THE BEST LEAST ABSOLUTE DEVIATIONS LINE – PROPERTIES AND TWO EFFICIENT METHODS FOR ITS DERIVATION

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Abstract

Given a set of points in the plane, the problem of existence and finding the least absolute deviations line is considered. The most important properties are stated and proved and two efficient methods for finding the best least absolute deviations line are proposed. Compared to other known methods, our proposed methods proved to be considerably more efficient.

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1. Introduction

Let $I = \{1, ..., m\}$, $m \ge 2$, be a set of indices, and let $\Lambda = \{T_i(x_i, y_i) \in \mathbb{R}^2 \mid i \in I\}$ be a set of points in the plane. The problem of determining parameters a and b of the linear function f(x; a, b) = ax + b, in order to have its graph pass as close as possible (in some sense) to the given points, is an old problem which has been solved in various ways. Most frequently it is assumed that errors can occur only in measured values of the independent variable. In this case, if we use the l_2 norm, we have the *ordinary least squares* (OLS) problem and the OLS line. In many technical and other applications (where so-called 'outliers' can be expected) using the l_1 norm is much more interesting. In the literature this approach is better known as the *least absolute deviations* (LAD) problem of finding the LAD line (see, for example, [8, 11, 21]). For example, in calculating movements of robots, based on the data obtained from a stereographic camera, it is important to estimate the position of a straight line in the

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plane efficiently and in real time (see [7, 14]). At the same time, the outliers in the data should not affect the results obtained. It is known that problems of this kind can be solved by applying the LAD approach (see, for example, [2, 6, 8, 21, 26, 32]). In this paper we give an overview of basic properties and facts related to estimation of parameters of the best LAD line, and propose two methods for finding them.

If errors are assumed to occur in measured values of both (dependent and independent) variables, and then in general the l_p norm is used, we have the *total least p* problem (see, for example, [1, 28, 31]).

In this paper the most important properties of the LAD line will be stated and proved and two efficient methods will be proposed. The first method basically relies upon [17] and for it the convergence theorem is proved. The second method for finding the best LAD line is a particular Gauss–Newton iterative process, which is based on solving a series of weighted least squares (WLS) line problems. Therefore, first some general properties and facts involved in this approach are given.

Basic properties of the LAD line are already known (see, for example, [2, 5, 6, 8, 9, 11, 17, 19, 21, 22, 26, 34, 37]). In this paper we present new and constructive proofs of those properties which enable us to construct efficient methods and prove the convergence theorem. Our methods have been compared to numerous other methods known from literature, and have proved to be much more efficient.

2. The best WLS line

The best WLS line is the graph of the function

$$f(x; a^*, b^*) = a^*x + b^*, \quad a^*, b^* \in \mathbb{R},$$
 (2.1)

whose parameters a^* , b^* are determined by minimizing the functional

$$F_2(a,b) = \sum_{i=1}^{m} \omega_i (y_i - ax_i - b)^2,$$
 (2.2)

where $T_i(x_i, y_i)$, $i = 1, ..., m, m \ge 2$, are points in the plane, and $\omega_i > 0$ are corresponding data weights.

Using some natural conditions on the data it can be shown (see, for example, [4]) that there exist unique optimal parameters a^* , b^* of the best WLS line.

The following lemma contains the well-known fact that the best l_2 weighted approximation of the measured data is the weighted arithmetical mean of the measured data. This lemma is used in proving the fact that the best WLS line passes through the centroid of the data, and its proof is trivial.

LEMMA 2.1. Let (ω_i, y_i) , i = 1, ..., m, be the data, where $y_1, ..., y_m$ are real numbers, and $\omega_i > 0$ corresponding data weights. Then

$$\sum_{i=1}^{m} \omega_i (y_i - \lambda)^2 \ge \sum_{i=1}^{m} \omega_i (y_i - \overline{y})^2, \quad \overline{y} = \frac{1}{\omega} \sum_{i=1}^{m} \omega_i y_i, \quad \omega = \sum_{i=1}^{m} \omega_i, \quad (2.3)$$

where the equality holds if and only if $\lambda = \overline{y}$.

LEMMA 2.2. For the given data (ω_i, x_i, y_i) , $i = 1, ..., m, m \ge 2$, in the plane with weights $\omega_i > 0$, i = 1, ..., m, the best WLS line passes through the centroid of the data $(\overline{x}, \overline{y})$, where

$$\overline{x} = \frac{1}{\omega} \sum_{i=1}^{m} \omega_i x_i, \quad \overline{y} = \frac{1}{\omega} \sum_{i=1}^{m} \omega_i y_i, \quad \omega = \sum_{i=1}^{m} \omega_i.$$

If $\min x_i < \max x_i$, then there exists a unique best WLS line whose parameters are given by

$$a^* = \frac{\sum_{i=1}^{m} \omega_i (x_i - \overline{x})(y_i - \overline{y})}{\sum_{i=1}^{m} \omega_i (x_i - \overline{x})^2}, \quad b^* = \overline{y} - a^* \overline{x}.$$
 (2.4)

If $x_1 = \cdots = x_m =: \xi$, then there exist infinitely many best WLS lines, which take the form $y = a^*(x - \xi) + \overline{y}$, where a^* is an arbitrary real number.

PROOF. First note that there exist optimal parameters a^* , $b^* \in \mathbb{R}$ of the functional F_2 given by (2.2). Following [27] and according to Lemma 2.1, it is easy to see that

$$F_2(a^*, b^*) \ge F_2(a^*, \overline{y} - a^* \overline{x}),$$

from which we conclude that the best WLS line must pass through the centroid of the data, that is, the best WLS line should be searched for in the form $x \mapsto a(x - \overline{x}) + \overline{y}$ by minimizing the functional

$$\overline{F}_2(a) = \sum_{i=1}^m \omega_i [(y_i - \overline{y}) - a(x_i - \overline{x})]^2$$

whence, under condition min $x_i < \max x_i$, it is easy to obtain formulae (2.4).

If $x_1 = \cdots = x_m =: \xi$, then according to Lemma 2.1,

$$F_2(a, b) = \sum_{i=1}^m \omega_i (y_i - a\xi - b)^2 \ge \sum_{i=1}^m \omega_i (y_i - \overline{y})^2,$$

where the equality holds if and only if $a\xi + b = \overline{y}$. Hence, in this case there exist infinitely many best WLS lines which take the form $\overline{f}(x; a^*) = f(x; a^*, -\xi a^* + \overline{y}) = a^*(x - \xi) + \overline{y}$, where a^* is an arbitrary real number.

3. Weighted median of the data

Let us first prove the following lemma, which gives properties and a solution of the weighted median problem. This lemma is used in the proof of the existence of the best LAD line passing through at least two different points of the data and other important theorems.

LEMMA 3.1. Let (ω_i, y_i) , $i \in I$, $I = \{1, ..., m\}$, $m \ge 2$, be the data, where $y_1 \le y_2 \le ... \le y_m$ are real numbers, and $\omega_i > 0$ corresponding data weights. Denote

$$J = \left\{ v \in I \mid 2 \sum_{i=1}^{\nu} \omega_i - \sum_{i=1}^{m} \omega_i \le 0 \right\}.$$

For $J \neq \emptyset$, let $v_0 = \max J$. Furthermore, let $F : \mathbb{R} \to \mathbb{R}$ be a function defined as

$$F(\alpha) = \sum_{i=1}^{m} \omega_i |y_i - \alpha|. \tag{3.1}$$

- (i) If $J = \emptyset$ (that is, $2\omega_1 > \sum_{i=1}^m \omega_i$), then the minimum of F is attained at the point
- (ii) If $J \neq \emptyset$ and $2\sum_{i=1}^{\nu_0} \omega_i < \sum_{i=1}^m \omega_i$, then the minimum of F is attained at the
- point $\alpha^* = y_{\nu_0+1}$.

 (iii) If $J \neq \emptyset$ and $2\sum_{i=1}^{\nu_0} \omega_i = \sum_{i=1}^m \omega_i$, then the minimum of F is attained at every point α^* from the segment $[y_{\nu_0}, y_{\nu_0+1}]$.

PROOF. Notice that on each interval

$$(-\infty, y_1), [y_1, y_2), \ldots, [y_{m-1}, y_m), [y_m, \infty),$$

F is a linear function and slopes of those linear functions are consecutively d_{ν} , $\nu =$ $0, \ldots, m$, where

$$d_0 = -\sum_{i=1}^{m} \omega_i, \quad d_m = \sum_{i=1}^{m} \omega_i,$$

$$d_v = 2\sum_{i=1}^{v} \omega_i - \sum_{i=1}^{m} \omega_i = d_{v-1} + 2\omega_v, \quad v = 1, \dots, m-1.$$

If $J = \emptyset$, then for every $v = 1, \ldots, m$, $2 \sum_{i=1}^{v} \omega_i - \sum_{i=1}^{m} \omega_i > 0$ and $d_0 < 0$ $< d_{\nu}$. It follows that F is strongly decreasing on $(-\infty, y_1)$ and strongly increasing on (y_1, ∞) , therefore the minimum of F is attained for $\alpha^* = y_1$.

If $J \neq \emptyset$, note that $v_0 = \max\{v \in I \mid d_v \leq 0\}$. Since $d_{v+1} - d_v = 2\omega_{v+1} > 0$ and $d_0 < 0$ and $d_m > 0$, the sequence (d_v) is increasing and

$$d_0 < d_1 < \dots < d_{\nu_0} \le 0 < d_{\nu_0 + 1} < \dots < d_m.$$
(3.2)

If $d_{\nu_0} < 0$, that is, $2\sum_{i=1}^{\nu_0} \omega_i < \sum_{i=1}^m \omega_i$, it follows from (3.2) that F is strongly decreasing on $(-\infty, y_{\nu_0+1})$ and strongly increasing on (y_{ν_0+1}, ∞) , therefore the

minimum of F is attained for $\alpha^* = y_{\nu_0+1}$. If $d_{\nu_0} = 0$, that is, $2\sum_{i=1}^{\nu_0} \omega_i = \sum_{i=1}^m \omega_i$, it follows from (3.2) that F is strongly decreasing on $(-\infty, y_{\nu_0})$, is constant on $[y_{\nu_0}, y_{\nu_0+1}]$ and strongly increasing on (y_{ν_0+1}, ∞) , therefore the minimum of F is attained at every point α^* from the segment $[y_{\nu_0}, y_{\nu_0+1}].$

COROLLARY 3.2. Let $y_1 \le y_2 \le \cdots \le y_m$, m > 1, be the data with weights $\omega_1 = \cdots = \omega_m = 1$. Then

- (i) if m is odd (m = 2k + 1), then the minimum of F is attained at the point $\alpha^{\star} = y_{k+1}$;
- (ii) if m is even (m=2k), the minimum of F is attained at every point α^* from the segment $[y_k, y_{k+1}]$.

PROOF. First, note that in this case the set J from Lemma 3.1 is always nonempty. Let m = 2k + 1. According to Lemma 3.1(ii),

$$\nu_0 = \max\{\nu \in I \mid 2\nu - m \le 0\} = \max\{\nu \in I \mid \nu \le k + \frac{1}{2}\} = k,$$

$$d_{\nu_0} = d_k = 2k - m = 2k - 2k - 1 < 0,$$

and therefore $\alpha^* = y_{k+1}$.

Let m = 2k. According to Lemma 3.1(iii),

$$v_0 = \max\{v \in I \mid 2v - m \le 0\} = \max\{v \in I \mid v = k\} = k,$$

$$d_{v_0} = d_k = 2k - m = 2k - 2k = 0.$$

It follows that the minimum of F is attained at every point α^* from the segment $[y_k, y_{k+1}]$.

REMARK 1. If the minimum of the functional F defined by (3.1) is attained at the real number α^* , then

$$F(\alpha) = \sum_{i=1}^{m} \omega_i |y_i - \alpha| \ge \sum_{i=1}^{m} \omega_i |y_i - \alpha^*|,$$

where the equality holds if and only if $\alpha = \alpha^*$.

4. The best LAD line

Let $I = \{1, \ldots, m\}$, $m \ge 2$, be a set of indices and $\Lambda = \{T_i(x_i, y_i) \in \mathbb{R}^2 \mid i \in I\}$ a set of points in the plane. The best LAD line is to be determined, that is, optimal parameters a^* , $b^* \in \mathbb{R}$ of the function f(x; a, b) = ax + b are to be determined such that

$$G(a^*, b^*) = \min_{(a,b) \in \mathbb{R}^2} G(a, b), \quad G(a, b) = \sum_{i=1}^m |y_i - ax_i - b|.$$
 (4.1)

The following theorem is straightforward, and it can be proved by the principle applied in [9, 13, 15, 16].

THEOREM 4.1. Let $I = \{1, ..., m\}$, $m \ge 2$, be a set of indices and $\Lambda = \{T_i(x_i, y_i) \in \mathbb{R}^2 \mid i \in I\}$ a set of points in the plane. Then there is a best LAD line, that is, problem (4.1) has a solution. In particular, if $x_1 = \cdots = x_m =: \xi$, then there exist infinitely many best LAD lines, which take the form $y = a^*(x - \xi) + \mu$, where a^* is an arbitrary real number, and μ is the median of the data y_1, \ldots, y_m .

The following lemma shows that for the linear function whose graph passes through a certain point $T_0(x_0, y_0) \in \mathbb{R}^2$ there exists a best LAD line whose graph also passes through a certain point $T_i(x_i, y_i) \in \Lambda$, for which $x_i \neq x_0$. In particular, the point T_0 can be one of the points of the set Λ . In this case the lemma states that there

exists a best LAD line whose graph passes through one more point $T_i(x_i, y_i) \in \Lambda$ for which $x_i \neq x_0$.

LEMMA 4.2. Let $I = \{1, ..., m\}$, $m \ge 2$, be a set of indices and

- (i) $\Lambda = \{T_i(x_i, y_i) \in \mathbb{R}^2 \mid i \in I\}$ a set of points in the plane, such that $(x_1 \leq \cdots \leq x_m)$ and $(x_1 < x_m)$;
- (ii) $T_0(x_0, y_0) \in \mathbb{R}^2$;
- (iii) $\overline{f}(x; a) = a(x x_0) + y_0, a \in \mathbb{R}$, a linear function whose graph passes through the point $T_0(x_0, y_0) \in \mathbb{R}^2$.

Then there exists $a^* \in \mathbb{R}$ such that

$$\overline{G}(a^*) = \min_{a \in \mathbb{R}} \overline{G}(a), \quad \overline{G}(a) = \sum_{i=1}^m |y_i - \overline{f}(x_i; a)| = \sum_{i=1}^m |y_i - a(x_i - x_0) - y_0|,$$
(4.2)

and the graph of the linear function $x \mapsto \overline{f}(x; a^*)$ passes through at least one more point $T_{\nu}(x_{\nu}, y_{\nu}) \in \Lambda$, where $x_{\nu} \neq x_0$.

PROOF. Write $I_0 = \{i \in I \mid x_i = x_0\}$. It can be seen that $I \setminus I_0 \neq \emptyset$, that is, that there exists $i_0 \in I$ such that $x_{i_0} \neq x_0$. Otherwise $x_i = x_0$, for all $i \in I$, which contradicts assumption (i). $\overline{G}(a)$ in (4.2) can be written in the form

$$\overline{G}(a) = \sum_{i=1}^{m} |y_i - a(x_i - x_0) - y_0| = \sum_{i \in I_0} |y_i - y_0| + \sum_{i \in I \setminus I_0} |x_i - x_0| \left| \frac{y_i - y_0}{x_i - x_0} - a \right|.$$
(4.3)

Let $s = \operatorname{card}(I \setminus I_0)$. We rearrange the data $\{(|x_i - x_0|, (y_i - y_0)/(x_i - x_0)) : i \in I \setminus I_0\}$ so that the new data $\{(|x_i' - x_0|, (y_i' - y_0)/(x_i' - x_0)) : i = 1, \ldots, s\}$ are such that $((y_1' - y_0)/(x_1' - x_0), \ldots, (y_s' - y_0)/(x_s' - x_0))$ is an increasing sequence. Notice that it still remains the case that $x_i' - x_0 \neq 0$, for all $i = 1, \ldots, s$. Therefore, the problem of minimizing (4.3) is the weighted median problem which can be written in the form

$$\overline{G}(a) = \sum_{i \in I_0} |y_i - y_0| + \sum_{i=1}^s |x_i' - x_0| \left| \frac{y_i' - y_0}{x_i' - x_0} - a \right| \to \min.$$
 (4.4)

Write $J = \{v : 2 \sum_{i=1}^{\nu} |x_i' - x_0| - \sum_{i=1}^{s} |x_i' - x_0| \le 0\}$. For $J \ne \emptyset$ let us choose $\nu_0 \in \{1, \ldots, s\}$, such that $\nu_0 = \max J$ and denote

$$W_0 = 2 \sum_{i=1}^{\nu_0} |x_i' - x_0|, \quad W = \sum_{i=1}^{s} |x_i' - x_0|.$$

According to Lemma 3.1, the functional (4.4) always has a minimum; furthermore,

(i) if $J = \emptyset$, it is obtained for $a^* = (y_1' - y_0)/(x_1' - x_0)$, that is, the required linear function \overline{f} is of the form

$$\overline{f}(x; a^*) = a^*(x - x_0) + y_0$$

$$= \frac{y_1' - y_0}{x_1' - x_0}(x - x_0) + y_0,$$

meaning that its graph also passes through the point $T_1'(x_1', y_1') \in \Lambda$, where $x_1' \neq x_0$;

(ii) if $J \neq \emptyset$ and $W_0 < W$, the minimum is obtained for $a^* = (y'_{\nu_0+1} - y_0)/(x'_{\nu_0+1} - x_0)$, that is, the required linear function \overline{f} is of the form

$$\overline{f}(x; a^*) = a^*(x - x_0) + y_0$$

$$= \frac{y'_{v_0+1} - y_0}{x'_{v_0+1} - x_0}(x - x_0) + y_0,$$

meaning that its graph also passes through the point $T'_{\nu_0+1}(x'_{\nu_0+1}, y'_{\nu_0+1}) \in \Lambda$ for which $\nu_0 + 1 \in I \setminus I_0$, that is, $x'_{\nu_0+1} \neq x_0$;

(iii) if $J \neq \emptyset$ and $W_0 = W$, the minimum of functional \overline{G} is attained at any point $a^* \in \left[(y'_{\nu_0} - y_0)/(x'_{\nu_0} - x_0), (y'_{\nu_0+1} - y_0)/(x'_{\nu_0+1} - x_0) \right]$, and similarly to previous cases it can be shown that if we choose $a^* = (y'_{\nu_0} - y_0)/(x'_{\nu_0} - x_0)$, then the graph of the searched linear function \overline{f} also passes through the point $T'_{\nu_0}(x'_{\nu_0}, y'_{\nu_0}) \in \Lambda$ for which $x_{\nu_0} \neq x_0$, and if we choose $a^* = (y'_{\nu_0+1} - y_0)/(x'_{\nu_0+1} - x_0)$, then the graph of the required linear function \overline{f} also passes through the point $T'_{\nu_0+1}(x'_{\nu_0+1}, y'_{\nu_0+1})$ for which $x'_{\nu_0+1} \neq x_0$.

Thus, there always exists $a^* \in \mathbb{R}$ such that the graph of the function $x \mapsto \overline{f}(x; a^*)$ passes through at least one more point $T_{\nu}(x_{\nu}, y_{\nu}) \in \Lambda$ for which $x_{\nu} \neq x_0$.

THEOREM 4.3. Let $I = \{1, ..., m\}$, $m \ge 2$, be a set of indices, and $\Lambda = \{T_i(x_i, y_i) \in \mathbb{R}^2 \mid i \in I\}$ a set of points in the plane, such that $(x_1 \le \cdots \le x_m)$ and $(x_1 < x_m)$. Then there exists a best LAD line which passes through at least two different points from Λ .

PROOF. According to Theorem 4.1, there exists a best LAD line $f(x; a^*, b^*) = a^*x + b^*$ with optimal parameters a^*, b^* . By means of a^* and data $(x_i, y_i), i \in I$, let us define the sequence

$$\Delta_m = (y_1 - a^* x_1, \dots, y_m - a^* x_m),$$

which, without loss of generality, we can assume is increasing.

If m = 2k + 1, according to Corollary 3.2(i), the minimum of the functional

$$G(a^*, b) = \sum_{i=1}^{m} |y_i - a^* x_i - b|$$
 (4.5)

is attained for $b^+ = y_{k+1} - a^* x_{k+1}$. Since

$$G(a^*, b^*) = \min_{b \in \mathbb{R}} G(a^*, b) = G(a^*, b^+),$$

at the point (a^*, b^+) the functional G also attains its minimum, and since $y_{k+1} = a^*x_{k+1} + b^+$, it means that there exists a best LAD line passing through the point $T_1(x_{k+1}, y_{k+1})$ and it can be written as

$$\overline{f}(x; a^*) := f(x; a^*, y_{k+1} - a^* x_{k+1}) = a^* (x - x_{k+1}) + y_{k+1}.$$

According to Lemma 4.2, then there exists at least one more point $T_2(x_\mu, y_\mu) \in \Lambda$, through which the best LAD line passes, and for which $x_\mu \neq x_{k+1}$.

If m=2k, according to Corollary 3.2(ii), the minimum of functional (4.5) is attained at any real number from segment $[y_k - a^*x_k, y_{k+1} - a^*x_{k+1}]$. Let us choose $b^+ := y_{k+1} - a^*x_{k+1}$; by deduction similar to the previous case we conclude that at least one more point $T_2(x_\mu, y_\mu) \in \Lambda$ exists, through which the best LAD line passes, and for which $x_\mu \neq x_{k+1}$.

5. Methods for finding the best LAD line

To solve this problem general methods of minimization can be used that do not involve derivatives, such as differential evolutions, Nelder–Mead, random search, and simulated annealing (see, for example, [18, 20, 23, 38]). There are also a certain number of methods based on linear programming (see, for example, [2, 3, 24, 33]) or different special cases of the Gauss–Newton method (see, for example, [9, 25, 30, 35]). There are also some specialized methods for solving this problem (see, for example, [17, 21, 26, 37]). Numerous methods mentioned in the literature are listed in [8]. In this section two effective methods are proposed, and their properties and characteristics are given along with proofs of the convergence theorem.

5.1. Two-points method The method described in this subsection resulted from the improved method referred to in [17], for which we give theoretical justification and prove the convergence theorem. It will be shown that this method gives a solution of LAD problem (4.1) in finitely many steps (significantly less than m).

With the objective of developing an algorithm for finding the best LAD line, first note that Theorem 4.3 refers to the fact that the best LAD line should be searched for among those lines which pass through at least two different points of the sequence Λ . The following algorithm is based on that fact. To get as close as possible from the beginning to the best LAD line, we can choose the point $T_p(x_p, y_p)$ as the initial point, where

$$x_p = \frac{1}{m} \sum_{i=1}^m x_i, \quad y_p = \frac{1}{m} \sum_{i=1}^m y_i$$
 (centroid of the data), or (5.1)

 $x_p = \text{median } (x), \quad y_p = \text{median } (y) \quad (\text{median of the data}),$

which are quickly calculated and probably pass close to the best LAD line. Thereafter, in accordance with Lemma 4.2, we construct the following algorithm.

Algorithm [Two Points]

Step 1: Set $m \ge 2$, input points $T_i(x_i, y_i)$, $i \in I$, $I = \{1, ..., m\}$, according to (5.1), determine the point $T_p(x_p, y_p)$ and define the set $I_0 = \{i \in I \mid x_i = x_p\}$.

Step 2: In accordance with Lemma 4.2:

- solve the LAD problem for the function $\overline{f}(x; a) = a(x x_p) + y_p$ by minimizing functional (4.3), denote the solution by a_1 and determine a new point $T_{i_1}(x_{i_1}, y_{i_1}) \in \Lambda$ for which $x_{i_1} \neq x_p$;
- put $b_1 = -a_1 x_p y_p$ and calculate $G_1 = \sum_{i=1}^m |y_i a_1 x_i b_1|$.

Step 3: Define the set $I_0 = \{i \in I \mid x_i = x_{i_1}\}$. In accordance with Lemma 4.2:

- solve the LAD problem for the function $\overline{f}(x; a) = a(x x_{i_1}) + y_{i_1}$ by minimizing functional (4.3), denote the solution by a_2 and determine a new point $T_{i_2}(x_{i_2}, y_{i_2}) \in \Lambda$ for which $x_{i_2} \neq x_{i_1}$;
- put $b_2 = -a_2x_{i_1} y_{i_1}$ and calculate $G_2 = \sum_{i=1}^m |y_i a_2x_i b_2|$.

Step 4: If $G_2 < G_1$, put $\{i_1 = i_2, G_1 = G_2\}$ and go to step 3; if not, stop.

The following theorem proves that the two-points algorithm leads to the best LAD line in finitely many steps. From the algorithm and Lemma 4.2 it is clear that the number of steps is less than the number of given points T_1, \ldots, T_m . In practice, with a favourable choice of the initial point according to (5.1), the number of steps will be considerably less than m. In this way maximum efficiency of the algorithm is ensured, which is implementable in real time.

THEOREM 5.1. Let $I = \{1, ..., m\}$, $m \ge 2$, be a set of indices, and $\Lambda = \{T_i(x_i, y_i) \mid i \in I\}$ a set of points in the plane, such that $(x_1 \le ... \le x_m)$ and $(x_1 < x_m)$. Then the sequence (a_n, b_n) , defined by the iterative method in the two-points algorithm in $N \le m$ steps leads to the solution of the LAD problem

$$G(a, b) = \sum_{i=1}^{m} |y_i - ax_i - b| \to \min, \quad \text{where}$$

$$G(a_{n+1}, b_{n+1}) < G(a_n, b_n), \quad n = 1, \dots, N.$$
(5.2)

PROOF. If we determine the coefficient b of the linear function f(x) = ax + b such that its graph passes through the point $T_p(x_p, y_p)$ chosen as in (5.1), the functional G given by (5.2) can be written as

$$\overline{G}(a) = G(a, -ax_p + y_p) = \sum_{i=1}^{m} |y_i - a(x_i - x_p) - y_p|,$$

and according to Lemma 4.2, we can solve the corresponding LAD problem, the solution of which is denoted by a_1 . The value of G at the point (a_1, b_1) is $G(a_1, b_1) = G(a_1, -a_1x_p + y_p) = \overline{G}(a_1)$. According to Lemma 4.2, in this way the linear

function $\overline{f}_1(x) = a_1(x - x_p) + y_p$ is defined, whose graph passes through one more new point $T_{i_1}(x_{i_1}, y_{i_1}) \in \Lambda$ for which $x_{i_1} \neq x_p$. Therefore, function \overline{f}_1 can be written as

$$\overline{f}_1(x) = a_1(x - x_{i_1}) + y_{i_1}.$$

Again according to Lemma 4.2, for this function we solve the LAD problem and denote the solution by a_2 . If (a_2, b_2) , $b_2 = -a_2x_{i_1} + y_{i_1}$ is not the point of the minimum of functional G, it is

$$G(a_1, b_1) > \sum_{i=1}^{m} |y_i - a_2(x_i - x_{i_1}) - y_{i_1}| = G(a_2, b_2).$$

Since according to Lemma 4.2 the graph of the function $\overline{f}_2(x) = a_2(x - x_{i_1}) + y_{i_1}$ also passes through a new point $T_{i_2}(x_{i_2}, y_{i_2}) \in \Lambda$, for which $x_{i_2} \neq x_{i_1}$, we can write

$$\overline{f}_2(x) = a_2(x - x_{i_2}) + y_{i_2}.$$

Now again according to Lemma 4.2, for this function we solve the LAD problem and denote the solution by a_3 . If (a_3, b_3) , $b_3 = -a_3x_{i_2} + y_{i_2}$ is not the point of the minimum of functional G, it is

$$G(a_2, b_2) > \sum_{i=1}^{m} |y_i - a_3(x_i - x_{i_2}) - y_{i_2}| = G(a_3, b_3).$$

By repeating this procedure, since the set Λ has finitely many points, this iterative method will end in finitely many steps.

5.2. Iterative reweighted least squares method The idea of the method presented in this subsection appears in different versions in the literature (see, for example, [2, 9, 24, 25, 29]). A general description of the method on which our iterative reweighted least squares (IRLS) method is also based can be found in, for example, [9, 24, 29, 36].

The idea is to write the minimizing functional (4.1) in the form

$$G(a,b) = \sum_{i=1}^{m} |y_i - ax_i - b| = \sum_{i=1}^{m} \frac{1}{|y_i - ax_i - b|} (y_i - ax_i - b)^2$$
 (5.3)

and construct the iterative method so that in every step we solve one WLS problem according to Lemma 2.2. The iterative method is specified in the following algorithm. Since the best LAD line must pass through at least two data points (Theorem 4.3), then at least two weights in step 2 near the solution can become infinitely large. This fact will be used in step 3 to stop the iterative process.

Algorithm [IRLS]

Step 1: Set $m \ge 2$ and M > 0 and input points $T_i(x_i, y_i)$, $i \in I$, $I = \{1, ..., m\}$.

Step 2: By using explicit formulae for solving the OLS problem (see Lemma 2.2) determine $a_0, b_0 \in \mathbb{R}$:

$$a_0 = \frac{\sum (x_i - \overline{x})(y_i - \overline{y})}{\sum (x_i - \overline{x})^2}, \quad b_0 = \overline{y} - a_0 \overline{x},$$
where $\overline{x} = \frac{1}{m} \sum x_i, \quad \overline{y} = \frac{1}{m} \sum y_i.$

Step 3: Calculate $\omega_i = 1/(|y_i - a_0x_i - b_0|)$, solve the WLS problem

$$G(a, b) = \sum \omega_i (y_i - ax_i - b)^2 \to \min$$

by using explicit formulae from Lemma 2.2 and denote the solution by a_1, b_1 :

$$a_1 = \frac{\sum \omega_i (x_i - x_p)(y_i - y_p)}{\sum \omega_i (x_i - x_p)^2}, \quad b_1 = y_p - a_1 x_p, \quad \text{where}$$

$$x_p = \frac{1}{\omega} \sum \omega_i x_i, \quad y_p = \frac{1}{\omega} \sum \omega_i y_i \quad \text{and} \quad \omega = \sum \omega_i.$$

Step 4: If $\max_{i=1,m} \omega_i < M$, put $a_0 = a_1$, $b_0 = b_1$ and go to step 3; otherwise stop.

As shown in [9, 29], this algorithm defines a sequence of approximations $(\theta^{(k)})$ = $(a_k, b_k)^T$, for which the sequence $G_k = G(\theta^{(k)})$ is strictly decreasing. It can be shown that this is actually a special case of the well-known Gauss–Newton method (see, for example, [9, 10, 29])

$$\theta^{(k+1)} = \theta^{(k)} - \lambda_k p^{(k)}, \quad k = 0, 1, \dots,$$

where λ_k is a length of steps in the direction of vector $p^{(k)}$, which is a solution of the WLS problem

$$\sqrt{\Omega^{(k)}}J^{(k)}p \simeq \sqrt{\Omega^{(k)}}r^{(k)}$$

where $J^{(k)}$ is a Jacobian of the function f(x; a, b) = ax + b at the point $\theta^{(k)}$, $r^{(k)}$ a vector of residuals at the point $\theta^{(k)}$, and $\Omega^{(k)}$ a diagonal matrix with elements $\omega_{i}^{(k)} = 1/(|y_i - a_k x_i - b_k|)$.

6. Numerical experiments

In the first example below we graphically illustrate the behaviour of the two-points algorithm; in the second, for a large set of points, we will compare the efficiency of the two-points and IRLS algorithms by using some other methods which can be found in the aforementioned references.

EXAMPLE 1. We are given the set of points $\Lambda = \{T_i(x_i, y_i) \in \mathbb{R}^2 \mid i = 1, ..., 8\}$, where

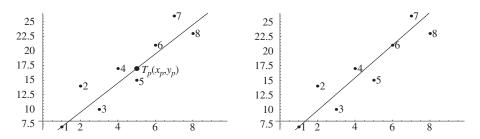


FIGURE 1. Illustration of the two-points algorithm.

10 100 500 1000 5000 10000 2(0)Two-points algorithm 3(0.03)3(0.42)2(1) 2(24.5)3(75)IRLS algorithm 18(0.05) 16(0)32(0.1)17(0.11) 7(0.22)44(1.4) 1(529) (Li–Arce, [21]) 2(0)2(0.04)3(1.03)4(4.53) 1(105.8)(Wesolowsky, [37]) 3(0)3(0.04)3(1.09)3(4.34)3(127.8)3(635) (0.44)Differential Evolution (0.3)(1.86)(6.95)(194)(825)Nelder-Mead (0.14)(0.16)(1.36)(6.42)(186)(775)Random Search (0.25)(0.47)(3.2)(14.75)(322)(1168)Simulated Annealing (0.25)(0.17)(1.66)(6.53)(209)(852)

TABLE 1. Comparison of algorithms for solving the LAD problem.

The two-points algorithm is initialized so that first the centroid of the data is calculated: $T_p(5, 17) \notin \Lambda$. Then the algorithm chooses the first point $T_1(1, 7) \in \Lambda$ and determines the linear function $f_1(x) = 2.5x + 4.5$, whose graph passes through those two points (see the left-hand illustration in Figure 1). The sum of absolute deviations is $G_1 = 18$.

Then the algorithm fixes the point $T_1(1, 7)$ and chooses a new point $T_6(6, 21)$ and a new linear function $f_2(x) = 2.8x + 4.2$, whose graph passes through those two points (see the right-hand illustration in Figure 1). The sum of absolute deviations is now $G_2 = 17.4$, which is a global minimum for this problem.

Of course, the same result is obtained by applying the module NMinimize using the *Nelder–Mead* method from the Mathematica software (see also [20, 23, 38]).

EXAMPLE 2. We are given the set of points $\Lambda = \{T_i(x_i, y_i) \in \mathbb{R}^2 \mid i = 1, ..., m\}$, where

$$x_i = \frac{10i}{m}, \quad i = 1, \dots, m,$$

$$y_i = 3x_i + 2 + \varepsilon_i, \quad \varepsilon_i \sim N(0, \sigma^2).$$

The efficiency of the two-points and IRLS algorithms will be compared to some special methods for finding the best LAD line [21, 37], but also to general minimization

algorithms, which are also included in Mathematica: DifferentialEvolution, NelderMead, RandomSearch, and SimulatedAnnealing (see also [18, 20, 23, 38]).

For m=10, 100, 500, 1000, 5000, 10 000, Table 1 shows (in parentheses) the time in seconds, and for the two-points, IRLS, Wesolowsky and Li–Arce algorithms the number of iterations 1. It has been shown that the two-points algorithm does not have significantly different properties if it is initialized with the centroid of the data $(\overline{x}, \overline{y})$ or with the point (M_x, M_y) , where M_x (M_y) is the median of the sequence x (y), as proposed in (5.1). Note that for the purpose of computing time efficiency the centroid of the data would be a better choice.

As can be seen, the two-points algorithm reaches a global minimum in only few steps (most often 2–3 steps), while the IRLS algorithm requires a few more iterations. The IRLS algorithm requires a significantly shorter time than the other algorithms considered. The time required by the two-points algorithm is a bit longer, which is probably the result of a direct application of Mathematica module Sort (see [38]). Several fast Sort algorithms can be found in [12]. From Table 1 it can be seen that both proposed algorithms show significant superiority over other methods, which can be further improved by careful programming.

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¹ The corresponding Mathematica modules were written and the Wesolowsky and Li–Arce algorithms tested by I. Kuzmanović, Department of Mathematics, University of Osijek.

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