}}{(x_{i+1} - x_{i-1})(x_{i+1} - x_i)} \tag{3}$$

is the i-th second divided difference on the components of $\underline{y}$. We call $\underline{y}$ a best ℓ_1 convex fit to $\underline{\phi}$, and also we call feasible any n-vector that satisfies the constraints (2). The constraints on $\underline{y}$ are linear and in order to simplify our notation, we denote the constraint normals with respect to $\underline{y}$ by $\underline{a}_j$, $j = 1, 2, ..., n-2$, and we set

$$y[x_j, x_{j+1}, x_{j+2}] = \underline{a}_j^T \underline{y}, \ j = 1, 2, ..., n-2. \tag{4}$$

Since each divided difference depends on only 3 adjacent components of $\underline{y}$, it immediately follows that the constraints have linearly independent normals.

The optimization problem may also be considered when the data come from processes that show increasing rates of change (cf. convexity), but one does not have sufficient information to set up a parametric form for the underlying function (see [6]). Thus, by writing the i-th second difference in the form

$$y\left[x_{i-1}, x_i, x_{i+1}\right] = \frac{1}{x_{i+1} - x_{i-1}} \left[\frac{y_{i+1} - y_i}{x_{i+1} - x_i} - \frac{y_i - y_{i-1}}{x_i - x_{i-1}}\right], \tag{5}$$

the inequalities on the rates of change of the sequence $\{y_i : \ i = 1, 2, ..., n\}$

$$\frac{y_{i+1} - y_i}{x_{i+1} - x_i} \geq \frac{y_i - y_{i-1}}{x_i - x_{i-1}} \tag{6}$$

imply the inequalities (2). Therefore, an alternative expression of the constraints (2) is that we require increasing rates of change on $[x_1, x_n]$, a property that is quite common in fields like economics and evolution processes, where a potential shape for the underlying function is that of a convex curve (see [5], [7], [14], [15]). The piecewise linear interpolant of the smoothed values (x_i, y_i), $i = 1, 2, ..., n$ provides some useful geometric description.

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We begin by noting that if all the divided differences are zero then the smoothed values lie on a straight line. Otherwise some divided differences are nonnegative and at least one of them is positive. This gives to the piecewise linear interpolant the convexity property.

Besides that the convexity shape is likely to strike immediately a user's eye when he inspects the data, two properties of our calculation that provide some advantages over other smoothing calculations are as follows. First, the approximation process is a projection because, if the data satisfy the convexity constraints, then they provide the required approximation. Second, there is no need to choose a set of approximating functions, because the missing property of convexity is imposed as a smoothing condition, namely inequalities (2), and the optimization calculation defined in the beginning of the section undertakes the smoothing process.

Similar problems are studied and characterized by [11], where (1) is replaced by the supremum norm

$$\|\underline{\phi} - \underline{y}\|_\infty = \max_{1 \le i \le n} |\phi_i - y_i| \tag{7}$$

and by [4], where (1) is replaced by the least squares norm

$$\|\underline{\phi} - \underline{y}\|_2 = \sum_{i=1}^{n} (\phi_i - y_i)^2. \tag{8}$$

Expression (7) is appropriate when the data errors have a uniform distribution, for example, if the measuring process rounds each measurement to the nearest integer, while expression (8) is appropriate when the data errors have a normal distribution. On the other hand, methods that rely upon (1) are well suited to long tailed error distributions, like Cauchy or Laplace, and have the remarkable property of ignoring some gross errors in the data (in the bibliography this property is called robustness). This occurs because a best ℓ_1 fit $\underline{y}^*$ depends on the data through the signs of the differences $(\phi_i - y_i^*)$, so that once a difference exceeds a certain amount, this difference is ignored in the calculation (see [9]).

We express the constraints (2) in the matrix form $C^T\underline{y} \ge \underline{0}$, where C^T is the $(n-2) \times n$ matrix whose rows are the constraints normals $\underline{a}_j^T$, $j = 1, 2, ..., n-2$, and we formulate the linear programming problem that gives a best ℓ_1 convex fit to the data by following [2]:

$$\text{Minimize } (\underline{u} + \underline{v}) \tag{9}$$

subject to

$$\begin{cases} \underline{y}' - \underline{y}'' + \underline{u} - \underline{v} = \underline{\phi} \\ C^T(\underline{y}' - \underline{y}'') = \underline{u}'' \\ \underline{y}', \underline{y}'', \underline{u}, \underline{v}, \underline{u}'' \ge \underline{0}, \end{cases} \tag{10}$$

where for the n-vector $\underline{y}$ we put $\underline{y} = \underline{y}' - \underline{y}''$; $\underline{u}$ and $\underline{v}$ are n-vectors and $\underline{u}''$ is a $(n-2)$-vector. Therefore, it is rather straightforward to solve problem (1)-(2) by applying standard linear programming techniques to (9)-(10) or to its dual (see [1], [3]), where one should take account of the constraints structure. However, since several thousand data points may occur in many calculations, we need a special technique for this problem, which is faster than applying a general linear programming algorithm.

The purpose of this article is to express conditions for the solution of problem (1)-(2) in terms of Karush-Kuhn-Tucker multipliers. Thus, in Section 2, necessary and sufficient conditions for a best ℓ_1 convex fit are obtained that are more useful than the linear programming form of the problem. In Section 3, we state some concluding remarks.

2 The characterization theorem

It is well known that a best ℓ_1 fit from a linear subspace to $\underline{\phi}$ satisfies certain interpolation conditions (see [10], [12]), which in our case may be expressed in the form of the following theorem.

Theorem 1 *Let A be a nonempty subset of $\{1, 2, \ldots, n-2\}$ and denote by $|A|$ the number of elements of A. Then there exists a vector $\underline{y}$ that minimizes (1) subject to the equality constraints*

$$\underline{a}_j^T \underline{y} = 0, \ j \in A, \tag{11}$$

and that has the property

$$y_i = \phi_i, \ i \in I \subseteq \{1, 2, \ldots, n\}, \tag{12}$$

with set I containing at least $n - |A|$ indices.

Proof: See [8]. ■

It follows that a best ℓ_1 fit $\underline{y}$ to $\underline{\phi}$ subject to (11) may be calculated by seeking a set I that allows $\underline{y}$ to be obtained by interpolation to the points $\{\phi_i : i \in I\}$. Therefore, in order to minimize (1) subject to (2), Theorem 1 suggests searching for a best ℓ_1 fit among feasible vectors defined by the conditions of this theorem. Theorem 4 below is useful for testing whether a feasible vector that satisfies the conditions of Theorem 1 is optimal, in terms of some parameters λ_i, $i \notin I$. Theorem 4 makes use of a characterization of a best ℓ_1 fit subject to linear equality constraints (Lemma 2) and the separating hyperplane theorem (Theorem 3). Let s_i be the sign of $y_i - \phi_i$. Obviously, s_i is ± 1, if $i \notin I$.

Lemma 2 *A vector $\underline{y} \in \mathbb{R}^n$ minimizes (1) subject to (11) if and only if there exists a vector $\underline{v}$ in*

$$V = \{\underline{v} \in \mathbb{R}^n : \ |v_i| \le 1, \ v_i = s_i, \ i \notin I\}$$

such that

$$\underline{y}^T \underline{v} = 0.$$

Proof: Let $\{B_j : j = 1,2,\dots,n-|A|\}$ be a basis for the linear subspace that is defined by (11) (see [8] for a suitable construction), where each B_j is defined on the abscissae x_i, $i = 1,2,...,n$. We define B to be the $n \times (n-|A|)$ matrix with (i,j) elements

$$B_j(x_i),\ j = 1,2,...,n-|A|,\ i = 1,2,...,n. \tag{13}$$

Then $\underline{y}$ is written as $\underline{y} = \sum_{j=1}^{n-|A|} \sigma_j B_j = B\underline{\sigma}$, where $\underline{\sigma}$ has to be determined by the minimization of $\|\underline{\phi} - B\underline{\sigma}\|_1$. In view of Theorem 6.1 of [12], $\underline{\sigma}$ is optimal if and only if there exists $\underline{v} \in V$ such that

$$B^T \underline{v} = 0$$

or

$$\underline{\sigma}^T B^T \underline{v} = 0 \text{ or } \underline{y}^T \underline{v} = 0. \blacksquare$$

Theorem 3 *(Separating Hyperplane) For any $m \times n$ matrix M and any $m-$vector $\underline{v}$, either $M\underline{\lambda} = \underline{v}$, $\underline{\lambda} \geq \underline{0}$ has a solution $\underline{\lambda}$, or $M^T\underline{d} \geq \underline{0}$, $\underline{v}^T\underline{d} < 0$ has a solution $\underline{d}$, but not both.*

Proof: See, for example, [13]. $\blacksquare$

Theorem 4 *We assume that a vector $\underline{y}^*$ satisfies the conditions of Theorem 1. Then, $\underline{y}^*$ minimizes (1) subject to $\underline{a}_j^T \underline{y} \geq 0$, $j = 1,2,...,n-2$, if and only if there exist multipliers λ_j, $j \in A$, such that*

$$\sum_{i \notin I} s_i^* \underline{e}_i = \sum_{j \in A} \lambda_j \underline{a}_j, \tag{14}$$

$$\lambda_j \geq 0,\ j \in A, \tag{15}$$

where s_i^* is the sign of $y_i^* - \phi_i$.

Proof: Let $\underline{y}^*$ be a feasible vector that satisfies the conditions (11) and (12) of Theorem 1. To prove the first part of the theorem, suppose there exist λ_j, $j \in A$, that satisfy (14) and (15). Then we define the function

$$F(\underline{y}) = \sum_{i=1}^{n} s_i^*(y_i - \phi_i) \tag{16}$$

which, due to the choice of $\underline{s}^*$ and $\underline{y}^*$, obtains the value

$$F(\underline{y}^*) = \|\underline{y}^* - \underline{\phi}\|_1. \tag{17}$$

We show next that the problem of minimizing $F(\underline{y})$ subject to the constraints

$$\underline{a}_j^T \underline{y} \geq 0,\ j \in A, \tag{18}$$

is solved by the specific $\underline{y}^*$. Indeed, since inequalities (18) are satisfied, for the active set conditions

$$\underline{a}_j^T \underline{y}^* = 0,\ j \in A, \tag{19}$$

are satisfied, since $F(\underline{y})$ is a differentiable function of $\underline{y}$, since $\nabla F = \underline{s}^*$ and (14) imply the equation

$$\nabla F = \sum_{j \in A} \lambda_j \underline{a}_j \tag{20}$$

and since, by assumption, the nonnegativity conditions (15) hold, we have sufficient conditions for $\underline{y}^*$ to be optimal for the problem of minimizing $F(\underline{y})$ subject to (18). In addition, these are also sufficient conditions for $\underline{y}^*$ to minimize $F(\underline{y})$ subject to the constraints

$$\underline{a}_j^T \underline{y} \geq 0,\ j = 1,2,...n-2, \tag{21}$$

because $\underline{y}^*$ is feasible and, for the specific set A, (20) and (15) hold.

Now, for every $\underline{y}$

$$\sum_{i=1}^{n} s_i^*(y_i - \phi_i) \leq \sum_{i=1}^{n} |s_i^*||y_i - \phi_i| \leq \sum_{i=1}^{n} |y_i - \phi_i|, \tag{22}$$

but at the specific (feasible) $\underline{y}^*$ due to (17) this inequality is satisfied as an equation. Since the left-hand side of inequality (22) is also the minimum value of F at $\underline{y}^*$ over all feasible vectors, it follows that (14) and (15) provide sufficient conditions for $\underline{y}^*$ to minimize (1) subject to the constraints (2), which completes the proof of this part of the theorem.

To prove the converse result, suppose that $\underline{y} = y^*$ minimizes (1) subject to (2) and that there are no nonnegative λ_j, $j \in [1, n-2]$, that satisfy the conditions (14).

Since, by assumption, $\underline{y}$ minimizes (1) subject to the constraints (11), in view of Lemma 2, there exists a vector $\underline{v} \in V$ such that

$$\underline{y}^T \underline{v} = 0. \tag{23}$$

We are going to construct such a vector $\underline{v}$. Suppose $\underline{v}$ is written as a linear combination of $\underline{a}_j$, $j \in A$,

$$\underline{v} = \sum_{j \in A} \lambda_j \underline{a}_j. \tag{24}$$

which allows (23) to be satisfied, since $\underline{a}_j^T \underline{y} = 0$, $j \in A$. Then, in view of the free signs of λ_j in (24) and Theorem 3, there exists a vector $\underline{d} \in \mathbb{R}^n$, that gives

$$\underline{a}_j^T \underline{d} \geq 0,\ j \in A, \text{ and } \underline{v}^T \underline{d} < 0. \tag{25}$$

It follows that there exists a small and positive number α, such that $\underline{y} + \alpha\underline{d}$ is feasible, whenever $\underline{y}$ is feasible. In addition, the value of the objective function is reduced along $\underline{d}$. Indeed,

$$\begin{aligned}
&\sum_{i=1}^{n} |y_i + \alpha d_i - \phi_i| = \\
&\sum_{i\in I} |y_i + \alpha d_i - \phi_i| + \sum_{i\notin I} |y_i + \alpha d_i - \phi_i| = \\
&\sum_{i\in I} \alpha\, |d_i| + \sum_{i\notin I} s_i\,(y_i + \alpha d_i - \phi_i) = \\
&\sum_{i\in I} \alpha\, |d_i| + \sum_{i\notin I} s_i\,(y_i - \phi_i) + \sum_{i\notin I} s_i \alpha d_i = \\
&\sum_{i=1}^{n} |y_i - \phi_i| + \alpha[\sum_{i\in I} |d_i| + \sum_{i\notin I} s_i d_i] = \\
&\sum_{i=1}^{n} |y_i - \phi_i| + \alpha[\sum_{i\in I} sign\,(d_i)\, d_i + \sum_{i\notin I} s_i d_i] = \\
&\sum_{i=1}^{n} |y_i - \phi_i| + \alpha \underline{d}^T \underline{v},
\end{aligned}$$

where $\underline{v} \in \mathbb{R}^n$ is defined by

$$v_i = \begin{cases} sign\,(d_i)\,, & i \in I \\ s_i, & i \notin I. \end{cases}$$

Thus, the construction of $\underline{v}$ is complete, this vector belonging to set V, since

$$v_i = s_i,\ i \notin I,\ |v_i| \le 1,\ i \in I.$$

Hence the conditions of Lemma 2 are satisfied.

Since the value of the objective function is reduced as we move from $\underline{y}$ along $\underline{d}$, for $\underline{d}^T\underline{v} < 0$, a contradiction to the optimality of $\underline{y}$ is derived. Therefore the assumption on the signs of λ_j is not true, and the proof of the second part of the theorem is complete. ■

Theorem 4 is useful, because one can find out whether a trial ℓ_1 convex fit to $\underline{\phi}$, which is at a linear subspace of the space of variables, is optimal by checking only the conditions (14) and (15). Moreover, the proof of the second part of the theorem provides a constructive method for obtaining another convex fit that is better than $\underline{y}^*$ if condition (15) is not satisfied.

3 Concluding remarks

We have provided characterization conditions for a best ℓ_1 convex fit to univariate data, where convexity is defined by nonnegative second divided differences, in terms of Karush-Kuhn-Tucker multipliers.

The corresponding least squares and supremum norm problems had been studied and characterized by [4] and [11].

It is straightforward to generalize the theorems of this paper to the case of a discrete best ℓ_1 approximation with linear inequality constraints.

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