

LEAST QUANTILE REGRESSION VIA MODERN OPTIMIZATION

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We address the Least Quantile of Squares (LQS) (and in particular the Least Median of Squares) regression problem using modern optimization methods. We propose a Mixed Integer Optimization (MIO) formulation of the LQS problem which allows us to find a provably global optimal solution for the LQS problem. Our MIO framework has the appealing characteristic that if we terminate the algorithm early, we obtain a solution with a guarantee on its sub-optimality. We also propose continuous optimization methods based on first-order subdifferential methods, sequential linear optimization and hybrid combinations of them to obtain near optimal solutions to the LQS problem. The MIO algorithm is found to benefit significantly from high quality solutions delivered by our continuous optimization based methods. We further show that the MIO approach leads to (a) an optimal solution for *any* dataset, where the data-points (y_i, \mathbf{x}_i) 's are not necessarily in general position, (b) a simple proof of the breakdown point of the LQS objective value that holds for any dataset and (c) an extension to situations where there are polyhedral constraints on the regression coefficient vector. We report computational results with both synthetic and real-world datasets showing that the MIO algorithm with warm starts from the continuous optimization methods solve small ($n = 100$) and medium ($n = 500$) size problems to provable optimality in under two hours, and outperform all publicly available methods for large-scale ($n = 10,000$) LQS problems.

1. Introduction. Consider a linear model with response $\mathbf{y} \in \mathfrak{R}^n$, model matrix $\mathbf{X}_{n \times p}$, regression coefficients $\boldsymbol{\beta} \in \mathfrak{R}^p$ and error $\boldsymbol{\varepsilon} \in \mathfrak{R}^n$:

$$\mathbf{y} = \mathbf{X}\boldsymbol{\beta} + \boldsymbol{\varepsilon}.$$

We will assume that \mathbf{X} contains a column of ones to account for the intercept in the model. Given data for the i th sample (y_i, \mathbf{x}_i) , $i = 1, \dots, n$ (where, $\mathbf{x}_i \in \mathfrak{R}^{p \times 1}$) and regression coefficients $\boldsymbol{\beta}$, the i th residual is given by the usual notation $r_i = y_i - \mathbf{x}_i' \boldsymbol{\beta}$ for $i = 1, \dots, n$. The traditional Least Squares (LS) estimator given by

$$(1.1) \quad \hat{\boldsymbol{\beta}}^{(\text{LS})} \in \arg \min_{\boldsymbol{\beta}} \sum_{i=1}^n r_i^2$$

is a popular and effective method for estimating the regression coefficients when the error vector $\boldsymbol{\varepsilon}$ has *small* ℓ_2 -norm. However, in the presence of outliers, the LS

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estimators do not work favorably—a single outlier can have an arbitrarily large effect on the estimate. The robustness of an estimator vis-a-vis outliers is often quantified by the notion of its finite sample breakdown point [Donoho and Huber (1983), Hampel (1971)]. The LS estimate (1.1) has a limiting (in the limit $n \rightarrow \infty$ with p fixed) breakdown point [Hampel (1971)] of zero.

The Least Absolute Deviation (LAD) estimator given by

$$(1.2) \quad \hat{\beta}^{(\text{LAD})} \in \arg \min_{\beta} \sum_{i=1}^n |r_i|$$

considers the ℓ_1 -norm on the residuals, thereby implicitly assuming that the error vector \mathbf{e} has small ℓ_1 -norm. The LAD estimator is not resistant to large deviations in the covariates and, like the optimal LS solutions, has a breakdown point of zero (in the limit $n \rightarrow \infty$ with p fixed).

M-estimators [Huber (1973)] are obtained by minimizing a loss function of the residuals of the form $\sum_{i=1}^n \rho(r_i)$, where $\rho(r)$ is a symmetric function with a unique minimum at zero. Examples include the Huber function and the Tukey function [Huber (2011), Rousseeuw and Leroy (1987)], among others. M-estimators often simultaneously estimate the scale parameter along with the regression coefficient. M-estimators too are severely affected by the presence of outliers in the covariate space. A generalization of M-estimators are Generalized M-estimators [Huber (2011), Rousseeuw and Leroy (1987)], which bound the influence of outliers in the covariate space by the choice of a weight function dampening the effect of outlying covariates. In some cases, they have an improved finite-sample breakdown point of $1/(p+1)$.

The repeated median estimator [Siegel (1982)] with breakdown point of approximately 50%, was one of the earliest estimators to achieve a very high breakdown point. The estimator however, is not equivariant under linear transformations of the covariates.

Rousseeuw (1984) introduced Least Median of Squares (LMS) [see also Hampel (1975)] which minimizes the median of the absolute residuals¹

$$(1.3) \quad \hat{\beta}^{(\text{LMS})} \in \arg \min_{\beta} \left(\text{median}_{i=1, \dots, n} |r_i| \right).$$

The LMS problem is equivariant and has a limiting breakdown point of 50%—making it the first equivariant estimator to achieve the maximal possible breakdown point in the limit $n \rightarrow \infty$ with p fixed.

Instead of considering the median, one may consider more generally, the q th order statistic, which leads to the Least Quantile of Squares (LQS) estimator:

$$(1.4) \quad \hat{\beta}^{(\text{LQS})} \in \arg \min_{\beta} |r_{(q)}|,$$

¹Note that the original definition of LMS [Rousseeuw (1984)] considers the squared residuals instead of the absolute values. However, we will work with the absolute values, since the problems are equivalent.

where $r_{(q)}$ denotes the residual, corresponding to the q th ordered absolute residual:

$$(1.5) \quad |r_{(1)}| \leq |r_{(2)}| \leq \cdots \leq |r_{(n)}|.$$

Rousseeuw (1984) showed that if the sample points (y_i, \mathbf{x}_i) , $i = 1, \dots, n$ are in general position, that is, for any subset of $\mathcal{I} \subset \{1, \dots, n\}$ with $|\mathcal{I}| = p$, the $p \times p$ submatrix $X_{\mathcal{I}}$ has rank p ; an optimal LMS solution (1.3) exists and has a finite sample breakdown point of $(\lfloor n/2 \rfloor - p + 2)/n$, where $\lfloor s \rfloor$ denotes the largest integer smaller than or equal to s . Rousseeuw (1984) showed that the finite sample breakdown point of the estimator (1.3) can be further improved to achieve the maximum possible finite sample breakdown point if one considers the estimator (1.4) with $q = \lfloor n/2 \rfloor + \lfloor (p+1)/2 \rfloor$. The LMS estimator has low efficiency [Rousseeuw (1984)]. This can, however, be improved by using certain post-processing methods on the LMS estimator—the one step M-estimator of Bickel (1975) or a reweighted least-squares estimator, where points with large values of LMS residuals are given small weight are popular methods that are used in this vein.

Related work. It is a well recognized fact that the LMS problem is computationally demanding due to the combinatorial nature of the problem. Bernholt (2005a) showed that computing an optimal LMS solution is NP-hard.

Many algorithms based on different approaches have been proposed for the LMS problem over the past thirty years. State of the art algorithms, however, fail to obtain a global minimum of the LMS problem for problem sizes larger than $n = 50$, $p = 5$. This severely limits the use of LMS for important real world multivariate applications, where n can easily range in the order of a few thousands. It goes without saying that a poor local minimum for the LMS problem may be misleading from a statistical inference point of view [see also Stromberg (1993) and references therein for related discussions on this matter]. The various algorithms presented in the literature for the LMS can be placed into two very broad categories. One approach computes an optimal solution to the LMS problem using geometric characterizations of the fit—they typically rely on complete enumeration and have complexity $O(n^p)$. The other approach gives up on obtaining an optimal solution and resorts to heuristics and/or randomized algorithms to obtain approximate solutions to the LMS problem. These methods, to the best of our knowledge, do not provide certificates about the quality of the solution obtained. We describe below a brief overview of existing algorithms for LMS.

Among the various algorithms proposed in the literature for the LMS problem, the most popular seems to be PROGRESS (Program for Robust Regression) [Rousseeuw and Hubert (1997), Rousseeuw and Leroy (1987)]. The algorithm does a complete enumeration of all p -subsets of the n sample points, computes the hyperplane passing through them and finds the configuration leading to the smallest value of the objective. The algorithm has a run-time complexity of $O(n^p)$ and assumes that the data points are in general position. For computational scalability, heuristics that randomly sample subsets are often used. See

also Barreto and Maharry (2006) for a recent work on algorithms for the bivariate regression problem.

Steele and Steiger (1986) proposed exact algorithms for LMS for $p = 2$ with complexity $O(n^3)$ and some probabilistic speed-up methods with complexity $O((n \log(n))^2)$.

Stromberg (1993) proposed an exact algorithm for LMS with run-time $O(n^{(p+2)} \log(n))$ using some insightful geometric properties of the LMS fit. This method does a brute force search among $\binom{n}{p+1}$ different regression coefficient values and scales up to problem sizes $n = 50$ and $p = 5$.

Agullo (1997) proposed a finite branch and bound technique with run-time complexity $O(n^{p+2})$ to obtain an optimal solution to the LMS problem motivated by the work of Stromberg (1993). The algorithm showed superior performance compared to methods preceding it and can scale up to problem sizes $n \approx 70$, $p \approx 4$.

Erickson, Har-Peled and Mount (2006) give an exact algorithm with run-time $O(n^p \log(n))$ for LMS and also show that computing an optimal LMS solution requires $O(n^p)$ time. For the two-dimensional case $p = 2$, Souvaine and Steele (1987) proposed an exact algorithm for LMS with complexity $O(n^2)$ using the topological sweep-line technique.

Giloni and Padberg (2002) propose integer optimization formulations for the LMS problem, however, no computational experiments are reported—the practical performance of the proposed method thus remains unclear.

Mount et al. (2007) present an algorithm based on branch and bound for $p = 2$ for computing approximate solutions to the LMS problem. Mount et al. (2000) present a quantile approximation algorithm with approximation factor ε with complexity $O(n \log(n) + (1/\varepsilon)^{O(p)})$. Chakraborty and Chaudhuri (2008) present probabilistic search algorithms for a class of problems in robust statistics. Nunkesser and Morell (2010) describe computational procedures based on heuristic search strategies using evolutionary algorithms for some robust statistical estimation problems including LMS. Hawkins (1993) proposes a probabilistic algorithm for LMS known as the “Feasible Set Algorithm” capable of solving problems up to sizes $n = 100$, $p = 3$.

Bernholt (2005b) describes a randomized algorithm for computing the LMS running in $O(n^p)$ time and $O(n)$ space, for fixed p . Olson (1997) describes an approximation algorithm to compute an optimal LMS solution within an approximation factor of two using randomized sampling methods—the method has (expected) run-time complexity of $O(n^{p-1} \log(n))$.

Related approaches in robust regression. Other estimation procedures that achieve a high breakdown point and good statistical efficiency include the least trimmed squares estimator [Rousseeuw (1984), Rousseeuw and Leroy (1987)], which minimizes the sum of squares of the q smallest squared residuals. Another popular approach is based on S-estimators [Rousseeuw (1984), Rousseeuw and

Leroy (1987)], which are a type of M-estimators of scale on the residuals. These estimation procedures like the LMS estimator are NP-hard [Bernholt (2005a)].

We refer the interested reader to Hubert, Rousseeuw and Van Aelst (2008) for a nice review of various robust statistical methods and their applications [Meer et al. (1991), Rousseeuw et al. (2006), Stewart (1999)].

What this paper is about. In this paper, we propose a computationally tractable framework to compute a globally optimal solution to the LQS problem (1.4), and in particular the LMS problem via modern optimization methods: first-order methods from continuous optimization and mixed integer optimization (MIO), see Bertsimas and Weismantel (2005). Our view of computational tractability is not polynomial time solution times as these do not exist for the LQS problem unless $P = NP$. Rather it is the ability of a method to solve problems of practical interest in times that are appropriate for the application addressed. An important advantage of our framework is that it easily adapts to obtain solutions to more general variants of (1.4) under polyhedral constraints, that is,

$$(1.6) \quad \underset{\boldsymbol{\beta}}{\text{minimize}} \quad |r_{(q)}|, \quad \text{subject to} \quad \mathbf{A}\boldsymbol{\beta} \leq \mathbf{b},$$

where $\mathbf{A}_{m \times p}$, $\mathbf{b}_{m \times 1}$ are given parameters in the problem representing side constraints on the variable $\boldsymbol{\beta}$ and “ \leq ” denotes component wise inequality. This is useful if one would like to incorporate some form of regularization on the $\boldsymbol{\beta}$ coefficients, for example, ℓ_1 regularization [Tibshirani (1996)] or generalizations thereof.

Contributions. Our contributions in this paper may be summarized as follows:

(1) We use MIO to find a provably optimal solution to the LQS problem. Our framework has the appealing characteristic that if we terminate the algorithm early, we obtain a solution with a guarantee on its suboptimality. We further show that the MIO approach leads to an optimal solution for *any* dataset where the data-points (y_i, \mathbf{x}_i) 's are not necessarily in general position. Our framework enables us to provide a simple proof of the breakdown point of the LQS objective value, generalizing the existing results for the problem. Furthermore, our approach is readily generalizable to problems of the type (1.6).

(2) We introduce a variety of solution methods based on modern continuous optimization—first-order subdifferential based minimization, sequential linear optimization and a hybrid version of these two methods that provide near optimal solutions for the LQS problem. The MIO algorithm is found to significantly benefit from solutions obtained by the continuous optimization methods.

(3) We report computational results with both synthetic and real-world datasets that show that the MIO algorithm with warm starts from the continuous optimization methods solve small ($n = 100$) and medium ($n = 500$) size LQS problems

to provable optimality in under two hours, and outperform all publicly available methods for large-scale ($n = 10,000$) LQS problems, but without showing provable optimality in under two hours of computation time.

Structure of the paper. The paper is organized as follows. Section 2 describes MIO approaches for the LQS problem. Section 3 describes continuous optimization based methods for obtaining local minimizers of the LQS problem. Section 4 describes properties of an optimal LQS solution. Section 5 describes computational results and experiments. The last section contains our key conclusions.

2. Mixed integer optimization formulation. In this section, we present an exact MIO formulation for the LQS problem. For the sake of completeness, we will first introduce the definition of a linear MIO problem. The generic MIO framework concerns the following optimization problem:

$$\begin{aligned}
 \text{minimize} \quad & \mathbf{c}'\boldsymbol{\alpha} + \mathbf{d}'\boldsymbol{\theta}, \\
 & A\boldsymbol{\alpha} + B\boldsymbol{\theta} \geq \mathbf{b}, \\
 (2.1) \quad & \boldsymbol{\alpha} \in \mathfrak{N}_+^n, \\
 & \boldsymbol{\theta} \in \{0, 1\}^m,
 \end{aligned}$$

where $\mathbf{c} \in \mathfrak{N}^n$, $\mathbf{d} \in \mathfrak{N}^m$, $A \in \mathfrak{N}^{k \times n}$, $B \in \mathfrak{N}^{k \times m}$, $\mathbf{b} \in \mathfrak{N}^k$ are the given parameters of the problem; \mathfrak{N}_+^n denotes the nonnegative n -dimensional orthant, the symbol \geq denotes element-wise inequalities and we optimize over both continuous ($\boldsymbol{\alpha}$) and discrete ($\boldsymbol{\theta}$) variables. For background on MIO, see [Bertsimas and Weismantel \(2005\)](#).

Consider a list of n numbers $|r_1|, \dots, |r_n|$, with the ordering described in (1.5). To model the sorted q th residual, that is, $|r_{(q)}|$, we need to express the fact that $r_i \leq |r_{(q)}|$ for q many residuals $|r_i|$'s from $|r_1|, \dots, |r_n|$. To do so, we introduce the binary variables z_i , $i = 1, \dots, n$ with the interpretation

$$(2.2) \quad z_i = \begin{cases} 1, & \text{if } |r_i| \leq |r_{(q)}|, \\ 0, & \text{otherwise.} \end{cases}$$

We further introduce auxiliary continuous variables $\mu_i, \bar{\mu}_i \geq 0$, such that

$$(2.3) \quad |r_i| - \mu_i \leq |r_{(q)}| \leq |r_i| + \bar{\mu}_i, \quad i = 1, \dots, n,$$

with the conditions

$$(2.4) \quad \begin{aligned}
 & \text{if } |r_i| \geq |r_{(q)}|, & \text{then } \bar{\mu}_i = 0, \mu_i \geq 0 \quad \text{and} \\
 & \text{if } |r_i| \leq |r_{(q)}|, & \text{then } \mu_i = 0, \bar{\mu}_i \geq 0.
 \end{aligned}$$

We thus propose the following MIO formulation:

$$\begin{aligned}
 & \text{minimize} && \gamma, \\
 & \text{subject to} && |r_i| + \bar{\mu}_i \geq \gamma, \quad i = 1, \dots, n, \\
 & && \gamma \geq |r_i| - \mu_i, \quad i = 1, \dots, n, \\
 & && M_u z_i \geq \bar{\mu}_i, \quad i = 1, \dots, n, \\
 (2.5) \quad & && M_\ell (1 - z_i) \geq \mu_i, \quad i = 1, \dots, n, \\
 & && \sum_{i=1}^n z_i = q, \\
 & && \mu_i \geq 0, \quad i = 1, \dots, n, \\
 & && \bar{\mu}_i \geq 0, \quad i = 1, \dots, n, \\
 & && z_i \in \{0, 1\}, \quad i = 1, \dots, n,
 \end{aligned}$$

where, $\gamma, z_i, \mu_i, \bar{\mu}_i, i = 1, \dots, n$ are the optimization variables, M_u, M_ℓ are the so-called *Big-M* constants. Let us denote the optimal solution of problem (2.5), which depends on M_ℓ, M_u , by γ^* . Suppose we consider $M_u, M_\ell \geq \max_i |r_{(i)}|$ —it follows from formulation (2.5) that q of the μ_i 's are zero. Thus, γ^* has to be larger than at least q of the $|r_i|$ values. By arguments similar to the above, we see that, since $(n - q)$ of the z_i 's are zero, at least $(n - q)$ many $\bar{\mu}_i$'s are zero. Thus, γ^* is less than or equal to at least $(n - q)$ many of the $|r_i|, i = 1, \dots, n$ values. This shows that γ^* is indeed equal to $|r_{(q)}|$, for M_u, M_ℓ sufficiently large.

We found in our experiments that, in formulation (2.5), if $z_i = 1$, then $\bar{\mu}_i = M_u$ and if $z_i = 0$ then $\mu_i = M_\ell$. Though this does not interfere with the definition of $|r_{(q)}|$, it creates a difference in the strength of the MIO formulation. We describe below how to circumvent this shortcoming.

From (2.4), it is clear that $\bar{\mu}_i \mu_i = 0, \forall i = 1, \dots, n$. The constraint $\bar{\mu}_i \mu_i = 0$ can be modeled via integer optimization using Specially Ordered Sets of type 1 [Bertsimas and Weismantel (2005)], that is, SOS-1 constraints as follows:

$$(2.6) \quad \mu_i \bar{\mu}_i = 0 \iff (\mu_i, \bar{\mu}_i) : \text{SOS-1},$$

for every $i = 1, \dots, n$. In addition, observe that, for M_ℓ sufficiently large and every $i \in \{1, \dots, n\}$ the constraint $M_\ell(1 - z_i) \geq \mu_i \geq 0$ can be modeled² by a SOS-1 constraint— $(\mu_i, z_i) : \text{SOS-1}$. In light of this discussion, we see that

$$(2.7) \quad |r_i| - |r_{(q)}| = \mu_i - \bar{\mu}_i, \quad (\mu_i, \bar{\mu}_i) : \text{SOS-1}.$$

²To see why this is true, observe that $(\mu_i, z_i) : \text{SOS-1}$ is equivalent to $\mu_i z_i = 0$. Now, since $z_i \in \{0, 1\}$, we have the following possibilities: $z_i = 0$, in which case μ_i is free; if $z_i = 1$, then $\mu_i = 0$.

We next show that $|r_{(q)}| \geq \bar{\mu}_i$ and $\mu_i \leq |r_i|$ for all $i = 1, \dots, p$. When $|r_i| \leq |r_{(q)}|$, it follows from the above representation that

$$\mu_i = 0 \quad \text{and} \quad \bar{\mu}_i = |r_{(q)}| - |r_i| \leq |r_{(q)}|.$$

When $|r_i| > |r_{(q)}|$, it follows that $\bar{\mu}_i = 0$. Thus, it follows that $0 \leq \bar{\mu}_i \leq |r_{(q)}|$ for all $i = 1, \dots, n$. It also follows by a similar argument that $0 \leq \mu_i \leq |r_i|$ for all i .

Thus, by using SOS-1 type of constraints, we can avoid the use of *Big-M*'s appearing in formulation (2.5), as follows:

$$\begin{aligned}
 &\text{minimize} && \gamma, \\
 &\text{subject to} && |r_i| - \gamma = \mu_i - \bar{\mu}_i, \quad i = 1, \dots, n, \\
 & && \sum_{i=1}^n z_i = q, \\
 & && \gamma \geq \bar{\mu}_i, \quad i = 1, \dots, n, \\
 (2.8) \quad & && \bar{\mu}_i \geq 0, \quad i = 1, \dots, n, \\
 & && \mu_i \geq 0, \quad i = 1, \dots, n, \\
 & && (\bar{\mu}_i, \mu_i) : \text{SOS-1}, \quad i = 1, \dots, n, \\
 & && (z_i, \mu_i) : \text{SOS-1}, \quad i = 1, \dots, n, \\
 & && z_i \in \{0, 1\}, \quad i = 1, \dots, n.
 \end{aligned}$$

Note, however, that the constraints

$$(2.9) \quad |r_i| - \gamma = \mu_i - \bar{\mu}_i, \quad i = 1, \dots, n$$

are not convex in r_1, \dots, r_n . We thus introduce the following variables r_i^+, r_i^- , $i = 1, \dots, n$ such that

$$\begin{aligned}
 (2.10) \quad &r_i^+ + r_i^- = |r_i|, \quad y_i - \mathbf{x}'_i \boldsymbol{\beta} = r_i^+ - r_i^-, \\
 &r_i^+ \geq 0, r_i^- \geq 0, r_i^+ r_i^- = 0, i = 1, \dots, n.
 \end{aligned}$$

The constraint $r_i^+ r_i^- = 0$ can be modeled via SOS-1 constraints

$$(r_i^+, r_i^-) : \text{SOS-1} \quad \text{for every } i = 1, \dots, n.$$

This leads to the following MIO for the LQS problem that we use in this paper:

$$\begin{aligned}
 &\text{minimize} && \gamma, \\
 &\text{subject to} && r_i^+ + r_i^- - \gamma = \bar{\mu}_i - \mu_i, \quad i = 1, \dots, n, \\
 & && r_i^+ - r_i^- = y_i - \mathbf{x}'_i \boldsymbol{\beta}, \quad i = 1, \dots, n, \\
 (2.11) \quad & && \sum_{i=1}^n z_i = q,
 \end{aligned}$$

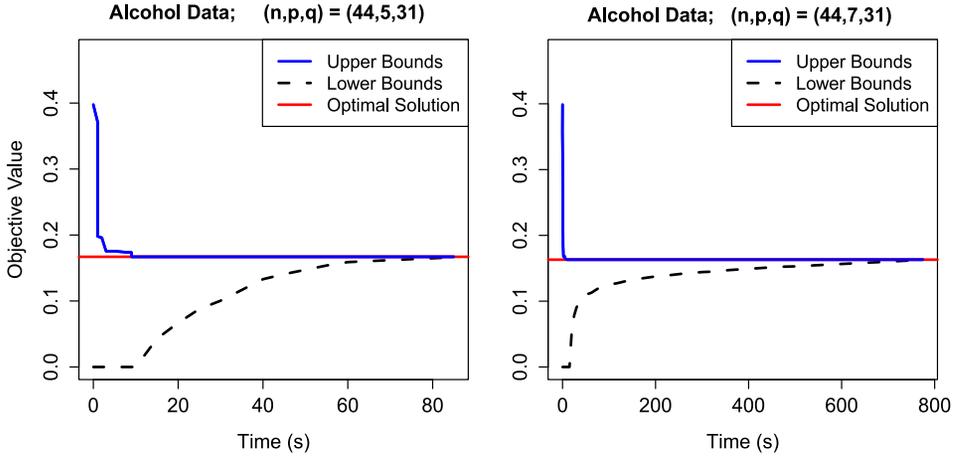


FIG. 1. Figure showing the typical evolution of the MIO formulation (2.11) for the “Alcohol” dataset with $n = 44$, $q = 31$ with $p = 5$ (left panel) and $p = 7$ (right panel). Global solutions for both the problems are found quite quickly in both examples, but it takes longer to certify global optimality via the lower bounds. As expected, the time taken for the MIO to certify convergence to the global optimum increases with increasing p .

$$\begin{aligned}
 \gamma &\geq \mu_i \geq 0, & i &= 1, \dots, n, \\
 \mu_i &\geq 0, & i &= 1, \dots, n, \\
 \bar{\mu}_i &\geq 0, & i &= 1, \dots, n, \\
 r_i^+ &\geq 0, r_i^- \geq 0, & i &= 1, \dots, n, \\
 (\bar{\mu}_i, \mu_i) &: \text{SOS-1}, & i &= 1, \dots, n, \\
 (r_i^+, r_i^-) &: \text{SOS-1}, & i &= 1, \dots, n, \\
 (z_i, \mu_i) &: \text{SOS-1}, & i &= 1, \dots, n, \\
 z_i &\in \{0, 1\}, & i &= 1, \dots, n.
 \end{aligned}$$

To motivate the reader, we show in Figure 1 an example that illustrates that the MIO formulation (2.11) leads to a provably optimal solution for the LQS problem. We give more details in Section 5.

3. Continuous optimization based methods. We describe two main approaches based on continuous optimization for the LQS problem. Section 3.1 presents a method based on sequential linear optimization and Section 3.2 describes a first-order subdifferential based method for the LQS problem. Section 3.3 describes hybrid combinations of the aforementioned approaches, which we have found, empirically, to provide high quality solutions. Section 3.4 describes initialization strategies for the algorithms.

3.1. *Sequential linear optimization.* We describe a sequential linear optimization approach to obtain a local minimum of problem (1.4). We first describe the algorithm, present its convergence analysis and describe its iteration complexity.

Main description of the algorithm. We decompose the q th ordered absolute residual as follows:

$$(3.1) \quad |r_{(q)}| = |y_{(q)} - \mathbf{x}'_{(q)}\boldsymbol{\beta}| = \underbrace{\sum_{i=q}^n |y_{(i)} - \mathbf{x}'_{(i)}\boldsymbol{\beta}|}_{H_q(\boldsymbol{\beta})} - \underbrace{\sum_{i=q+1}^n |y_{(i)} - \mathbf{x}'_{(i)}\boldsymbol{\beta}|}_{H_{q+1}(\boldsymbol{\beta})},$$

where, we use the notation $H_m(\boldsymbol{\beta}) = \sum_{i=m}^n |y_{(i)} - \mathbf{x}'_{(i)}\boldsymbol{\beta}|$ to denote the sum of the largest m ordered residuals $|r_{(i)}| := |y_{(i)} - \mathbf{x}'_{(i)}\boldsymbol{\beta}|$, $i = 1, \dots, n$ in absolute value. The function $H_m(\boldsymbol{\beta})$ can be written as

$$(3.2) \quad \begin{aligned} H_m(\boldsymbol{\beta}) &:= \max_{\mathbf{w}} \sum_{i=1}^n w_i |y_i - \mathbf{x}'_i \boldsymbol{\beta}| \\ \text{subject to} \quad &\sum_{i=1}^n w_i = n - m + 1, \\ &0 \leq w_i \leq 1, \quad i = 1, \dots, n. \end{aligned}$$

Let us denote the feasible set in problem (3.2) by

$$\mathcal{W}_m := \left\{ \mathbf{w} : \sum_{i=1}^n w_i = n - m + 1, w_i \in [0, 1], i = 1, \dots, n \right\}.$$

Observe that for every $\mathbf{w} \in \mathcal{W}_m$ the function $\sum_{i=1}^n w_i |y_i - \mathbf{x}'_i \boldsymbol{\beta}|$ is convex in $\boldsymbol{\beta}$. Furthermore, since $H_m(\boldsymbol{\beta})$ is the point-wise supremum with respect to \mathbf{w} over \mathcal{W}_m , the function $H_m(\boldsymbol{\beta})$ is convex in $\boldsymbol{\beta}$ [see [Boyd and Vandenberghe \(2004\)](#)]. Equation (3.1) thus shows that $|r_{(q)}|$ can be written as the difference of two convex functions, namely, $H_q(\boldsymbol{\beta})$ and $H_{q+1}(\boldsymbol{\beta})$. By taking the dual of problem (3.2) and invoking strong duality, we have

$$(3.3) \quad \begin{aligned} H_m(\boldsymbol{\beta}) &= \min_{\theta, \mathbf{v}} \theta(n - m + 1) + \sum_{i=1}^n v_i \\ \text{subject to} \quad &\theta + v_i \geq |y_i - \mathbf{x}'_i \boldsymbol{\beta}|, \quad i = 1, \dots, n, \\ &v_i \geq 0, \quad i = 1, \dots, n. \end{aligned}$$

Representation (3.2) also provides a characterization of the set of subgradients of $H_m(\boldsymbol{\beta})$:

$$(3.4) \quad \partial H_m(\boldsymbol{\beta}) = \text{conv} \left\{ \sum_{i=1}^n -w_i^* \text{sgn}(y_i - \mathbf{x}'_i \boldsymbol{\beta}) \mathbf{x}_i : \mathbf{w}^* \in \arg \max_{\mathbf{w} \in \mathcal{W}_m} \mathcal{L}(\boldsymbol{\beta}, \mathbf{w}) \right\},$$

where $\mathcal{L}(\boldsymbol{\beta}, \mathbf{w}) = \sum_{i=1}^n w_i |y_i - \mathbf{x}'_i \boldsymbol{\beta}|$ and “conv(S)” denotes the convex hull of set S . An element of the set of subgradients (3.4) will be denoted by $\partial H_m(\boldsymbol{\beta})$.

Recall that (3.1) expresses the q th ordered absolute residual as a difference of two convex functions. Now, having expressed $H_q(\boldsymbol{\beta})$ as the value of a Linear Optimization (LO) problem (3.3) (with $m = q$) we linearize the function $H_{q+1}(\boldsymbol{\beta})$. If $\boldsymbol{\beta}_k$ denotes the value of the estimate at iteration k , we linearize $H_{q+1}(\boldsymbol{\beta})$ at $\boldsymbol{\beta}_k$ as follows:

$$(3.5) \quad H_{q+1}(\boldsymbol{\beta}) \approx H_{q+1}(\boldsymbol{\beta}_k) + \langle \partial H_{q+1}(\boldsymbol{\beta}_k), \boldsymbol{\beta} - \boldsymbol{\beta}_k \rangle,$$

where $\partial H_{q+1}(\boldsymbol{\beta}_k)$ is a subgradient of $H_{q+1}(\boldsymbol{\beta}_k)$ as defined in (3.4), with $m = (q + 1)$.

Combining (3.3) and (3.5), we obtain that, the minimum of problem (3.1) with respect to $\boldsymbol{\beta}$ can be approximated by solving the following LO problem:

$$(3.6) \quad \begin{aligned} \min_{\mathbf{v}, \theta, \boldsymbol{\beta}} \quad & \theta(n - q + 1) + \sum_{i=1}^n v_i - \langle \partial H_{q+1}(\boldsymbol{\beta}_k), \boldsymbol{\beta} \rangle \\ \text{subject to} \quad & \theta + v_i \geq |y_i - \mathbf{x}'_i \boldsymbol{\beta}|, \quad i = 1, \dots, n, \\ & v_i \geq 0, \quad i = 1, \dots, n. \end{aligned}$$

Let $\boldsymbol{\beta}_{k+1}$ denote a minimizer of problem (3.6). This leads to an iterative optimization procedure as described in Algorithm 1.

We next study the convergence properties of Algorithm 1.

Convergence analysis of Algorithm 1. In representation (3.1), we replace $H_q(\boldsymbol{\beta})$ by its dual representation (3.3) to obtain

$$(3.7) \quad \begin{aligned} f_q(\boldsymbol{\beta}) := \min_{\mathbf{v}, \theta} \quad & F(\mathbf{v}, \theta, \boldsymbol{\beta}) := \theta(n - q + 1) + \sum_{i=1}^n v_i - H_{q+1}(\boldsymbol{\beta}) \\ \text{subject to} \quad & \theta + v_i \geq |y_i - \mathbf{x}'_i \boldsymbol{\beta}|, \quad i = 1, \dots, n, \\ & v_i \geq 0, \quad i = 1, \dots, n. \end{aligned}$$

Algorithm 1 Sequential linear optimization algorithm for the LQS problem

1. Initialize with $\boldsymbol{\beta}_1$, and for $k \geq 1$ perform the following steps 2–3 for a pre-defined tolerance parameter “Tol.”
2. Solve the linear optimization problem (3.6) and let $(\mathbf{v}_{k+1}, \theta_{k+1}, \boldsymbol{\beta}_{k+1})$ denote a minimizer.
3. If $(|y_{(q)} - \mathbf{x}'_{(q)} \boldsymbol{\beta}_k| - |y_{(q)} - \mathbf{x}'_{(q)} \boldsymbol{\beta}_{k+1}|) \leq \text{Tol} \cdot |y_{(q)} - \mathbf{x}'_{(q)} \boldsymbol{\beta}_k|$ exit; else go to step 2.

Note that the minimum of problem (3.7)

$$\begin{aligned}
 & \min_{\mathbf{v}, \theta, \boldsymbol{\beta}} \quad F(\mathbf{v}, \theta, \boldsymbol{\beta}) \\
 (3.8) \quad & \text{subject to} \quad \theta + v_i \geq |y_i - \mathbf{x}'_i \boldsymbol{\beta}|, \quad i = 1, \dots, n, \\
 & \quad \quad \quad v_i \geq 0, \quad i = 1, \dots, n
 \end{aligned}$$

equals to $\min_{\boldsymbol{\beta}} f_q(\boldsymbol{\beta})$, which is also the minimum of (1.4), that is, $\min_{\boldsymbol{\beta}} f_q(\boldsymbol{\beta}) = \min_{\boldsymbol{\beta}} |r_{(q)}|$. The objective function $F(\mathbf{v}, \theta, \boldsymbol{\beta})$ appearing in (3.7) is the sum of a linear function in (\mathbf{v}, θ) and a concave function in $\boldsymbol{\beta}$ and the constraints are convex.

Note that the function

$$\begin{aligned}
 (3.9) \quad & Q((\mathbf{v}, \theta, \boldsymbol{\beta}); \bar{\boldsymbol{\beta}}) \\
 & = \theta(n - q + 1) + \sum_{i=1}^n v_i - \langle \partial H_{q+1}(\bar{\boldsymbol{\beta}}), \boldsymbol{\beta} - \bar{\boldsymbol{\beta}} \rangle - H_{q+1}(\bar{\boldsymbol{\beta}}),
 \end{aligned}$$

which is linear in the variables $(\mathbf{v}, \theta, \boldsymbol{\beta})$ is a linearization of $F(\mathbf{v}, \theta, \boldsymbol{\beta})$ at the point $\bar{\boldsymbol{\beta}}$. Since $H_{q+1}(\boldsymbol{\beta})$ is convex in $\boldsymbol{\beta}$, the function $Q((\mathbf{v}, \theta, \boldsymbol{\beta}); \bar{\boldsymbol{\beta}})$ is a majorizer of $F(\mathbf{v}, \theta, \boldsymbol{\beta})$ for any fixed $\bar{\boldsymbol{\beta}}$ with equality holding at $\bar{\boldsymbol{\beta}} = \boldsymbol{\beta}$, that is,

$$Q((\mathbf{v}, \theta, \boldsymbol{\beta}); \bar{\boldsymbol{\beta}}) \geq F(\mathbf{v}, \theta, \boldsymbol{\beta}) \quad \forall \boldsymbol{\beta} \quad \text{and} \quad Q((\mathbf{v}, \theta, \bar{\boldsymbol{\beta}}); \bar{\boldsymbol{\beta}}) = F(\mathbf{v}, \theta, \bar{\boldsymbol{\beta}}).$$

Observe that problem (3.6) minimizes the function $Q((\mathbf{v}, \theta, \boldsymbol{\beta}); \boldsymbol{\beta}_k)$.

It follows that for every fixed $\bar{\boldsymbol{\beta}}$, an optimal solution of the following linear optimization problem:

$$\begin{aligned}
 & \min_{\mathbf{v}, \theta, \boldsymbol{\beta}} \quad Q((\mathbf{v}, \theta, \boldsymbol{\beta}); \bar{\boldsymbol{\beta}}) \\
 (3.10) \quad & \text{subject to} \quad \theta + v_i \geq |y_i - \mathbf{x}'_i \boldsymbol{\beta}|, \quad i = 1, \dots, n, \\
 & \quad \quad \quad v_i \geq 0, \quad i = 1, \dots, n,
 \end{aligned}$$

provides an upper bound to the minimum of problem (3.8), and hence the global minimum of the LQS objective function. We now define the first-order optimality conditions of problem (3.7).

DEFINITION 1. A point $(\mathbf{v}_*, \theta_*, \boldsymbol{\beta}_*)$ satisfies the first-order optimality conditions for the minimization problem (3.8) if (a) $(\mathbf{v}_*, \theta_*, \boldsymbol{\beta}_*)$ is feasible for problem (3.7) and (b) $(\mathbf{v}_*, \theta_*, \boldsymbol{\beta}_*)$ is a minimizer of the following LO problem:

$$\begin{aligned}
 (3.11) \quad & \Delta_* := \min_{\mathbf{v}, \theta, \boldsymbol{\beta}} \left\langle \nabla F(\mathbf{v}_*, \theta_*, \boldsymbol{\beta}_*), \begin{pmatrix} \mathbf{v} - \mathbf{v}_* \\ \theta - \theta_* \\ \boldsymbol{\beta} - \boldsymbol{\beta}_* \end{pmatrix} \right\rangle \\
 & \text{subject to} \quad \theta + v_i \geq |y_i - \mathbf{x}'_i \boldsymbol{\beta}|, \quad i = 1, \dots, n, \\
 & \quad \quad \quad v_i \geq 0, \quad i = 1, \dots, n,
 \end{aligned}$$

where, $\nabla F(\mathbf{v}_*, \theta_*, \boldsymbol{\beta}_*)$ is a subgradient of the function $F(\mathbf{v}_*, \theta_*, \boldsymbol{\beta}_*)$.

It is easy to see that, if $(\mathbf{v}_*, \theta_*, \boldsymbol{\beta}_*)$ satisfies the first-order optimality conditions as in Definition 1, then $\Delta_* = 0$.

REMARK 1. Note that if $(\mathbf{v}_*, \theta_*, \boldsymbol{\beta}_*)$ satisfies the first-order optimality conditions for the minimization problem (3.8), then $\boldsymbol{\beta}_*$ satisfies the first-order stationarity conditions for the LQS minimization problem (1.4).

Let us define Δ_k as a measure of suboptimality of the tuple $(\mathbf{v}_k, \theta_k, \boldsymbol{\beta}_k)$ from first-order stationary conditions, given in Definition 1

$$(3.12) \quad \Delta_k := \left\langle \nabla F(\mathbf{v}_k, \theta_k, \boldsymbol{\beta}_k), \begin{pmatrix} \mathbf{v}_{k+1} - \mathbf{v}_k \\ \theta_{k+1} - \theta_k \\ \boldsymbol{\beta}_{k+1} - \boldsymbol{\beta}_k \end{pmatrix} \right\rangle,$$

where $\{(\mathbf{v}_k, \theta_k, \boldsymbol{\beta}_k)\}_{k \geq 1}$ are as defined in Algorithm 1.

Note that $\Delta_k \leq 0$. If $\Delta_k = 0$, then the point $(\mathbf{v}_k, \theta_k, \boldsymbol{\beta}_k)$ satisfies the first-order stationary conditions. If $\Delta_k < 0$, then we can improve the solution further. The following theorem presents the rate at which $\Delta_k \rightarrow 0$.

THEOREM 3.1. (a) *The sequence $(\mathbf{v}_k, \theta_k, \boldsymbol{\beta}_k)$ generated by Algorithm 1 leads to a decreasing sequence of objective values $F(\mathbf{v}_{k+1}, \theta_{k+1}, \boldsymbol{\beta}_{k+1}) \leq F(\mathbf{v}_k, \theta_k, \boldsymbol{\beta}_k)$, $k \geq 1$ that converge to a value F_* .*

(b) *The measure of suboptimality $\{\Delta_k\}_{K \geq k \geq 1}$ admits a $O(1/K)$ convergence rate, that is,*

$$\frac{F(\mathbf{v}_1, \theta_1, \boldsymbol{\beta}_1) - F_*}{K} \geq \min_{k=1, \dots, K} (-\Delta_k),$$

where $F(\mathbf{v}_k, \theta_k, \boldsymbol{\beta}_k) \downarrow F_*$.

(c) *As $K \rightarrow \infty$ the sequence satisfies the first-order stationary conditions as in Definition 1 for problem (3.8).*

PROOF. Part (a). Since the objective function in (3.10) is a linearization of the concave function (3.7), Algorithm 1 leads to a decreasing sequence of objective values:

$$f_q(\boldsymbol{\beta}_{k+1}) = F(\mathbf{v}_{k+1}, \theta_{k+1}, \boldsymbol{\beta}_{k+1}) \leq F(\mathbf{v}_k, \theta_k, \boldsymbol{\beta}_k) = f_q(\boldsymbol{\beta}_k).$$

Thus, the sequence $F(\mathbf{v}_k, \theta_k, \boldsymbol{\beta}_k)$ is decreasing and bounded below, hence it converges—we denote the limit as F_* .

Part (b). We make use of the concavity of $F(\mathbf{v}, \theta, \boldsymbol{\beta})$ which follows since it can be written as the sum of a linear function in (\mathbf{v}, θ) and $-H_{q+1}(\boldsymbol{\beta})$, which is a concave function in $\boldsymbol{\beta}$. This gives rise to the following inequality:

$$(3.13) \quad \begin{aligned} & F(\mathbf{v}_{k+1}, \theta_{k+1}, \boldsymbol{\beta}_{k+1}) - F(\mathbf{v}_k, \theta_k, \boldsymbol{\beta}_k) \\ & \leq \left\langle \nabla F(\mathbf{v}_k, \theta_k, \boldsymbol{\beta}_k), \begin{pmatrix} \mathbf{v}_{k+1} - \mathbf{v}_k \\ \theta_{k+1} - \theta_k \\ \boldsymbol{\beta}_{k+1} - \boldsymbol{\beta}_k \end{pmatrix} \right\rangle. \end{aligned}$$

Considering inequality (3.13) for $k = 1, \dots, K$, the notation (3.12) and adding up the terms we have

$$(3.14) \quad \sum_{k=1}^K (F(\mathbf{v}_k, \theta_k, \boldsymbol{\beta}_k) - F(\mathbf{v}_{k+1}, \theta_{k+1}, \boldsymbol{\beta}_{k+1})) \geq \sum_{k=1}^K (-\Delta_k),$$

that is,

$$(3.15) \quad F(\mathbf{v}_1, \theta_1, \boldsymbol{\beta}_1) - F(\mathbf{v}_{K+1}, \theta_{K+1}, \boldsymbol{\beta}_{K+1}) \geq K \left(\min_{k=1, \dots, K} (-\Delta_k) \right),$$

that is,

$$(3.16) \quad \frac{F(\mathbf{v}_1, \theta_1, \boldsymbol{\beta}_1) - F_*}{K} \geq \left(\min_{k=1, \dots, K} (-\Delta_k) \right).$$

In the above, while moving from line (3.15) to (3.16) we made use of the fact that $F(\mathbf{v}_{K+1}, \theta_{K+1}, \boldsymbol{\beta}_{K+1}) \geq F_*$, where the decreasing sequence $F(\mathbf{v}_k, \theta_k, \boldsymbol{\beta}_k)$ converges to F_* . Equation (3.16) provides a convergence rate for the algorithm.

Part (c). As $K \rightarrow \infty$, we see that $\Delta_k \rightarrow 0$ —corresponding to the first-order stationarity condition (3.11). This also corresponds to a local minimum of (1.4).

This completes the proof of the theorem. \square

3.2. *A first-order subdifferential based algorithm for the LQS problem.* Subgradient descent methods have a long history in nonsmooth convex optimization [Nesterov (2004), Shor (1985)]. If computation of the subgradients turns out to be inexpensive, then subgradient based methods are quite effective in obtaining a moderate accuracy solution with relatively low computational cost. For nonconvex and nonsmooth functions, a subgradient need not exist, so the notion of a subgradient needs to be generalized. For nonconvex, nonsmooth functions having certain regularity properties (e.g., Lipschitz functions) subdifferentials exist and form a natural generalization of subgradients [Clarke (1990)]. Algorithms based on subdifferential information oracles [see, e.g., Shor (1985)] are thus used as natural generalizations of subgradient methods for nonsmooth, nonconvex optimization problems. While general subdifferential-based methods can become quite complicated based on appropriate choices of the subdifferential and step-size sequences, we propose a simple subdifferential based method for approximately minimizing $f_q(\boldsymbol{\beta})$ as we describe below. Recall that $f_q(\boldsymbol{\beta})$ admits a representation as the difference of two simple convex functions of the form (3.1). It follows that $f_q(\boldsymbol{\beta})$ is Lipschitz [Rockafellar (1996)], almost everywhere differentiable and any element belonging to the set difference

$$\partial f_q(\boldsymbol{\beta}) \in \partial H_q(\boldsymbol{\beta}) - \partial H_{q+1}(\boldsymbol{\beta}),$$

where, $\partial H_m(\boldsymbol{\beta})$ (for $m = q, q + 1$) is the set of subgradients defined in (3.4); is a subdifferential [Shor (1985)] of $f_q(\boldsymbol{\beta})$.

Algorithm 2 Subdifferential based algorithm for the LQS problem

1. Initialize β_1 , for $\text{MaxIter} \geq k \geq 1$ do the following:
 2. $\beta_{k+1} = \beta_k - \alpha_k \partial f_q(\beta_k)$ where α_k is a step-size.
 3. Return $\min_{1 \leq k \leq \text{MaxIter}} f_q(\beta_k)$ and β_{k^*} at which the minimum is attained, where $k^* = \arg \min_{1 \leq k \leq \text{MaxIter}} f_q(\beta_k)$.
-

In particular, the quantity

$$\partial f_q(\beta) = -\text{sgn}(y_{(q)} - \mathbf{x}'_{(q)}\beta)\mathbf{x}_{(q)}$$

is a subdifferential of the function $f_q(\beta)$ at β .

Using the definitions above, we propose a first-order subdifferential based method for the LQS problem as described in Algorithm 2, below.

While various step-size choices are possible, we found the following simple fixed step-size sequence to be quite useful in our experiments:

$$\alpha_k = \frac{1}{\max_{i=1, \dots, n} \|\mathbf{x}_i\|_2},$$

where, the quantity $\max_{i=1, \dots, n} \|\mathbf{x}_i\|_2$ may be interpreted as an upper bound to the subdifferentials of $f_q(\beta)$. Similar constant step-size based rules are often used in subgradient descent methods for convex optimization.

3.3. *A hybrid algorithm.* Let $\hat{\beta}_{\text{GD}}$ denote the estimate produced by Algorithm 2. Since Algorithm 2 runs with a fixed step-size, the estimate $\hat{\beta}_{\text{GD}}$ need not be a local minimum of the LQS problem. Algorithm 1, on the other hand, delivers an estimate $\hat{\beta}_{\text{LO}}$, say, which is a *local* minimum of the LQS objective function. We found that if $\hat{\beta}_{\text{GD}}$ obtained from the subdifferential method is used as a warm-start for the sequential linear optimization algorithm, the estimator obtained improves upon $\hat{\beta}_{\text{GD}}$ in terms of the LQS objective value. This leads to the proposal of a hybrid version of Algorithms 1 and 2, as presented in Algorithm 3 below.

3.4. *Initialization strategies for the algorithms.* Both Algorithms 1 and 2 are sensitive to initializations β_1 . We run each algorithm for a prescribed number of

Algorithm 3 A hybrid algorithm for the LQS problem

1. Run Algorithm 2 initialized with β_1 for MaxIter iterations. Let $\hat{\beta}_{\text{GD}}$ be the solution.
 2. Run Algorithm 1 with $\hat{\beta}_{\text{GD}}$ as the initial solution and Tolerance parameter “Tol” to obtain $\hat{\beta}_{\text{LO}}$.
 3. Return $\hat{\beta}_{\text{LO}}$ as the solution to Algorithm 3.
-

runs “RUNS” (say), and consider the solution that gives the best objective value among them. For the initializations, we found two strategies to be quite useful.

Initialization around LAD solutions. One method is based on the LAD solution, that is, $\hat{\beta}^{(LAD)}$ and random initializations around $\hat{\beta}^{(LAD)}$ given by $[\hat{\beta}_i^{(LAD)} - \eta|\hat{\beta}_i^{(LAD)}|, \hat{\beta}_i^{(LAD)} + \eta|\hat{\beta}_i^{(LAD)}|]$, for $i = 1, \dots, p$, where η is a predefined number say $\eta \in \{2, 4\}$. This initialization strategy leads to β^1 , which we denote by the “LAD” initialization.

Initialization around Chebyshev fits. Another initialization strategy is inspired by a geometric characterization of the LQS solution [see [Stromberg \(1993\)](#) and also Section 4]. Consider a subsample $\mathcal{J} \subset \{1, \dots, n\}$ of size of size $(p + 1)$ and the associated ℓ_∞ regression fit (also known as the Chebyshev fit) on the subsample $(y_i, \mathbf{x}_i), i \in \mathcal{J}$ given by

$$\hat{\beta}_{\mathcal{J}} \in \arg \min_{\beta} \left(\max_{i \in \mathcal{J}} |y_i - \mathbf{x}'_i \beta| \right).$$

Consider a number of random subsamples \mathcal{J} and the associated coefficient-vector $\hat{\beta}_{\mathcal{J}}$ for every \mathcal{J} . The estimate $\hat{\beta}_{\mathcal{J}^*}$ that produces the minimum value of the LQS objective function is taken as β_1 . We denote β_1 chosen in this fashion as the best Chebyshev fit or “Cheb” in short.

Algorithm 3, in our experience, was found to be less sensitive to initializations. Experiments demonstrating the different strategies described above are discussed in Section 5.

4. Properties of the LQS solutions for arbitrary datasets. In this section, we prove that key properties of optimal LQS solutions hold without assuming that the data (\mathbf{y}, \mathbf{X}) are in general position as it is done in the literature to date [[Rousseeuw \(1984\)](#), [Rousseeuw and Leroy \(1987\)](#), [Stromberg \(1993\)](#)]. For this purpose, we utilize the MIO characterization of the LQS problem. Specifically:

(1) We show in [Theorem 4.1](#) that an optimal solution to the LQS problem (and in particular the LMS problem) always exists, for *any* (\mathbf{y}, \mathbf{X}) and q . The theorem also shows that an optimal LQS solution is given by the ℓ_∞ or Chebyshev regression fit to a subsample of size q from the sample $(y_i, \mathbf{x}_i), i = 1, \dots, n$, thereby generalizing the results of [Stromberg \(1993\)](#), which require (\mathbf{y}, \mathbf{X}) to be in general position.

(2) We show in [Theorem 4.2](#) that the absolute values of some of the residuals are equal to the optimal solution value of the LQS problem, without assuming that the data is in general position.

(3) We show in [Theorem 4.3](#) a new result that the breakdown point of the optimal value of the LQS objective is $(n - q + 1)/n$ without assuming that the data is in general position. For the LMS problem $q = n - \lfloor n/2 \rfloor$, which leads to the sample breakdown point of LQS objective of $(\lfloor n/2 \rfloor + 1)/n$, independent of the

number of covariates p . In contrast, it is known that LMS solutions have a sample breakdown point of $(\lfloor n/2 \rfloor - p + 2)/n$ (when the data is in general position).

THEOREM 4.1. *The LQS problem is equivalent to the following:*

$$(4.1) \quad \min_{\boldsymbol{\beta}} |r_{(q)}| = \min_{\mathcal{I} \in \Omega_q} \left(\min_{\boldsymbol{\beta}} \|\mathbf{y}_{\mathcal{I}} - \mathbf{X}_{\mathcal{I}}\boldsymbol{\beta}\|_{\infty} \right),$$

where, $\Omega_q := \{\mathcal{I} : \mathcal{I} \subset \{1, \dots, n\}, |\mathcal{I}| = q\}$ and $(\mathbf{y}_{\mathcal{I}}, \mathbf{X}_{\mathcal{I}})$ denotes the subsample $(y_i, \mathbf{x}_i), i \in \mathcal{I}$.

PROOF. Consider the MIO formulation (2.11) for the LQS problem. Let us take a vector of binary variables $\bar{z}_i \in \{0, 1\}, i = 1, \dots, n$ with $\sum_i \bar{z}_i = q$, feasible for problem (2.11). This vector $\bar{\mathbf{z}} := (\bar{z}_1, \dots, \bar{z}_n)$ gives rise to a subset $\mathcal{I} \in \Omega_q$ given by

$$\mathcal{I} = \{i | \bar{z}_i = 1, i \in \{1, \dots, n\}\}.$$

Corresponding to this subset \mathcal{I} consider the subsample $(\mathbf{y}_{\mathcal{I}}, \mathbf{X}_{\mathcal{I}})$ and the associated optimization problem

$$(4.2) \quad T_{\mathcal{I}} = \min_{\boldsymbol{\beta}} \|\mathbf{y}_{\mathcal{I}} - \mathbf{X}_{\mathcal{I}}\boldsymbol{\beta}\|_{\infty},$$

and let $\boldsymbol{\beta}_{\mathcal{I}}$ be a minimizer of (4.2). Observe that $\bar{\mathbf{z}}, \boldsymbol{\beta}_{\mathcal{I}}$ and $\bar{r}_i = y_i - \mathbf{x}'_i \boldsymbol{\beta}_{\mathcal{I}}, i = 1, \dots, n$ is feasible for problem (2.11). Furthermore, it is easy to see that, if \mathbf{z} is taken to be equal to $\bar{\mathbf{z}}$, then the minimum value of problem (2.11) with respect to the variables $\boldsymbol{\beta}$ and $r_i^+, r_i^-, \mu_i, \bar{\mu}_i$ for $i = 1, \dots, n$ is given by $|\bar{r}_{(q)}| = T_{\mathcal{I}}$. Since every choice of $\mathbf{z} \in \{0, 1\}^n$ with $\sum_i z_i = q$ corresponds to a subset $\mathcal{I} \in \Omega_q$, it follows that the minimum value of problem (2.11) is given by the minimum value of $T_{\mathcal{I}}$ as \mathcal{I} varies over Ω_q .

Note that the minimum in problem (4.1) is attained since it is a minimum over finitely many subsets $\mathcal{I} \in \Omega_q$. This shows that an optimal solution to the LQS problem always exists, without any assumption on the geometry or orientation of the sample points (\mathbf{y}, \mathbf{X}) . This completes the proof of the equivalence (4.1). \square

COROLLARY 1. *Theorem 4.1 shows that an optimal LQS solution for any sample (\mathbf{y}, \mathbf{X}) is given by the Chebyshev or ℓ_{∞} regression fit to a subsample of size q from the n sample points. In particular, for every optimal LQS solution there is a $\mathcal{I}_* \in \Omega_q$ such that*

$$(4.3) \quad \hat{\boldsymbol{\beta}}^{(\text{LQS})} \in \arg \min_{\boldsymbol{\beta}} \|\mathbf{y}_{\mathcal{I}_*} - \mathbf{X}_{\mathcal{I}_*}\boldsymbol{\beta}\|_{\infty}.$$

We next show that, at an optimal solution of the LQS problem, some of the absolute values of the residuals are all equal to the minimum objective value of the LQS

problem, generalizing earlier work by [Stromberg \(1993\)](#). Note that problem (4.2) can be written as the following linear optimization problem:

$$(4.4) \quad \begin{aligned} & \underset{t, \beta}{\text{minimize}} && t, \\ & \text{subject to} && -t \leq y_i - \mathbf{x}'_i \beta \leq t, \quad i \in \mathcal{I}_*. \end{aligned}$$

The Karush Kuhn Tucker (KKT) [[Boyd and Vandenberghe \(2004\)](#)] optimality conditions of problem (4.4) are given by

$$(4.5) \quad \begin{aligned} & \sum_{i \in \mathcal{I}_*} (v_i^- + v_i^+) = 1, \\ & \sum_{i \in \mathcal{I}_*} (v_i^- - v_i^+) \mathbf{x}_i = \mathbf{0}, \\ & v_i^+ (y_i - \mathbf{x}'_i \hat{\beta} - t^*) = 0 \quad \forall i \in \mathcal{I}_*, \\ & v_i^- (y_i - \mathbf{x}'_i \hat{\beta} + t^*) = 0 \quad \forall i \in \mathcal{I}_*, \\ & v_i^+, v_i^- \geq 0 \quad \forall i \in \mathcal{I}_*, \end{aligned}$$

where $\hat{\beta}, t^*$ are optimal solutions³ to (4.4).

Let us denote

$$(4.6) \quad \mathcal{I}^+ := \{i \mid i \in \mathcal{I}_*, |v_i^+ - v_i^-| > 0\},$$

clearly, on this set of indices at least one of v_i^+ or v_i^- is nonzero, which implies $|y_i - \mathbf{x}'_i \hat{\beta}| = t^*$. This gives the following bound:

$$|\mathcal{I}^+| \leq |\{i \in \mathcal{I}_* : |y_i - \mathbf{x}'_i \hat{\beta}| = t^*\}|.$$

It follows from (4.5) that $|\mathcal{I}^+| > \text{rank}([\mathbf{x}_i, i \in \mathcal{I}^+])$. We thus have

$$|\{i \in \mathcal{I}_* : |y_i - \mathbf{x}'_i \hat{\beta}| = t^*\}| \geq |\mathcal{I}^+| > \text{rank}([\mathbf{x}_i, i \in \mathcal{I}^+]).$$

In particular, if the \mathbf{x}_i 's come from a continuous distribution then with probability one:

$$\text{rank}([\mathbf{x}_i, i \in \mathcal{I}^+]) = p \quad \text{and} \quad |\{i \in \mathcal{I}_* : |y_i - \mathbf{x}'_i \hat{\beta}| = t^*\}| \geq (p + 1).$$

This leads to the following theorem.

THEOREM 4.2. *Let $\mathcal{I}_* \in \Omega_q$ denote a subset of size q which corresponds to an optimal LQS solution (see Corollary 1). Consider the KKT optimality conditions of the Chebyshev fit to this subsample $(\mathbf{y}_{\mathcal{I}_*}, \mathbf{X}_{\mathcal{I}_*})$ as given by (4.5). Then*

$$|\{i \in \mathcal{I}_* : |y_i - \mathbf{x}'_i \hat{\beta}| = t^*\}| \geq |\mathcal{I}^+| > \text{rank}([\mathbf{x}_i, i \in \mathcal{I}^+]),$$

where $\hat{\beta}, \mathcal{I}^+$ are as defined in (4.5) and (4.6).

³We use the shorthand $\hat{\beta}$ in place of $\hat{\beta}^{(LQS)}$.

4.1. *Breakdown point and stability of solutions.* In this section, we revisit the notion of a breakdown point of estimators and derive sharper results for the problem without the assumption that the data is in general position. Let $\Theta(\mathbf{y}, \mathbf{X})$ denote an estimator based on a sample (\mathbf{y}, \mathbf{X}) . Suppose the original sample is (\mathbf{y}, \mathbf{X}) and m of the sample points have been replaced arbitrarily—let $(\mathbf{y} + \Delta_{\mathbf{y}}, \mathbf{X} + \Delta_{\mathbf{X}})$ denote the perturbed sample. Let

$$(4.7) \quad \alpha(m; \Theta; (\mathbf{y}, \mathbf{X})) = \sup_{(\Delta_{\mathbf{y}}, \Delta_{\mathbf{X}})} \|\Theta(\mathbf{y}, \mathbf{X}) - \Theta(\mathbf{y} + \Delta_{\mathbf{y}}, \mathbf{X} + \Delta_{\mathbf{X}})\|,$$

denote the maximal change in the estimator under this perturbation, where $\|\cdot\|$ denotes the standard Euclidean norm. The finite sample breakdown point of the estimator Θ is defined as follows:

$$(4.8) \quad \eta(\Theta; (\mathbf{y}, \mathbf{X})) := \min_m \left\{ \frac{m}{n} \mid \alpha(m; \Theta; (\mathbf{y}, \mathbf{X})) = \infty \right\}.$$

We will derive the breakdown point of the minimum value of the LQS objective function, that is, $|r_{(q)}| = |y_{(q)} - \mathbf{x}'_{(q)} \hat{\boldsymbol{\beta}}^{(LQS)}|$, as defined in (3.1).

THEOREM 4.3. *Let $\hat{\boldsymbol{\beta}}^{(LQS)}$ denote an optimal solution and $\Theta := \Theta(\mathbf{y}, \mathbf{X})$ denote the optimum objective value to the LQS problem for a given dataset (\mathbf{y}, \mathbf{X}) , where the (y_i, \mathbf{x}_i) 's are not necessarily in general position. Then the finite sample breakdown point of Θ is $(n - q + 1)/n$.*

PROOF. We will first show that the breakdown point of Θ is strictly greater than $(n - q)/n$. Suppose we have a corrupted sample $(\mathbf{y} + \Delta_{\mathbf{y}}, \mathbf{X} + \Delta_{\mathbf{X}})$, with $m = n - q$ replacements in the original sample. Consider the equivalent LQS formulation (4.1) and let \mathcal{I}_0 denote the unchanged sample indices. Consider the inner convex optimization problem appearing in (4.1), corresponding to the index set \mathcal{I}_0 :

$$(4.9) \quad T_{\mathcal{I}_0}(\mathbf{y} + \Delta_{\mathbf{y}}, \mathbf{X} + \Delta_{\mathbf{X}}) = \min_{\boldsymbol{\beta}} \|\mathbf{y}_{\mathcal{I}_0} - \mathbf{X}_{\mathcal{I}_0} \boldsymbol{\beta}\|_{\infty},$$

with $\boldsymbol{\beta}_{\mathcal{I}_0}(\mathbf{y} + \Delta_{\mathbf{y}}, \mathbf{X} + \Delta_{\mathbf{X}})$ denoting a minimizer of the convex optimization problem (4.9). Clearly, both a minimizer and the minimum objective value are finite and neither depends upon $(\Delta_{\mathbf{y}}, \Delta_{\mathbf{X}})$. Suppose

$$T_{\mathcal{I}_*}(\mathbf{y} + \Delta_{\mathbf{y}}, \mathbf{X} + \Delta_{\mathbf{X}}) = \min_{\mathcal{I} \in \Omega_q} T_{\mathcal{I}}(\mathbf{y} + \Delta_{\mathbf{y}}, \mathbf{X} + \Delta_{\mathbf{X}})$$

denotes the minimum value of the LQS objective function corresponding to the perturbed sample, for some $\mathcal{I}_* \in \Omega_q$, then it follows that: $T_{\mathcal{I}_*}(\mathbf{y} + \Delta_{\mathbf{y}}, \mathbf{X} + \Delta_{\mathbf{X}}) \leq T_{\mathcal{I}_0}(\mathbf{y} + \Delta_{\mathbf{y}}, \mathbf{X} + \Delta_{\mathbf{X}})$ —which clearly implies that the quantity $\|T_{\mathcal{I}_0}(\mathbf{y} + \Delta_{\mathbf{y}}, \mathbf{X} + \Delta_{\mathbf{X}}) - \Theta\|$ is bounded above and the bound does not depend upon $(\Delta_{\mathbf{y}}, \Delta_{\mathbf{X}})$. This shows that the breakdown point of Θ is strictly larger than $\frac{(n-q)}{n}$.

We will now show that the breakdown point of the estimator is less than or equal to $(n - q + 1)/n$. If the number of replacements is given by $m = n - q + 1$, then it is easy to see that every $\mathcal{I} \in \Omega_q$ includes a sample i_0 (say) from the replaced sample units. If $(\delta_{y_{i_0}}, \delta'_{\mathbf{x}_{i_0}})$ denotes the perturbation corresponding to the i_0 th sample, then it is easy to see that

$$T_{\mathcal{I}}(\mathbf{y} + \Delta_{\mathbf{y}}, \mathbf{X} + \Delta_{\mathbf{X}}) \geq |(y_{i_0} - \mathbf{x}_{i_0} \boldsymbol{\beta}_{\mathcal{I}}) + (\delta_{y_{i_0}} - \delta'_{\mathbf{x}_{i_0}} \boldsymbol{\beta}_{\mathcal{I}})|,$$

where $\boldsymbol{\beta}_{\mathcal{I}}$ is a minimizer for the corresponding problem (4.9) (with $\mathcal{I}_0 = \mathcal{I}$). It is possible to choose $\delta_{y_{i_0}}$ such that the r.h.s. of the above inequality becomes arbitrarily large. Thus, the finite-sample breakdown point of the estimator Θ is $\frac{(n-q)+1}{n}$. \square

For the LMS problem $q = n - \lfloor n/2 \rfloor$, which leads to the sample breakdown point of Θ of $(\lfloor n/2 \rfloor + 1)/n$, independent of the number of covariates p . In contrast, LMS solutions have a sample breakdown point of $(\lfloor n/2 \rfloor - p + 2)/n$. In other words, the optimal solution value is more robust than optimal solutions to the LMS problem.

5. Computational experiments. In this section, we perform computational experiments demonstrating the effectiveness of our algorithms in terms of quality of solutions obtained, scalability and speed.

All computations were done in MATLAB version R2011a on a 64-bit linux machine, with 8 cores and 32 GB RAM. For the MIO formulations we used GUROBI [Gurobi Optimization (2013)] via its MATLAB interface.

We consider a series of examples including synthetic and real-world datasets showing that our proposed methodology consistently finds high quality solutions of problems of sizes up to $n = 10,000$ and $p = 20$. For moderate-large sized examples, we observed that global optimum solutions are obtained usually within a few minutes (or even faster), but it takes longer to deliver a certificate of global optimality. Our continuous optimization based methods enhance the performance of the MIO formulation, the margin of improvement becomes more significant with increasing problem sizes. In all the examples, there is an appealing common theme—if the MIO algorithm is terminated early, the procedure provides a bound on its suboptimality.

In Section 5.1, we describe the synthetic datasets used in our experiments. Section 5.2 presents a deeper understanding of Algorithms 1, 2 and 3. Section 5.3 presents comparisons of Algorithms 1, 2 and 3 as well as the MIO algorithm with state of the art algorithms for the LQS. In Section 5.4, we illustrate the performance of our algorithms on real-world data sets. Section 5.5 discusses the evolution of lower bounds and global convergence certificates for the problem. Section 5.6 describes scalability considerations for larger problems.

5.1. *Synthetic examples.* We considered a set of synthetic examples, following Rousseeuw and Driessen (2006). We generated the model matrix $\mathbf{X}_{n \times p}$ with i.i.d. Gaussian entries $N(0, 100)$ and took $\boldsymbol{\beta} \in \Re^p$ to be a vector of all ones. Subsequently, the response is generated as $\mathbf{y} = \mathbf{X}\boldsymbol{\beta} + \boldsymbol{\varepsilon}$, where $\varepsilon_i \sim N(0, 10)$, $i = 1, \dots, n$. Once (\mathbf{y}, \mathbf{X}) have been generated, we corrupt a certain proportion π of the sample in two different ways:

(A) $\lfloor \pi n \rfloor$ of the samples are chosen at random and the first coordinate of the data matrix \mathbf{X} , that is, x_{1j} 's are replaced by $x_{1j} \leftarrow x_{1j} + 1000$.

(B) $\lfloor \pi n \rfloor$ of the samples are chosen at random out of which the covariates of half of the points are changed as in item (A); for the remaining half of the points the responses are corrupted as $y_j \leftarrow y_j + 1000$. In this set-up, outliers are added in *both* the covariate and response spaces.

We considered seven different examples for different values of (n, p, π) :

Moderate-scale: We consider four moderate-scale examples Ex-1–Ex-4:

Ex-1: Data is generated as per (B) with $(n, p, \pi) = (201, 5, 0.4)$.

Ex-2: Data is generated as per (B) with $(n, p, \pi) = (201, 10, 0.5)$.

Ex-3: Data is generated as per (A) with $(n, p, \pi) = (501, 5, 0.4)$.

Ex-4: Data is generated as per (A) with $(n, p, \pi) = (501, 10, 0.4)$.

Large-scale: We consider three large-scale examples, Ex-5–Ex-7:

Ex-5: Data is generated as per (B) with $(n, p, \pi) = (2001, 10, 0.4)$.

Ex-6: Data is generated as per (B) with $(n, p, \pi) = (5001, 10, 0.4)$.

Ex-7: Data is generated as per (B) with $(n, p, \pi) = (10, 001, 20, 0.4)$.

5.2. *A deeper understanding of Algorithms 1, 2 and 3.* For each of the synthetic examples Ex-1–Ex-4, we compared the performances of the different continuous optimization based algorithms proposed in this paper—Algorithms 1, 2 and 3. For each of the Algorithms 1, 2, we considered two different initializations, following the strategy described in Section 3.4:

(LAD) This is the initialization from the LAD solution, with $\eta = 2$ and number of random initializations taken to be 100. This is denoted in Table 1 by the moniker “LAD.”

(Cheb) This is the initialization from the Chebyshev fit. For every initialization, forty different subsamples were taken to estimate $\boldsymbol{\beta}_1$, 100 different initializations were considered. This method is denoted by the moniker “Cheb” in Table 1.

Algorithm 1, initialized at the “LAD” method (described above) is denoted by Algorithm 1 (LAD), the same notation carries over to the other remaining combinations of Algorithms 1 and 2 with initializations “LAD” and “Cheb.” Each of the methods Algorithms 2 (LAD) and 2 (Cheb), lead to an initialization for Algorithm 3—denoted by Algorithms 3 (LAD) and 3 (Cheb), respectively.

TABLE 1

Table showing performances of different continuous optimization based methods proposed in this paper, for examples, Ex-1–Ex-4. For every example, the top row “Accuracy” is Relative Accuracy [see (5.1)] and the numbers inside parenthesis denotes standard errors (across the random runs); the lower row denotes the time taken (in cpu seconds). Results are averaged over 20 different random instances of the problem. Algorithm 3 seems to be the clear winner among the different examples, in terms of the quality of solutions obtained. Among all the algorithms considered, Algorithm 3 seems to be least sensitive to initializations

Example (n, p, π) q		Algorithm used					
		Algorithm 1		Algorithm 2		Algorithm 3	
		(LAD)	(Cheb)	(LAD)	(Cheb)	(LAD)	(Cheb)
Ex-1 (201, 5, 0.4) $q = 121$	Accuracy	49.399 (2.43)	0.0 (0.0)	0.233 (0.03)	0.240 (0.02)	0.0 (0.0)	0.0 (0.0)
	Time (s)	24.05	83.44	3.29	83.06	36.13	118.43
Ex-2 (201, 10, 0.5) $q = 101$	Accuracy	43.705 (2.39)	5.236 (1.73)	1.438 (0.07)	1.481 (0.10)	0.0 (0.0)	0.0 (0.0)
	Time (s)	54.39	133.79	3.22	73.14	51.89	125.55
Ex-3 (501, 5, 0.4) $q = 301$	Accuracy	2.897 (0.77)	0.0 (0.0)	0.249 (0.05)	0.274 (0.06)	0.0 (0.0)	0.0 (0.0)
	Time (s)	83.01	158.41	3.75	62.36	120.90	179.34
Ex-4 (501, 10, 0.4) $q = 301$	Accuracy	8.353 (2.22)	11.926 (2.31)	1.158 (0.06)	1.083 (0.06)	0.0	0.0
	Time (s)	192.02	240.99	3.76	71.45	155.36	225.09

In all the examples, we set the MaxIter counter for Algorithm 2 at 500 and took the step-size sequence as described in Section 3.2. The tolerance criterion “Tol” used in Algorithm 1 (and consequently Algorithm 3), was set to 10^{-4} .

Results comparing these methods are summarized in Table 1. To compare the different algorithms in terms of the quality of solutions obtained, we do the following. For every instance, we run all the algorithms and obtain the best solution among them, say, f_* . If f_{alg} denotes the value of the LQS objective function for algorithm “alg,” then we define the relative accuracy of the solution obtained by “alg” as

$$(5.1) \quad \text{Relative Accuracy} = (f_{\text{alg}} - f_*)/f_* \times 100.$$

To obtain the entries in Table 1, the relative accuracy is computed for every algorithm (six in all: Algorithms 1—3, two types for each “LAD” and “Cheb”) for every random problem instance corresponding to a particular example type; and the results are averaged (over 20 runs). The times reported for Algorithms 1 (LAD) and 1 (Cheb) includes the times taken to perform the LAD and Chebyshev fits, respectively. The same thing applies to Algorithms 2 (LAD) and 2 (Cheb). For Algorithm 3 (Cheb) [resp., Algorithm 3 (LAD)], the time taken equals the time taken by Algorithm 2 (Cheb) [resp., Algorithm 2 (LAD)] and the time taken to perform the Chebyshev (resp., LAD) fits.

In Table 1, we see that Algorithm 2 (LAD) converges quite quickly in all the examples. The quality of the solution, however, depends upon the choice of p —for $p = 10$ the algorithm converges to a lower quality solution when compared to $p = 5$. The time till convergence for Algorithm 2 is less sensitive to the problem dimensions—this is in contrast to the other algorithms, where computation times show a monotone trend depending upon the sizes of (n, p) . Algorithm 2 (Cheb) takes more time than Algorithm 2 (LAD), since it spends a considerable amount of time in performing multiple Chebyshev fits (to obtain a good initialization). Algorithm 1 (LAD) seems to be sensitive to the type of initialization used; Algorithm 1 (Cheb) is more stable and it appears that the multiple Chebyshev initialization guides Algorithm 1 (Cheb) to higher quality solutions. Algorithm 3 (both variants) seem to be the clear winner among the various algorithms—this does not come as a surprise since, intuitively it aims at combining the *best features* of its constituent algorithms. Based on computation times, Algorithm 3 (LAD) outperforms Algorithm 3 (Cheb), since it avoids the computational overhead of computing several Chebyshev fits.

5.3. Comparisons: Quality of the solutions obtained. In this section, we shift our focus from studying the detailed dynamics of Algorithms 1—3; and compare the performances of Algorithm 3 (which seems to be the best among the algorithms we propose in the paper), the MIO formulation (2.11) and state-of-the art implementations of the LQS problem as implemented in the popular R-package MASS (available from CRAN). For the MIO formulation (2.11), we considered two

TABLE 2

Table showing performances of various algorithms for the LQS problem for different moderate-scale examples as described in the text. For each example, “Accuracy” is Relative Accuracy [see (5.1)], the numbers within brackets denote the standard errors; the lower row denotes the averaged cpu time (in secs) taken by the algorithm. All results are averaged over 20 random examples. The MIO formulation (2.11) warm-started with Algorithm 3 seems to be the best performer in terms of obtaining the best solution. The combined time taken by MIO formulation (2.11) (warm-start) and Algorithm 3 (which is used as a warm-start) equals the run-time of MIO formulation (2.11) (cold-start)

Example (n, p, π) q		Algorithm used			
		LQS (MASS)	Algorithm 3	MIO formulation (2.11)	
				(Cold-start)	(Warm-start)
Ex-1 (201, 5, 0.4) $q = 121$	Accuracy	24.163 (1.31)	0.0 (0.0)	60.880 (5.60)	0.0 (0.0)
	Time (s)	0.02	36.13	71.46	35.32
Ex-2 (201, 10, 0.5) $q = 101$	Accuracy	105.387 (5.26)	0.263 (0.26)	56.0141 (3.99)	0.0 (0.0)
	Time (s)	0.05	51.89	193.00	141.10
Ex-3 (501, 5, 0.4) $q = 301$	Accuracy	9.677 (0.99)	0.618 (0.27)	11.325 (1.97)	0.127 (0.11)
	Time (s)	0.05	120.90	280.66	159.76
Ex-4 (501, 5, 0.4) $q = 301$	Accuracy	29.756 (1.99)	0.341 (0.33)	27.239 (2.66)	0.0 (0.0)
	Time (s)	0.08	155.36	330.88	175.52

variations: MIO formulation (2.11) (cold-start), where the MIO algorithm is not provided with any advanced warm-start and MIO formulation (2.11) (warm-start), where the MIO algorithm is provided with an advanced warm-start obtained by Algorithm 3. The times taken by MIO formulation (2.11) (warm-start) do not include the times taken by Algorithm 3, the combined times are similar to the times taken by MIO formulation (2.11) (cold-start).

The focus here is on comparing the quality of upper bounds to the LQS problem. We consider the same datasets used in Section 5.2 for our experiments. The results are shown in Table 2. We see that MIO formulation (2.11) (warm-start) is the clear winner among all the examples, Algorithm 3 comes a close second. MIO formulation (2.11) (cold-start) in the absence of advanced warm-starts as provided by Algorithm 3 requires more time to obtain high quality upper bounds. The state-of-the-art algorithm for LQS (obtained from the R-package MASS) delivers a solution very quickly, but the solutions obtained are quite far from the global minimum.

5.4. *Performance on some real-world datasets.* We considered a few real-world datasets popularly used in the context of robust statistical estimation, as available from the R-package `robustbase` [Rousseeuw et al. (2013), Todorov and Filzmoser (2009)]. We used the “Alcohol” dataset (available from the same package), which is aimed at studying the solubility of alcohols in water to understand alcohol transport in living organisms. This dataset contains physicochemical

characteristics of $n = 44$ aliphatic alcohols and measurements on seven numeric variables: SAG solvent accessible surface-bounded molecular volume (x_1), logarithm of the octanol-water partitions coefficient (x_2), polarizability (x_3), molar refractivity (x_4), mass (x_5), volume (x_6) and the response (y) is taken to be the logarithm of the solubility. We consider two cases from the Alcohol dataset—the first one has $n = 44$, $p = 5$ where the five covariates were x_1, x_2, x_4, x_5, x_6 ; the second example has all the six covariates and an intercept term, which leads to $p = 7$. We used the MIO formulation (2.11) (cold-start) for both the cases. The evolution of the MIO (with upper and lower bounds) for the two cases are shown in Figure 1. As expected, the time taken for the algorithm to converge is larger for $p = 7$ than for $p = 5$.

We considered a second dataset created by Hawkins, Bradu and Kass (1984) and available from the R-package `robustbase`. The dataset consists of 75 observations in four dimensions (one response and three explanatory variables), that is, $n = 75$, $p = 3$. We computed the LQS estimate for this example for $q \in \{60, 45\}$. We used both the MIO formulation (2.11) (cold-start) and MIO formulation (2.11) (warm-start) and observed that the latter showed superior convergence speed to global optimality (see Figure 2). As expected, the time taken for convergence was found to increase with decreasing q -values. The results are shown in Figure 2.

5.5. Certificate of lower bounds and global optimality. The MIO formulation (2.11) for the LQS problem converges to the global solution. With the aid of advanced MIO warm-starts as provided by Algorithm 3 the MIO obtains a very high quality solution very quickly—in most of the examples the solution thus obtained, indeed turns out to be the global minimum. However, the certificate of global optimality comes later as the lower bounds of the problem “evolve” slowly; see, for example, Figures 1 and 2. We will now describe a regularized version of the MIO formulation, which we found to be quite useful in speeding up the convergence of the MIO algorithm without any loss in the accuracy of the solution. The LQS problem formulation does not contain any explicit regularization on β , it is rather implicit (since $\hat{\beta}^{(\text{LQS})}$ will be generally bounded). We thus consider the following modified version of the LQS problem (1.4):

$$(5.2) \quad \begin{aligned} & \underset{\beta}{\text{minimize}} && |r_{(q)}|, \\ & \text{subject to} && \|\beta - \beta_0\|_\infty \leq M \end{aligned}$$

for some predefined β_0 and $M \geq 0$. If $\hat{\beta}_M$ solves problem (5.2), then it is the global minimum of the LQS problem in the ℓ_∞ -ball $\{\beta : -M\mathbf{1} \leq \beta - \beta_0 \leq M\mathbf{1}\}$. In particular, if $\hat{\beta}^{\text{LQS}}$ is the solution to problem (1.4), then by choosing $\beta_0 = \mathbf{0}$ and $M \geq \|\hat{\beta}^{\text{LQS}}\|_\infty$ in (5.2); both problems (1.4) and (5.2) will have the same solution. The MIO formulation of problem (5.2) is a very simple modification of (2.11) with additional box-constraints on β of the form $\{\beta : -M\mathbf{1} \leq \beta - \beta_0 \leq M\mathbf{1}\}$. Our

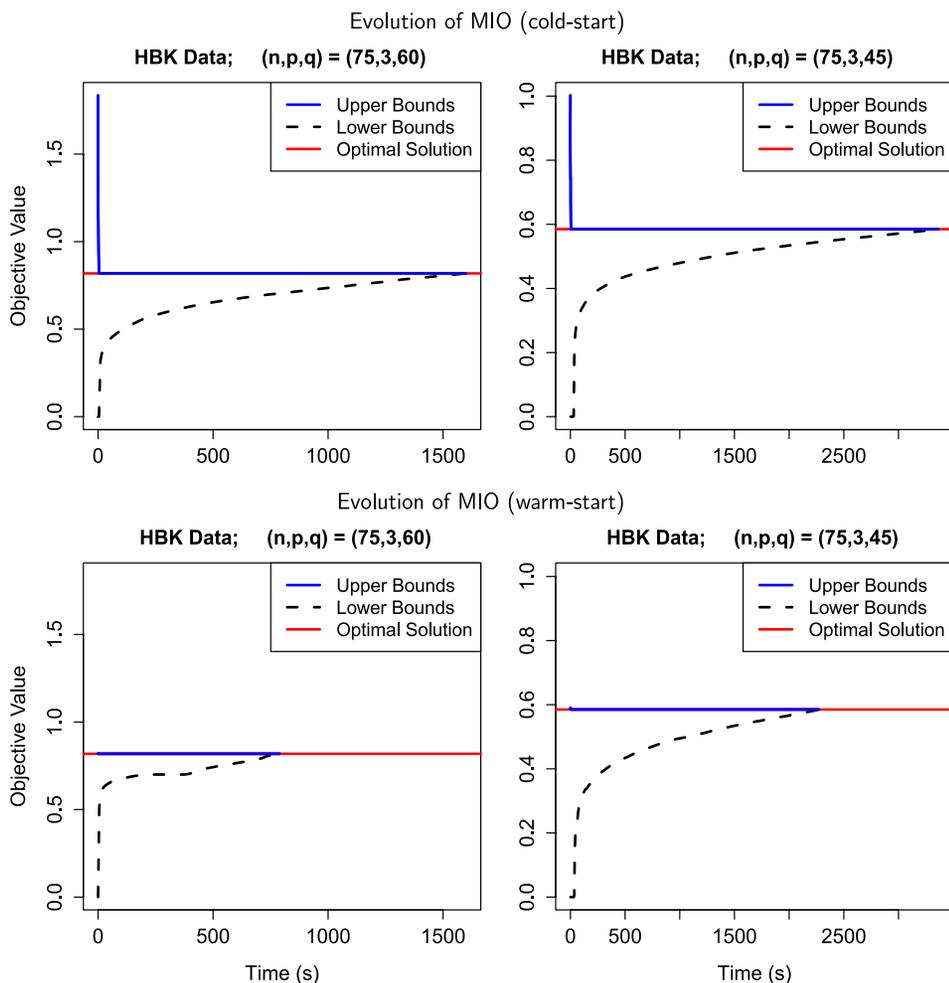


FIG. 2. Figure showing the evolution of the MIO formulation (2.11) for the HBK dataset with different values of q with and without warm-starts. (Top row) MIO formulation warm-started with the least squares solution (which we denote by “cold-start”), for $q = 60$ (left panel) and $q = 45$ (right panel). (Bottom row) MIO formulation warm-started with Algorithm 3 for $q = 60$ (left panel) and $q = 45$ (right panel).

empirical investigation suggests that the MIO formulation (2.11) in presence of box-constraints⁴ produces tighter lower bounds than the unconstrained MIO formulation (2.11), for a given time limit. As an illustration of formulation (5.2), see Figure 3, where we use the MIO formulation (2.11) with box constraints. We consider two cases corresponding to $M \in \{3, 40\}$; in both the cases we took

⁴Of course, a very large value of M will render the box-constraints to be ineffective.

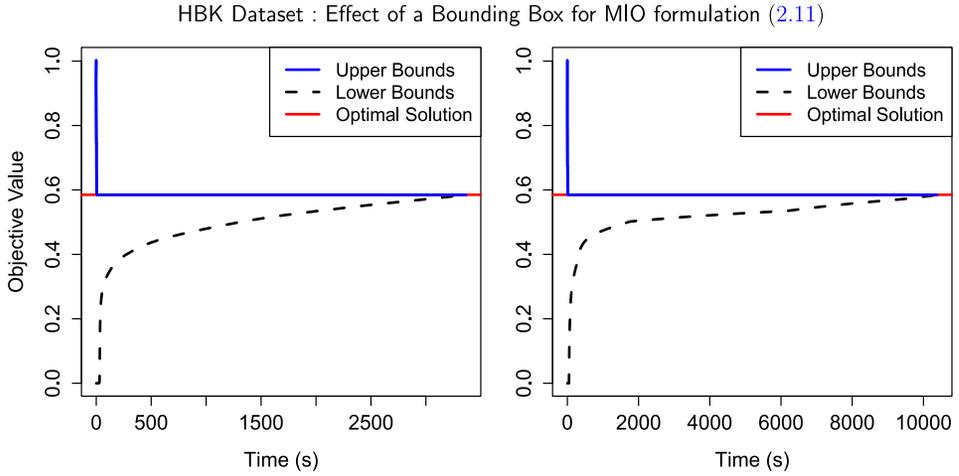


FIG. 3. Figure showing the effect of the bounding box for the evolution of the MIO formulation (2.11) for the HBK dataset, with $(n, p, q) = (75, 3, 45)$. The left panel considers a bounding box of diameter 6 and the right panel considers a bounding box of diameter 80 centered around the least squares solution.

$\beta_0 = \hat{\beta}^{(LS)} = (0.08, -0.36, 0.43)$. Both these boxes (which are in fact, quite large, given that $\|\hat{\beta}^{(LS)}\|_\infty = 0.43$) contains the (unconstrained) global solution for the problem. As the figure shows, the evolution of the lower bounds of the MIO algorithm toward the global optimum depends upon the radius of the box.

We argue that formulation (5.2) is a more desirable formulation—the constraint may behave as a regularizer to shrink coefficients or if one seeks an unconstrained LQS solution, there are effective ways to choose β_0 and M . For example, if β_0 denotes the solution obtained by Algorithm 3, then for $M = \eta \|\beta_0\|_\infty$, for $\eta \in [1, 2]$ (say), the solution to (5.2) corresponds to a global optimum of the LQS problem inside a box of diameter $2M$ centered at β_0 . For moderate sized problems with $n \in \{201, 501\}$, we found this strategy to be useful in certifying global optimality within a reasonable amount of time. Figure 4 shows some examples.

5.6. Scalability to large problems. We present our findings for large-scale experiments performed on synthetic and real data-set, below.

Synthetic large scale examples. For large-scale problems with $n \geq 5000$ with $p \geq 10$, we found that Algorithm 1 becomes computationally demanding due to the associated LO problems (3.6) appearing in step 2 of Algorithm 1. On the other hand, Algorithm 2 remains computationally inexpensive. So for larger problems, we propose using a modification of Algorithm 1—we run Algorithm 2 for several random initializations around the $\hat{\beta}^{(LAD)}$ solution and find the best solution among them. The regression coefficient thus obtained is used as an initialization

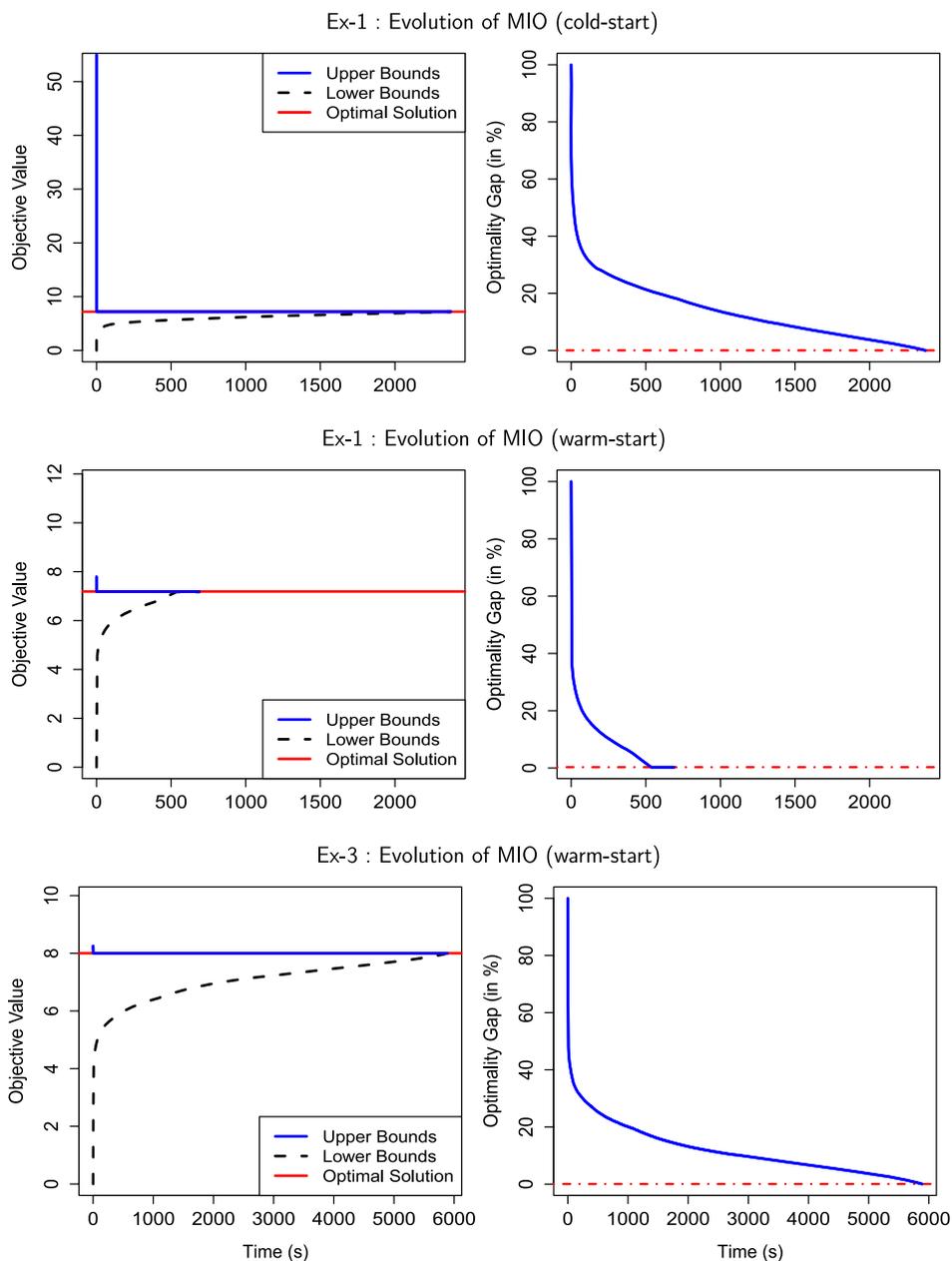


FIG. 4. Figure showing evolution of MIO in terms of upper/lower bounds (left panel) and Optimality gaps (in %) (right panel). Top and middle rows display an instance of Ex-1 with $(n, p, q) = (201, 5, 121)$ with different initializations, that is, MIO (2.11) (cold-start) and MIO (2.11) (warm-start), respectively. Bottom row considers an instance of Ex-3 with $(n, p, q) = (501, 5, 301)$.

TABLE 3

Table showing performances of various Algorithms for the LQS problem for different moderate/large-scale examples as described in the text. For each example, “Accuracy” is Relative Accuracy [see (5.1)] the numbers within brackets denote the standard errors; the lower row denotes the averaged cpu time (in secs) taken for the algorithm. All results are averaged over 20 random examples

Example (n, p, π) q		Algorithm used			
		LQS (MASS)	Algorithm 3 (large-scale)	MIO formulation (2.11)	
				(Cold-start)	(Warm-start)
Ex-5 (2001, 10, 0.4) $q = 1201$	Accuracy	65.125 (2.77)	0.0 (0.0)	273.543 (16.16)	0.0 (0.0)
	Time (s)	0.30	13.75	200	100
Ex-6 (5001, 10, 0.4) $q = 3001$	Accuracy	52.092 (1.33)	0.0	232.531 (17.62)	0.0 (0.0)
	Time (s)	0.69	205.76	902	450.35
Ex-7 (10,001, 20, 0.4) $q = 6001$	Accuracy	146.581 (3.77)	0.0 (0.0)	417.591 (4.18)	0.0 (0.0)
	Time (s)	1.80	545.88	1100	550

for Algorithm 1—we call this Algorithm 3 (large-scale). Note that this procedure deviates from the vanilla Algorithm 3 (described in Section 3.3), where, we do both steps 1 and 2 for every initialization β_1 . For each of the examples Ex-5–Ex-7, Algorithm 2 was run for MaxIter = 500, for 100 different initializations around the LAD solution, the best solution was used as an initialization for Algorithm 1. Table 3 presents the results obtained with Algorithm 3 (large-scale). In addition, the aforementioned algorithms, Table 3 also presents MIO (warm-start), that is, MIO formulation (2.11) warm-started with Algorithm 3 (large-scale) and the LQS algorithm from the R-package MASS.

Large scale examples with real datasets. In addition to the above, we considered a large environmental dataset from the R-package robustbase with hourly measurements of NOx pollution content in the ambient air. The dataset has $n = 8088$ samples with $p = 4$ covariates (including the intercept). The covariates are square-root of the windspeed (x_1), day number (x_2), log of hourly sum of NOx emission of cars (x_3) and intercept, with response being log of hourly mean of NOx concentration in ambient air (y). We considered three different values of $q \in \{7279, 6470, 4852\}$ corresponding to the 90th, 80th and 60th quantile, respectively. We added a small amount of contamination by changing $\lfloor 0.01n \rfloor$ sample points according to item (B) in Section 5.1. On the modified dataset, we ran three different algorithms: Algorithm 3 (large-scale),⁵ MIO (warm-start), that is, MIO

⁵In this example, we initialized Algorithm 2 with the best Chebyshev fit from forty different sub-samples. Algorithm 2 was run for MaxIter = 500, with five hundred random initializations. The best solution was taken as the starting point of Algorithm 3.

formulation (2.11) warm-started with Algorithm 3 (large-scale) and the LQS algorithm from the R-package MASS. In all the following cases, the MIO algorithm was run for a maximum of two hours. We summarize our key findings below:

(1) For $q = 7279$, the best solution was obtained by MIO (warm-start) in about 1.6 hours. Algorithm 3 (large-scale) delivered a solution with relative accuracy [see (5.1)] 0.39% in approximately six minutes. The LQS algorithm from R-package MASS, delivered a solution with relative accuracy 2.8%.

(2) For $q = 6470$, the best solution was found by MIO (warm-start) in 1.8 hours. Algorithm 3 (large-scale) delivered a solution with relative accuracy [see (5.1)] 0.19% in approximately six minutes. The LQS algorithm from R-package MASS, delivered a solution with relative accuracy 2.5%.

(3) For $q = 4852$, the best solution was found by MIO (warm-start) in about 1.5 hours. Algorithm 3 (large-scale) delivered a solution with relative accuracy [see (5.1)] 0.14% in approximately seven minutes. The LQS algorithm from R-package MASS, delivered a solution with relative accuracy 1.8%.

Thus, in all the examples above, MIO warm-started with Algorithm 3 (large-scale) obtained the best upper bounds. Algorithm 3 (large-scale) obtained very high quality solutions, too, but the solutions were all improved by MIO.

6. Conclusions. In this paper, we proposed algorithms for LQS problems based on a combination of first-order methods from continuous optimization and mixed integer optimization. Our key conclusions are:

(1) The MIO algorithm with warm start from the continuous optimization algorithms solves to provable optimality problems of small ($n = 100$) and medium ($n = 500$) size problems in under two hours.

(2) The MIO algorithm with warm starts finds high quality solutions for large ($n = 10,000$) scale problems in under two hours outperforming all state of the art algorithms that are publicly available for the LQS problem. For problems of this size, the MIO algorithm does not provide a certificate of optimality in a reasonable amount of time.

(3) Our framework enables us to show the existence of an optimal solution for the LQS problem for *any* dataset, where the data-points (y_i, \mathbf{x}_i) 's are not necessarily in general position. Our MIO formulation leads to a simple proof of the breakdown point of the LQS optimum objective value that holds for general datasets and our framework can easily incorporate extensions of the LQS formulation with polyhedral constraints on the regression coefficient vector.

REFERENCES

- AGULLO, J. (1997). Exact algorithms for computing the least median of squares estimate in multiple linear regression. In *L₁-Statistical Proceedness and Related Topics. Lecture Notes Monogr. Ser. 31* 133–146. IMS, Hayward, CA.

- BARRETO, H. and MAHARRY, D. (2006). Least median of squares and regression through the origin. *Comput. Statist. Data Anal.* **50** 1391–1397. [MR2222048](#)
- BERNHOLT, T. (2005a). Robust estimators are hard to compute. Technical Report 52/2005, Univ. Dortmund.
- BERNHOLT, T. (2005b). Computing the least median of squares estimator in time $O(n^d)$. In *Computational Science and Its Applications, ICCSA 2005. Lecture Notes in Computer Science* **3480** 697–706. Springer, Berlin.
- BERTSIMAS, D. and WEISMANTEL, R. (2005). *Optimization over Integers*. Dynamic Ideas, Belmont, MA.
- BICKEL, P. J. (1975). One-step Huber estimates in the linear model. *J. Amer. Statist. Assoc.* **70** 428–434. [MR0386168](#)
- BOYD, S. and VANDENBERGHE, L. (2004). *Convex Optimization*. Cambridge Univ. Press, Cambridge. [MR2061575](#)
- CHAKRABORTY, B. and CHAUDHURI, P. (2008). On an optimization problem in robust statistics. *J. Comput. Graph. Statist.* **17** 683–702. [MR2451342](#)
- CLARKE, F. H. (1990). *Optimization and Nonsmooth Analysis*, 2nd ed. SIAM, Philadelphia, PA. [MR1058436](#)
- DONOHO, D. and HUBER, P. J. (1983). The notion of breakdown point. In *A Festschrift for Erich L. Lehmann* 157–184. Wadsworth, Belmont, CA. [MR0689745](#)
- ERICKSON, J., HAR-PELED, S. and MOUNT, D. M. (2006). On the least median square problem. *Discrete Comput. Geom.* **36** 593–607. [MR2267548](#)
- GILONI, A. and PADBERG, M. (2002). Least trimmed squares regression, least median squares regression, and mathematical programming. *Math. Comput. Modelling* **35** 1043–1060. [MR1910678](#)
- GUROBI OPTIMIZATION, INC. (2013). Gurobi Optimizer Reference Manual.
- HAMPEL, F. R. (1971). A general qualitative definition of robustness. *Ann. Math. Statist.* **42** 1887–1896. [MR0301858](#)
- HAMPEL, F. R. (1975). Beyond location parameters: Robust concepts and methods. *Bull. Int. Stat. Inst.* **46** 375–382.
- HAWKINS, D. M. (1993). The feasible set algorithm for least median of squares regression. *Comput. Statist. Data Anal.* **16** 81–101.
- HAWKINS, D. M., BRADU, D. and KASS, G. V. (1984). Location of several outliers in multiple-regression data using elemental sets. *Technometrics* **26** 197–208. [MR0770368](#)
- HUBER, P. J. (1973). Robust regression: Asymptotics, conjectures and Monte Carlo. *Ann. Statist.* **1** 799–821. [MR0356373](#)
- HUBER, P. J. (2011). *Robust Statistics*. Springer, Berlin.
- HUBERT, M., ROUSSEEUW, P. J. and VAN AELST, S. (2008). High-breakdown robust multivariate methods. *Statist. Sci.* **23** 92–119. [MR2431867](#)
- MEER, P., MINTZ, D., ROSENFELD, A. and KIM, D. Y. (1991). Robust regression methods for computer vision: A review. *Int. J. Comput. Vis.* **6** 59–70.
- MOUNT, D. M., NETANYAHU, N. S., PIATKO, C. D., SILVERMAN, R. and WU, A. Y. (2000). Quantile approximation for robust statistical estimation and k -enclosing problems. *Internat. J. Comput. Geom. Appl.* **10** 593–608. [MR1808213](#)
- MOUNT, D. M., NETANYAHU, N. S., ROMANIK, K., SILVERMAN, R. and WU, A. Y. (2007). A practical approximation algorithm for the LMS line estimator. *Comput. Statist. Data Anal.* **51** 2461–2486. [MR2338982](#)
- NESTEROV, Y. (2004). *Introductory Lectures on Convex Optimization: A Basic Course*. Kluwer Academic, Boston, MA. [MR2142598](#)
- NUNKESSER, R. and MORELL, O. (2010). An evolutionary algorithm for robust regression. *Comput. Statist. Data Anal.* **54** 3242–3248. [MR2727749](#)
- OLSON, C. F. (1997). An approximation algorithm for least median of squares regression. *Inform. Process. Lett.* **63** 237–241. [MR1475335](#)

- ROCKAFELLAR, R. T. (1996). *Convex Analysis*. Princeton Univ. Press, Princeton, NJ.
- ROUSSEEUW, P. J. (1984). Least median of squares regression. *J. Amer. Statist. Assoc.* **79** 871–880. [MR0770281](#)
- ROUSSEEUW, P. J. and DRIESSEN, K. V. (2006). Computing LTS regression for large data sets. *Data Min. Knowl. Discov.* **12** 29–45. [MR2225526](#)
- ROUSSEEUW, P. and HUBERT, M. (1997). Recent developments in PROGRESS. In *L₁-Statistical Procedures and Related Topics* 201–214. IMS, Hayward, CA.
- ROUSSEEUW, P. J. and LEROY, A. M. (1987). *Robust Regression and Outlier Detection*. Wiley, New York. [MR0914792](#)
- ROUSSEEUW, P. J., DEBRUYNE, M., ENGELEN, S. and HUBERT, M. (2006). Robustness and outlier detection in chemometrics. *Crit. Rev. Anal. Chem.* **36** 221–242.
- ROUSSEEUW, P., CROUX, C., TODOROV, V., RUCKSTUHL, A., SALIBIAN-BARRERA, M., VERBEKE, T., KOLLER, M. and MAECHLER, M. (2013). robustbase: Basic Robust Statistics. R package version 0.9-10.
- SHOR, N. Z. (1985). *Minimization Methods for Nondifferentiable Functions*. Springer, Berlin. Translated from the Russian by K. C. Kiwiel and A. Ruszczyński. [MR0775136](#)
- SIEGEL, A. F. (1982). Robust regression using repeated medians. *Biometrika* **69** 242–244.
- SOUVAINE, D. L. and STEELE, J. M. (1987). Time- and space-efficient algorithms for least median of squares regression. *J. Amer. Statist. Assoc.* **82** 794–801. [MR0909984](#)
- STEELE, J. M. and STEIGER, W. L. (1986). Algorithms and complexity for least median of squares regression. *Discrete Appl. Math.* **14** 93–100. [MR0839533](#)
- STEWART, C. V. (1999). Robust parameter estimation in computer vision. *SIAM Rev.* **41** 513–537. [MR1719133](#)
- STROMBERG, A. J. (1993). Computing the exact least median of squares estimate and stability diagnostics in multiple linear regression. *SIAM J. Sci. Comput.* **14** 1289–1299.
- TIBSHIRANI, R. (1996). Regression shrinkage and selection via the lasso. *J. Roy. Statist. Soc. Ser. B* **58** 267–288. [MR1379242](#)
- TODOROV, V. and FILZMOSER, P. (2009). An object-oriented framework for robust multivariate analysis. *J. Stat. Softw.* **32** 1–47.

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