A Practical Approximation Algorithm for the LTS Estimator

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(For submission to CSDA)
Dedicated to the memory of our dear friend and longtime colleague, Ruth Silverman

Abstract

The linear least trimmed squares (LTS) estimator is a statistical technique for fitting a linear model to a set of points. It was proposed by Rousseeuw as a robust alternative to the classical least squares estimator. Given a set of n points in $\mathbb{R}^d$, the objective is to minimize the sum of the smallest 50% squared residuals (or more generally any given fraction). There exist practical heuristics for computing the linear LTS estimator, but they provide no guarantees on the accuracy of the final result. We present two results in this paper. First, we introduce a measure of the numerical condition of a set of points. We present a probabilistic analysis of the accuracy of the best LTS fit resulting from a set of random elemental fits. Our analysis shows that as the condition of the point set improves, the accuracy of the resulting fit increases as well. Second, we present an approximation algorithm for LTS, called Adaptive-LTS. Given bounds on the minimum and maximum slope coefficients, this algorithm returns an approximation to the optimal LTS fit whose slope coefficients lie within the given bounds. We present empirical evidence on a variety of data sets of this algorithm's efficiency and effectiveness.

Keywords: Robust estimation, linear estimation, least trimmed squares estimator, approximation algorithms, computational geometry

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1 Introduction

In standard *linear regression* (with intercept), an n-element point set $P = \{p_1, \ldots, p_n\}$ is given, where each point consists of some number of independent variables and one dependent variable. Letting d denote the total number of variables, we wish to express the dependent variable as a linear function of the $d-1$ independent variables. More formally, for $1 \leq i \leq n$, let $p_i = (x_{i,1}, \ldots, x_{i,d-1}, y_i) \in \mathbb{R}^d$. The objective is to compute a $(d-1)$-dimensional hyperplane, represented as a coefficient vector $\boldsymbol{\beta} = (\beta_1, \ldots, \beta_d) \in \mathbb{R}^d$ so that

$$y_i \;=\; \sum_{j=1}^{d-1} \beta_j x_{i,j} + \beta_d + e_i, \quad \text{for } i = 1, 2, \ldots, n,$$

where the e_i's are the errors. We refer to $(\beta_1, \ldots, \beta_{d-1})$ as the *slope coefficients* and β_d as the *y-intercept*. Given such a vector $\boldsymbol{\beta}$, the *ith residual*, denoted by $r_i(\boldsymbol{\beta}, P)$, is defined to be $y_i - \big(\sum_{j=1}^{d-1} \beta_j x_{i,j} + \beta_d\big)$. Let $r_{[i]}(\boldsymbol{\beta}, P)$ denote the ith smallest residual in terms of absolute value. Throughout, we consider the y-coordinate axis to be the *vertical* direction, and so the ith residual is just the signed vertical distance from the hyperplane to p_i.

Robust estimators (see, e.g., [21]) have been introduced in order to eliminate sensitivity to outliers, that is, points that fail to follow the linear pattern of the majority of the points. The basic measure of the robustness of an estimator is its *breakdown point*, that is, the fraction (up to 50%) of outlying data points that can corrupt the estimator arbitrarily. One of the most widely studied robust linear estimators is Rousseeuw's *least median of squares estimator* (LMS) [19], which is defined to be the hyperplane that minimizes the median squared residual. More generally, given an integer *trimming parameter* h, the objective is to find the hyperplane that minimizes the hth smallest squared residual. A number of papers, both practical and theoretical, have been devoted to solving this problem in the plane and in higher dimensions (see, e.g., [1,3,4,15,17,18,25]).

It has been observed by Rousseeuw and Leroy [21] that LMS may not be the best estimator from the perspective of statistical properties. They argue in support of the *least trimmed squares* (or LTS) linear estimator [19]. Given an n-element point set P and a positive integer *trimming parameter* $h \leq n$, this estimator is defined to be the nonvertical hyperplane that minimizes the *sum* (as opposed to the maximum) of the h smallest squared residuals. For the sake of preserving scale, we convert this into a quantity that more closely resembles a standard deviation. More formally, given a nonvertical hyperplane $\boldsymbol{\beta}$ define its *LTS cost* with respect to P and h to be

$$\Delta_{\boldsymbol{\beta}}(P, h) \;=\; \left(\frac{1}{h-1} \sum_{i=1}^{h} r_{[i]}^2(\boldsymbol{\beta}, P) \right)^{1/2}.$$

(Note that this differs from the definition of LTS cost as the sum of squared residuals given in our earlier paper [16]. We prefer the above definition because it is scale invariant, but clearly minimizing one is equivalent to minimizing the other.) The *LTS estimator* is a $(d-1)$-dimensional hyperplane of minimum LTS cost, which we denote by $\boldsymbol{\beta}^*(P, h)$. We let $\Delta^*(P, h)$ denote the associated LTS cost of this hyperplane. (When P and h are clear from context, we refer to these simply as $\boldsymbol{\beta}^*$ and Δ^*.) The *LTS problem* is that of computing this hyperplane. We refer to the points having the h smallest squared residuals as *inliers* and the remaining points as *outliers*. This generalizes the ordinary least squares estimator (when $h = n$). Typically, h is set to some constant fraction of n based on the expected number of outliers. In order to guarantee a unique solution, it is often assumed that h is at least $n/2$. The statistical properties of LTS are analyzed in [19] and [21].

The computational complexity of LTS is less well understood than that of LMS. Hössjer [11] presented an $O(n^2 \log n)$ algorithm for LTS in $\mathbb{R}^2$ based on plane sweep. In a companion paper [16], we presented an exact algorithm whose running time is $O(n^2)$ for the planar case and runs in $O(n^{d+1})$ time in any fixed dimension d. For large n these running times may be unacceptably slow, even in spaces of moderate dimension.

Given these relatively high running times, it is natural to consider whether this problem can be solved approximately. There are a few possible ways to formulate LTS as an approximation problem, either by approximating the residual, by approximating the quantile, or both. The following formulations were introduced in [16] (but they have been modified in light of our scale-invariant definition of LTS cost). The approximation parameters ε_r and ε_q denote the allowed residual and quantile errors, respectively.

Residual Approximation: The requirement of minimizing the sum of squared residuals is relaxed. Given $0 < \varepsilon_r$, an ε_r*-residual approximation* is any hyperplane $\boldsymbol{\beta}$ such that

$$\Delta_{\boldsymbol{\beta}}(P, h) \;\leq\; (1 + \varepsilon_r)\, \Delta^*(P, h).$$

Quantile Approximation: Much of the complexity of LTS arises because of the requirement that *exactly* h points be considered. We can relax this requirement by introducing a parameter $0 < \varepsilon_q < h/n$ and requiring that the fraction of inliers used is smaller by ε_q. Let $h^- = h - \lfloor n\varepsilon_q \rfloor$. An ε_q*-quantile approximation* is any hyperplane $\boldsymbol{\beta}$ such that

$$\Delta_{\boldsymbol{\beta}}(P, h^-) \;\leq\; \Delta^*(P, h).$$

Hybrid Approximation: The above approximations can be merged into a single approximation. Given ε_r and ε_q as in the previous two approximations, let h^- be as defined above. An $(\varepsilon_r, \varepsilon_q)$*-hybrid approximation* is any hyperplane $\boldsymbol{\beta}$ such that

$$\Delta_{\boldsymbol{\beta}}(P, h^-) \;\leq\; (1 + \varepsilon_r)\Delta^*(P, h).$$

LTS and LMS are robust versions of the well known least squares (L_2) and Chebyshev (L_∞) estimators, respectively. A third example is the *least trimmed sum of absolute residuals*, or *LTA*. This is a trimmed version of the L_1 estimator, in which the objective is to minimize the sum of squares of the h smallest *absolute values* of the residuals. By analogy, approximations can be defined for the other trimmed estimators. Such algorithms have been presented for LMS and LTA [4, 5, 9]. In an earlier paper [16], we presented an approximation algorithm for LTS with a running time of roughly $O(n^d/h)$. In the same paper, we presented lower bounds for the LTS and LTA problems, which suggest that substantial improvements to these bounds, either exact or approximate, are unlikely.

There is, however, a very simple and practical approach to LTS. This is the Fast-LTS heuristic of Rousseeuw and Van Driessen [22]. This algorithm (which will be described in detail in Section 2) is based on a combination of random sampling and local improvement. It is based on repeatedly fitting a hyperplane to a small random sample of points, which is called an *elemental fit*, and then applying a small number of local improvements, called *concentration steps* or *C-steps* (formal definitions are given below). Each C-step transforms an existing fit into one of equal or lower LTS cost. In practice this approach works very well. However, it provides no assurance on the quality of the final fit. Another example of a local search heuristic is Hawkins' feasible point algorithm [10]. It does not offer any formal performance guarantees either.

While Fast-LTS works well in practice, it does not represent a truly satisfactory algorithmic solution to the LTS problem. It implicitly assumes that the data are sufficiently well conditioned that, with reasonably high probability, a random elemental fit is close enough to the optimal fit that subsequent local improvements will converge to a fit that is nearly optimal. If the data are poorly conditioned, however, Fast-LTS may require a very large number of random trials before it succeeds. This raises the question of what constitutes a well-conditioned point set, and whether there is an algorithm that can provide guarantees on the quality of the result.

We present two principal results in this paper. First, in Section 2 we introduce a measure of the numerical condition of a set of points, and we present a probabilistic analysis of the accuracy of the LTS fit resulting from a series of random elemental fits. Our results show that as the condition of the point set improves, the expected accuracy the resulting fit improves as well. Second, in Section 3 we present a hybrid approximation algorithm for LTS, called *Adaptive-LTS*. Given P, h, bounds on the minimum and maximum slope coefficients, and approximation parameters ε_r and ε_q, the algorithm returns a hyperplane that is an $(\varepsilon_r, \varepsilon_q)$-hybrid approximation to the optimal hyperplane whose slope coefficients lie within the specified bounds. The most complex aspect of the algorithm involves the solution of a variant of the 1-dimensional LTS problem for a set of input intervals, which we call the *interval LTS problem*. In Section 4 we present an $O(n \log n)$ time solution to this problem. We have implemented the Adaptive-LTS algorithm, and in Section 5, we present empirical evidence that, for many distributions, this algorithm efficiently produces solutions that are provably good approximations to the optimal LTS fit.

2 Numerical Condition and Elemental Fits

In this section we consider the question of how the numerical conditioning of a point set influences the accuracy of an LTS fit based on random elemental fits. Consider a set of n points P in $\mathbb{R}^d$ and a trimming parameter $h \leq n$. We assume that the points are in general position, so that any subset of d points defines a unique $(d-1)$-dimensional hyperplane. (This can always be achieved through an infinitesimal perturbation.) Any hyperplane generated in this manner is called an *elemental fit*. Elemental fits play an important role in Fast-LTS (described below). In this section we introduce a measure on the numerical condition of a point set, and we establish formal bounds on the accuracy of random elemental fits in terms of this measure.

We begin with a brief presentation of Rousseeuw and van Driessen's Fast-LTS algorithm. (Our description is slightly simplified, and we refer the reader to [22] for details.) The algorithm consists of a series of stages. Each stage starts by generating a random subset of P of size d and fits a hyperplane $\boldsymbol{\beta}$ to these points. It then generates a series of local improvements as follows. The h points of P that have the smallest squared residuals with respect to $\boldsymbol{\beta}$ are determined. Let $\boldsymbol{\beta}'$ be the least squares linear estimator of these points. Clearly, the LTS cost of $\boldsymbol{\beta}'$ is not greater than that of $\boldsymbol{\beta}$. We set $\boldsymbol{\beta} \leftarrow \boldsymbol{\beta}'$ and repeat the process. This is called a *C-step*. C-steps are repeated a small fixed number of times.

The overall algorithm operates by performing a large number of stages, where each stage starts with a new random elemental fit. After all stages have completed, a small number of results with the lowest LTS costs are saved. For each of these, C-steps are repeatedly applied until converging to a local minimum. The algorithm's final output is the hyperplane with the lowest overall cost. Assuming constant dimension, each C-step can be performed in $O(n)$ time, and thus the overall running time is $O(kn)$, where k is the number of stages.

It is easy to see why Fast-LTS performs well under nominal circumstances. If we succeed in sampling d inliers (which would be expected to occur with probability roughly $(h/n)^d$, assuming at least h inliers) and these points are well distributed, then the resulting elemental fit should be sufficiently close to the optimal solution that the subsequent C-steps will converge to a fit that is very close to the optimum. Thus, although there are no guarantees of good performance, if the data are well conditioned, then after a sufficiently large number of random starts, it is reasonable to believe that at least one of the resulting fits will be sufficiently close to the optimum so that subsequent C-steps produce a nearly optimal solution.

The objective of this section is explore how we might formalize the notion of "well conditioned" data. We will ignore the effect of C-steps, and focus only on analyzing the performance of repeated random elemental fits. (An analysis of the effect of C-steps would be a valuable addition to our results, but this seems to be a significantly harder problem.) Our aim is to provide sufficient conditions on the properties of point sets so that with constant probability, a random elemental fit will provide a reasonably good approximation to the optimum LTS hyperplane.

Rousseeuw and Leroy provide an analysis of the number of elemental fits needed to obtain a good fit with a given probability (see Chapter 5 of [21]), but their analysis makes the tacit assumption that the inliers lie on the optimum LTS fit and determine a unique hyperplane. Such an argument ignores the potential effects of numerical instabilities. For example, if the inliers are clustered close to a low-dimensional flat, then the resulting elemental fit will be numerically unstable.

We fix P and h throughout the remainder of this section, and we let $\boldsymbol{\beta}^* = \boldsymbol{\beta}^*(P, h)$ denote the optimum LTS estimator. Define $\boldsymbol{x}_i$ to be the d-element column vector $(x_1, \ldots, x_{d-1}, 1)$ and $\boldsymbol{\beta}$ to be the row vector $(\beta_1, \ldots, \beta_d)$. The ith residual is just $y_i - \boldsymbol{\beta} \cdot \boldsymbol{x}_i$. Let $\mathcal{E}(P)$ denote the collection of d-element subsets of the index set $\{1, \ldots, n\}$. Given $E = \{i_1, \ldots, i_d\} \in \mathcal{E}$, let X_E denote the $d \times d$ matrix whose columns are the coordinate vectors of the corresponding independent variables:

$$X_E \;=\; \left[\boldsymbol{x}_{i_1} \;\middle|\; \ldots \;\middle|\; \boldsymbol{x}_{i_d} \right].$$

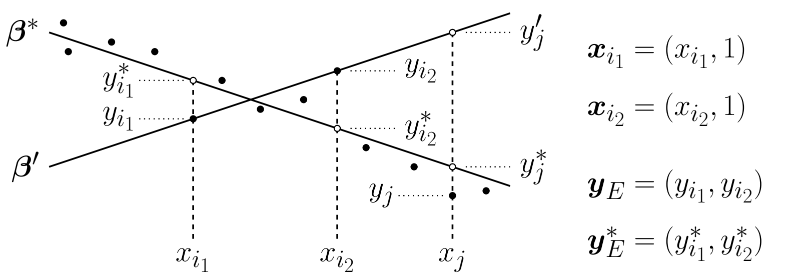
Let $\boldsymbol{y}_E$ be the row d-vector of associated dependent variables $(y_{i_1}, \ldots, y_{i_d})$. By our general position assumption, these vectors are linearly independent, and so there is a unique d-element row vector $\boldsymbol{\beta}'$ such that

$$\boldsymbol{y}_E \;=\; \boldsymbol{\beta}' X_E, \qquad \text{that is} \qquad \boldsymbol{\beta}' \;=\; \boldsymbol{y}_E X_E^{-1}.$$

(See Fig. 1.) For our subsequent analysis, we also define $\boldsymbol{y}_E^* = \boldsymbol{\beta}^* X_E$ to be the vector of y-values resulting from evaluating the optimum LTS hyperplane at the points of the elemental set. Thus, we have $\boldsymbol{\beta}^* = \boldsymbol{y}_E^* X_E^{-1}$.

We begin with a few standard definitions [6, 7]. Consider a d-vector $\boldsymbol{x}$ and a $d \times d$ matrix X. Let $X_{i,j}$ denote the element in row i and column j of X, and let X_j denote the jth column vector. The norms of $\boldsymbol{x}$ and X (in the L_2 and Frobenius norms, respectively) are defined to be

$$\|\boldsymbol{x}\| \;=\; \left(\sum_i x_i^2 \right)^{1/2} \qquad \|X\| \;=\; \left(\sum_j \sum_i X_{i,j}^2 \right)^{1/2} \;=\; \left(\sum_j \|X_j\|^2 \right)^{1/2}.$$



$\boldsymbol{\beta}^*$
$\boldsymbol{\beta}'$
$y^*_{i_1}$
y_{i_1}
y_{i_2}
$y^*_{i_2}$
y'_j
y^*_j
y_j
x_{i_1}
x_{i_2}
x_j
$\boldsymbol{x}_{i_1} = (x_{i_1}, 1)$
$\boldsymbol{x}_{i_2} = (x_{i_2}, 1)$
$\boldsymbol{y}_E = (y_{i_1}, y_{i_2})$
$\boldsymbol{y}^*_E = (y^*_{i_1}, y^*_{i_2})$

Fig. 1: Estimated and optimal fits for $E = \{i_1, i_2\}$ and $\boldsymbol{y}_E = (y_{i_1}, y_{i_2})$. Solid points indicate points of P and hollow points are computed quantities.

Let $\kappa(X)$ denote the *condition number* of X relative to this norm, that is, $\kappa(X) = \|X\| \cdot \|X^{-1}\|$. The concept of condition number is well known in matrix algebra as a means to characterize the stability of linear systems involving X [7]. It is a dimensionless quantity, where lower values mean greater stability.

Our condition measure is based on two properties of the independent variables of the inliers. Let $H \subseteq \{1, \ldots, n\}$ denote the h-element index set of the inliers relative to P's optimal LTS hyperplane. Intuitively, the first property states that a random elemental set of inliers provides a stable elemental fit. This is expressed by bounding the median condition number of X_E for $E \in \mathcal{E}(H)$. (That is, we are taking the median over the collection of all d-element subsets of the h inliers.) This property alone is not sufficient, since even a minuscule error in the placement of the hyperplane might be fatal if any inlier is located so far away that its associated residual dominates the overall cost. Such a point is called a *leverage point* [20]. Intuitively, the second property rules out leverage point inliers by bounding the ratio between the average squared norm and median squared norm of the points $\boldsymbol{x}_i$, for $i \in H$. More formally, given two positive real parameters γ and λ, we say that P is (γ, λ)-*well conditioned* if

$$\text{(i):} \quad \operatorname*{med}_{E \in \mathcal{E}(H)} \kappa(X_E) \;\le\; \gamma \qquad \text{and} \qquad \text{(ii):} \quad \frac{\sum_{j \in H} \|\boldsymbol{x}_j\|^2}{h \cdot \operatorname{med}_{j \in H} \|\boldsymbol{x}_j\|^2} \;\le\; \lambda^2.$$

Note that these assumptions constrain only the independent variables (not the dependent variables), and they apply only to the set of inliers of the optimal fit (and thus there are no assumptions imposed on the outliers). The use of the median in the two assumptions is not critical. At the expense of a constant factor in the analysis, we could have replaced the median with any constant quantile of h.

The main result of this section is given in the following theorem. It shows that depending on the condition of the point set, after a sufficiently large number of repetitions of random elemental fits, we can achieve a constant-factor (residual) approximation for LTS with arbitrarily high confidence.

Theorem 1 *Let P be an n-element point set in $\mathbb{R}^d$ that is (γ, λ)-well conditioned for some γ and λ. Let h be a trimming parameter, where $h = \lceil qn \rceil$, for some constant $0 < q \le 1$. Then for any $0 < \delta < 1$, after $O((\ln(1/\delta))/q^d)$ elemental fits, with probability at least $1 - \delta$, at least one of these fits $\boldsymbol{\beta}'$ satisfies*

$$\Delta_{\boldsymbol{\beta}'}(P, h) \;\le\; \big(1 + \sqrt{2}\gamma\lambda\big)\Delta^*(P, h).$$

The proof relies on the following lemma, which shows that with constant probability, a single elemental fit provides the desired approximation bound.

Lemma 1 *Given the preconditions of Theorem 1, let E be a random element of $\mathcal{E}(P)$, and let $\boldsymbol{\beta}'$ denote the resulting random elemental fit. With probability at least $q^d/2^{d+2}$,*

$$\Delta_{\boldsymbol{\beta}'}(P,h) \;\leq\; \big(1+\sqrt{2}\gamma\lambda\big)\Delta^*(P,h).$$

Assuming this lemma, Theorem 1 follows directly. In particular, by repeating m independent random elemental fits, the probability of failing to achieve the stated approximation bound is at most $(1-q^d/2^{d+2})^m \leq \exp(-mq^d/2^{d+2})$. By selecting $m \geq (\ln(1/\delta))2^{d+2}/q^d$, the probability of failure is at most δ, from which Theorem 1 follows.

The remainder of the section is devoted to proving Lemma 1. Recall the definitions given earlier for the norms of a matrix X, column vector $\boldsymbol{x}$, and row vector $\boldsymbol{y}$. The following are easy consequences of these definitions and the Cauchy-Schwarz inequality:

$$|\boldsymbol{y}\boldsymbol{x}| \;\leq\; \|\boldsymbol{y}\|\cdot\|\boldsymbol{x}\| \qquad\qquad \|\boldsymbol{y}X\| \;\leq\; \|\boldsymbol{y}\|\cdot\|X\|.$$

With probability at least q, a random index from $\{1,\ldots,n\}$ is drawn from H, and so the probability that a random element of $\mathcal{E}(P)$ lies in $\mathcal{E}(H)$ approaches q^d for all sufficiently large n. (Note that we sample without replacement.) The remainder of the proof is conditioned on this assumption.

Recall that $\boldsymbol{\beta}^*$ is the optimal LTS hyperplane, and Δ^* is its cost. Let $\Delta' = \Delta_{\boldsymbol{\beta}'}(P,h)$. Let H denote indices of the h points of P whose residuals with respect to $\boldsymbol{\beta}^*$ are the smallest. We make use of the following technical result.

Lemma 2 *Given Δ^* and Δ' as defined above,*

$$\frac{\Delta'}{\Delta^*}-1 \;\leq\; \left(\frac{\|\boldsymbol{y}_E-\boldsymbol{y}_E^*\|^2}{\sum_{j\in H}(y_j-y_j^*)^2}\right)^{1/2} \cdot\; \left(\|X_E^{-1}\|\cdot\|X_E\|\right) \;\cdot \left(\frac{\sum_{j\in H}\|\boldsymbol{x}_j\|^2}{\|X_E\|^2}\right)^{1/2}.$$

Proof: By definition of the LTS cost we have

$$(\Delta^*)^2(h-1) \;=\; \sum_{j\in H} r_j^2(\boldsymbol{\beta}^*,P) \;=\; \sum_{j\in H}(y_j-\boldsymbol{\beta}^*\boldsymbol{x}_j)^2.$$

Let H' denote the indices of the h points of P whose squared residuals with respect to $\boldsymbol{\beta}'$ are the smallest. Therefore,

$$(\Delta')^2(h-1) \;=\; \sum_{j\in H'} r_j^2(\boldsymbol{\beta}',P) \;=\; \sum_{j\in H'}(y_j-\boldsymbol{\beta}'\boldsymbol{x}_j)^2 \;\leq\; \sum_{j\in H}(y_j-\boldsymbol{\beta}'\boldsymbol{x}_j)^2.$$

Thus, we have

$$(\Delta'-\Delta^*)\sqrt{h-1} \;\leq\; \left(\sum\nolimits_{j\in H}(y_j-\boldsymbol{\beta}'\boldsymbol{x}_j)^2\right)^{1/2} - \;\left(\sum\nolimits_{j\in H}(y_j-\boldsymbol{\beta}^*\boldsymbol{x}_j)^2\right)^{1/2}.$$

We may interpret $\Delta'\sqrt{h-1}$ as the Euclidean distance between two points in $\mathbb{R}^h$, particularly $(y_1,\ldots,y_h)$ and $(\boldsymbol{\beta}'\boldsymbol{x}_1,\ldots,\boldsymbol{\beta}'\boldsymbol{x}_h)$. Similarly, we may interpret $\Delta^*\sqrt{h-1}$ as the Euclidean distance between $(y_1, \ldots, y_h)$ and $(\boldsymbol{\beta}^* \boldsymbol{x}_1, \ldots \boldsymbol{\beta}^* \boldsymbol{x}_h)$. Let $\|\boldsymbol{u} - \boldsymbol{v}\|$ denote the Euclidean distance between $\boldsymbol{u}$ and $\boldsymbol{v}$. By the triangle inequality and the above inequalities regarding norms, we have

$$\begin{aligned}
(\Delta' - \Delta^*)\sqrt{h-1} \;&\leq\; \sum\nolimits_{j \in H} \left(\|y_j - \boldsymbol{\beta}' \boldsymbol{x}_j\| - \|y_j - \boldsymbol{\beta}^* \boldsymbol{x}_j\|\right) \;\leq\; \sum\nolimits_{j \in H} \|\boldsymbol{\beta}' \boldsymbol{x}_j - \boldsymbol{\beta}^* \boldsymbol{x}_j\| \\
&\leq\; \left(\sum\nolimits_{j \in H} (\boldsymbol{\beta}' \boldsymbol{x}_j - \boldsymbol{\beta}^* \boldsymbol{x}_j)^2\right)^{1/2} \;=\; \left(\sum\nolimits_{j \in H} ((\boldsymbol{\beta}' - \boldsymbol{\beta}^*) \boldsymbol{x}_j)^2\right)^{1/2} \\
&=\; \left(\sum\nolimits_{j \in H} \|\boldsymbol{\beta}' - \boldsymbol{\beta}^*\|^2 \cdot \|\boldsymbol{x}_j\|^2\right)^{1/2} \;\leq\; \|\boldsymbol{\beta}' - \boldsymbol{\beta}^*\| \left(\sum\nolimits_{j \in H} \|\boldsymbol{x}_j\|^2\right)^{1/2}.
\end{aligned}$$

By the earlier observations relating $\boldsymbol{\beta}'$ and $\boldsymbol{\beta}^*$ to $\boldsymbol{y}_E$ and $\boldsymbol{y}_E^*$, we obtain

$$\begin{aligned}
(\Delta' - \Delta^*)\sqrt{h-1} \;&\leq\; \|\boldsymbol{y}_E X_E^{-1} - \boldsymbol{y}_E^* X_E^{-1}\| \left(\sum\nolimits_{j \in H} \|\boldsymbol{x}_j\|^2\right)^{1/2} \\
&\leq\; \|(\boldsymbol{y}_E - \boldsymbol{y}_E^*)\| \cdot \|X_E^{-1}\| \left(\sum\nolimits_{j \in H} \|\boldsymbol{x}_j\|^2\right)^{1/2}.
\end{aligned}$$

For each $\boldsymbol{x}_j \in P$, let $y_j^* = \boldsymbol{\beta}^* \boldsymbol{x}_j$. We can express Δ^* as $\sum_{j \in H} (y_j - y_j^*)^2$, from which it follows that

$$\frac{(\Delta' - \Delta^*)}{\Delta^*} \;\leq\; \|\boldsymbol{y}_E - \boldsymbol{y}_E^*\| \cdot \|X_E^{-1}\| \left(\sum\nolimits_{j \in H} \|\boldsymbol{x}_j\|^2\right)^{1/2} \Big/ \left(\sum\nolimits_{j \in H} (y_j - y_j^*)^2\right)^{1/2}.$$

By multiplying and dividing by $\|X_E\|$, we obtain

$$\frac{\Delta'}{\Delta^*} - 1 \;\leq\; \left(\frac{\|\boldsymbol{y}_E - \boldsymbol{y}_E^*\|^2}{\sum_{j \in H} (y_j - y_j^*)^2}\right)^{1/2} \cdot \left(\|X_E^{-1}\| \cdot \|X_E\|\right) \cdot \left(\frac{\sum_{j \in H} \|\boldsymbol{x}_j\|^2}{\|X_E\|^2}\right)^{1/2},$$

which completes the proof. □

Given this result, let us analyze each of these three factors separately. By definition, the middle factor is just $\kappa(X_E)$. To analyze the first factor, observe that $\|\boldsymbol{y}_E - \boldsymbol{y}_E^*\|^2 = \sum_{j \in E} (y_j - y_j^*)^2$. By our earlier assumption, E is a random subset of H, and so with probability approaching $1/2^d$ for large n, every element of $\{(y_j - y_j^*)^2 : j \in E\}$ is at most $\operatorname{med}_{j \in H} (y_j - y_j^*)^2$. Since at least half of the elements of the multiset $\{(y_j - y_j^*)^2 : j \in H\}$ are at least as large as the median of the set, it follows that $\sum_{j \in H} (y_j - y_j^*)^2 \geq (h/2) \operatorname{med}_{j \in H} (y_j - y_j^*)^2$. Thus, with probability approaching $1/2^d$ (and under the assumption that $E \subseteq H$) we have

$$\frac{\|\boldsymbol{y}_E - \boldsymbol{y}_E^*\|^2}{\sum_{j \in H} (y_j - y_j^*)^2} \;\leq\; \frac{\operatorname{med}_{j \in H} (y_j - y_j^*)^2}{(h/2) \operatorname{med}_{j \in H} (y_j - y_j^*)^2} \;\leq\; \frac{2}{h}.$$

To analyze the third factor, recall that from the definition of the Frobenius norm, $\|X_E\|^2 = \sum_{j \in E} \|\boldsymbol{x}_j\|^2$. By our earlier assumption, E is a random subset of H, and so with probability at least $1 - (1/2)^d \geq 1/2$, at least one element of $\{\|\boldsymbol{x}_j\|^2 : j \in E\}$ is at least as large as $\operatorname{med}_{j \in H} \|\boldsymbol{x}_j\|^2$. If so, $\|X_E\|^2$ is at least as large as the median as well. Combining this with property (ii) of well-conditioned sets, with probability at least 1/2 (and under the assumption that $E \subseteq H$) we have

$$\frac{\sum_{j \in H} \|\boldsymbol{x}_j\|^2}{\|X_E\|^2} \;\leq\; \frac{\lambda^2 \, h \cdot \operatorname{med}_{j \in H} \|\boldsymbol{x}_j\|^2}{\operatorname{med}_{j \in H} \|\boldsymbol{x}_j\|^2} \;\leq\; \lambda^2 h.$$

Combining our bounds on all three factors together with condition (i) of well-conditioned sets, we conclude that for large n, with probability approaching $q^d(1/2^d)(1/2) = q^d/2^{d+1}$, we have

$$\frac{\Delta'}{\Delta^*} - 1 \;\leq\; \left(\frac{2}{h}\right)^{1/2} \cdot \kappa(X_E) \cdot (\lambda\sqrt{h}) \;=\; \sqrt{2} \cdot \kappa(X_E) \cdot \lambda.$$

Since E is a random element of $\mathcal{E}(H)$, with probability at least $1/2$, $\kappa(X_E)$ is not greater than $\text{med}_{F \in \mathcal{E}(H)} \kappa(X_F)$, and so by condition (i) of well-conditioned sets we have $\kappa(X_E) \leq \gamma$. Therefore, with probability at least $q^d/2^{d+2}$,

$$\frac{\Delta'}{\Delta^*} \;\leq\; 1 + \sqrt{2} \cdot \kappa(X_E) \cdot \lambda \;\leq\; 1 + \sqrt{2}\gamma\lambda,$$

This completes the proof of Lemma 1 and establishes Theorem 1.

Note that the definition of well conditioning would appear to require the computation of medians over sets of size $O(h^d)$, which is quite large. It is clear from the proof, however, that replacing the medians with the rth quantile in the definition of well conditioning merely changes the factor $1/2^{d+2}$ of Lemma 1 to $1/r^{d+2}$. Thus, rather than computing the median exactly, it would suffice to employ random sampling to estimate its value, at the price of slightly increasing the number elemental fits.

Of course, Theorem 1 does not completely resolve the question of how the numerical conditioning of the point set affects the convergence of Fast-LTS. First, it ignores the effect of C-steps. Second, since its conditions apply only to the inliers, whose membership we do not normally know, it is not obvious how to turn this into an effective computational procedure. Nonetheless, if *a priori* knowledge about the inlier distribution is available, this result can provide useful bounds on the expected accuracy of any approach to LTS based on repeated random elemental fits in terms of easily computable quantities.

3 An Adaptive Approximation Algorithm

In this section we present an approximation algorithm for LTS, which we call *Adaptive-LTS.* The input to the algorithm is an n-element point set P, a trimming parameter $h \leq n$, a residual approximation parameter $\varepsilon_r \geq 0$, and a quantile approximation parameter ε_q, where $0 \leq \varepsilon_q < h/n$. The algorithm also accepts bounds on the minimum and maximum slope coefficients. (If these are not given, the algorithm can automatically estimate them from the point set.) The algorithm returns a hyperplane that is an $(\varepsilon_r, \varepsilon_q)$-hybrid approximation to the optimal hyperplane whose slope coefficients lie within the specified slope bounds.

This algorithm is based on a general technique called *geometric branch-and-bound*, which involves a recursive subdivision of the solution space in search of the optimal solution. Geometric branch-and-bound has been used in other applications of geometric optimization, notably point pattern matching by Huttenlocher and Rucklidge [12, 23, 24] and Hagedoorn and Veltkamp [8] and image registration by Mount *et al.* [14].

Before presenting the algorithm we provide a brief overview of the approach. The solution to the LTS problem can be represented as a d-dimensional vector $\boldsymbol{\beta} = (\beta_1, \ldots, \beta_d)$, consisting of the coefficients of the estimated hyperplane. Given P and h, we can associate each point $\boldsymbol{\beta} \in \mathbb{R}^d$ with its associated LTS cost, $\Delta_{\boldsymbol{\beta}}(P, h)$. This defines a scalar field over $\mathbb{R}^d$, called the *solution space.* The

LTS problem reduces to computing the point $\boldsymbol{\beta} \in \mathbb{R}^d$ that minimizes this cost, that is, the lowest point in this field. This is the context in which geometric branch-and-bound is applied.

Let us begin with an generic overview of how geometric branch-and-bound works. It recursively subdivides the solution space into a collection of disjoint regions, called *cells*. For a given cell C, let Δ_C denote the smallest value of $\Delta_{\boldsymbol{\beta}}$, for any $\boldsymbol{\beta} \in C$. (For the LTS problem, this is the minimum LTS cost under the constraint that the coefficient vector of the hyperplane is chosen from C.) The algorithm then computes a lower bound and an upper bound on Δ_C. Letting Δ_C^- and Δ_C^+ denote these bounds, respectively, we have $\Delta_C^- \leq \Delta_C \leq \Delta_C^+$. (Note that Δ_C^+ is an upper bound on the *minimum* cost within the cell, not an upper bound on all the costs within the cell.) The algorithm also maintains the hyperplane $\boldsymbol{\beta}'$ associated with the smallest upper bound encountered in any cell that has been seen so far. If C's lower bound exceeds the smallest upper bound seen so far, that is, if $\Delta_C^- > \Delta_{\widehat{\boldsymbol{\beta}}}$, we may safely eliminate C from further consideration, since any solution that it might provide cannot improve upon the current best solution. (A weaker condition can be applied if we desire only an approximate solution.) If so, we say that C is *killed* when this happens. Otherwise, C is said to be *active*.

A geometric branch-and-bound algorithm runs in a sequence of *stages*. At the start of any stage, the algorithm maintains a collection of all the currently active cells. During each stage, one of the active cells is selected and is processed by subdividing it into two (or generally more) smaller cells, called its *children*. We compute the aforementioned bounds for each child, and if possible, we kill them. If either or both cells survive, they are added to the collection of active cells for future processing. The algorithm terminates when no more active cells remain.

The precise implementation of any geometric branch-and-bound algorithm depends on the following elements:

- How are cells represented?
- What is the initial cell?
- How is a cell subdivided?
- How are the upper and lower bounds computed?
- Under what conditions is a cell killed?
- Among the active cells, which cell is selected next for processing?

Let us describe each of these elements in greater detail in the context of our approximation algorithm for LTS.

Cells and their representations. Although a solution to LTS is fully specified by the d-vector of coefficients, we will use a more concise representation. Recall that a hyperplane is represented by the equation $y = \sum_{j=1}^{d-1} \beta_j x_j + \beta_d$, where β_d is the intercept term. Rather than store all d-coefficients, we will store only the first $d-1$ coefficients, the *slope coefficients*. In particular, we represent a solution to LTS by a vector $\boldsymbol{\beta} = (\beta_1, \ldots, \beta_{d-1}) \in \mathbb{R}^{d-1}$. We will show in Section 4 that given such a vector, it is possible to compute the optimum value of β_d in $O(n \log n)$ time by solving a 1-dimensional LTS problem. Because the time to process a cell is already $O(n)$, this represents only a modest increase in the processing time for each cell. Because running times tend to grow exponentially with the dimension of the solution space, this reduction in dimension can significantly reduce the algorithm's overall running time. (Empirical evidence for this is provided in

Section 5.2.) Given $\boldsymbol{\beta} \in \mathbb{R}^{d-1}$, let $\Delta_{\boldsymbol{\beta}}(P,h)$ denote the minimum LTS cost achievable by extending $\boldsymbol{\beta}$ to a d-dimensional vector.

For our algorithm, a *cell* C is a closed, axis-parallel hyperrectangle in $\mathbb{R}^{d-1}$. It is represented by a pair of vectors $\boldsymbol{\beta}^-, \boldsymbol{\beta}^+ \in \mathbb{R}^{d-1}$, and consists of the Cartesian product of intervals $\prod_{i=1}^{d-1}[\beta_i^-, \beta_i^+]$. Let $\Delta_C(P,h) = \min_{\boldsymbol{\beta}\in C} \Delta_{\boldsymbol{\beta}}(P,h)$ denote the smallest LTS cost of any point of C.

Sampled elemental fits. We will employ random elemental fits to help guide the search algorithm. Before the algorithm begins, a user-specified number of randomly sampled elemental fits is generated. Each elemental fit is associated with a $(d-1)$-dimensional vector of slope coefficients. Let S_0 denote this set of vectors. For each active cell C, let $S(C)$ denote the elements of S_0 that lie within C. Each active cell C stores the elements of $S(C)$ in a list and the minimum axis-aligned hyperrectangle that contains $S(C)$.

Initial cell. The initial cell can be specified by the user or generated automatically by the program from the sampled elemental fits. If the user does not specify the initial cell, we generate the initial cell by computing the smallest axis-aligned hyperrectangle in $\mathbb{R}^{d-1}$ that encloses the elements of S_0. Because this hyperrectangle will be heavily influenced by outliers, we compute a subrectangle of small volume that contains a user-specified fraction of the points of S_0. (In our implementation we chose this fraction to be 1/2. Let m denote the number of points of S_0. For each coordinate axis x_i, we project the points of S_0 onto x_i and compute the smallest interval that contains all but $m/2d$ of these points. We remove these $m/2d$ points from S_0. Repeating this for each axis results in a set of d intervals, one per axis, whose Cartesian product defines the desired subrectangle. Since each of the d iterations eliminates $m/2d$ points, the number of points remaining is $m/2$.)

Cell subdivision. We will discuss how active cells are selected for processing below. Once a cell C is selected, it is subdivided into two hyperrectangles by an axis parallel hyperplane. This hyperplane is chosen as follows. First, if $S(C)$ is not empty, then the algorithm determines the longest side length of bounding rectangle containing $S(C)$ (with ties broken arbitrarily). It then sorts the vectors of $S(C)$ along the axis that is parallel to this side, and splits the set by a hyperplane that is orthogonal to this side and passes through the median of the sorted sequence (see Fig. 2(a)). If $S(C)$ is empty, the algorithm bisects the cell through its midpoint by a hyperplane that is orthogonal to the cell's longest side length (see Fig. 2(b)). The resulting cells, denoted C_0 and C_1 in the figure, are called C's *children*.

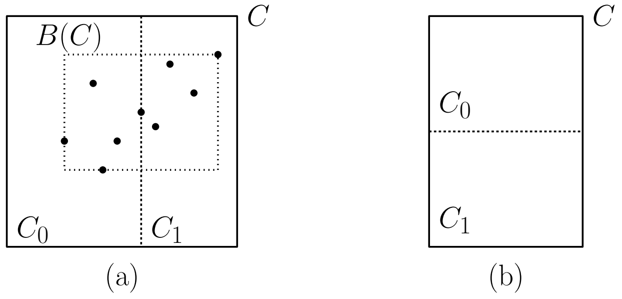


Fig. 2: Subdividing a cell (a) when $S(C)$ is nonempty and (b) when $S(C)$ is empty.

An example of the subdivision process is shown below in Fig. 3 for a 2-dimensional solution space. In (a) we show a cell C and its samples $S(C)$. In (b) we show the subdivision that results by repeatedly splitting each cell through its median sample. In (c) we show the effect of two additional steps of subdivision by bisecting the cell's longest side. (This assumes that all the cells are selected for processing and none are killed.) Note that the subdivision has the property that it tends to produce more cells in regions of space where the density of samples is higher.

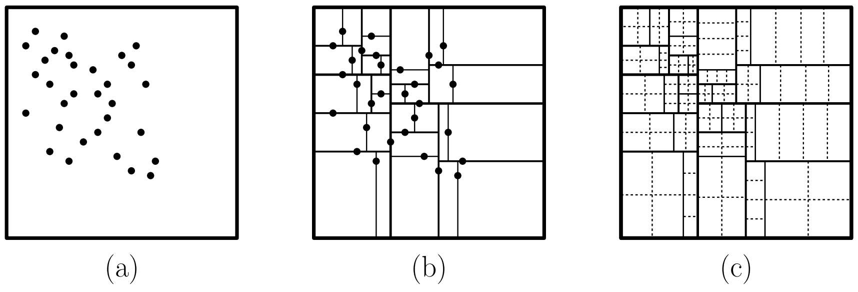


Fig. 3: Example of the subdivision process: (a) initial cell and samples, (b) sample-based subdivision, (c) two more stages of midpoint subdivision.

Upper and lower bounds. Recall that the upper bound for a cell C, which we denote by $\Delta^+(C)$, is an upper bound on the smallest LTS cost among all hyperplanes whose slope coefficients lie within C. To compute such an upper bound, it suffices to sample any representative slope from within the cell and then compute the y-intercept of the hyperplane with this slope that minimizes the LTS cost. We shall see that it suffices to use the reduced trimming parameter $h^- = h - \lfloor n\varepsilon_q \rfloor$.

Our algorithm chooses the representative slope as follows. If $S(C)$ is nonempty, we take the median sample point that was chosen in the cell-subdivision process. Otherwise, we take the cell's midpoint. In Section 4, we will show how to compute the optimum y-intercept by reduction to a 1-dimensional LTS problem, which can be solved in $O(n \log n)$ time. To further improve the upper bound, we then apply a user-specified number of C-steps. (We used two C-steps in our experiments.)

The computation of the lower bound for the cell C, denoted $\Delta^-(C)$, is more complex than the upper bound. Our approach is similar to the upper bound computation, but rather than computing the optimum y-intercept for a specific slope, we compute the optimum y-intercept under the assumption that the slope could be any point of C (using the full trimming parameter h, not h^-). In Section 4, we will show how to do this in $O(n \log n)$ time by solving a problem that we call the 1-dimensional interval LTS problem.

Killing cells. Recall that our objective is to report a hyperplane $\boldsymbol{\beta}$ that satisfies

$$\Delta_{\boldsymbol{\beta}}(P, h^-) \;\leq\; (1 + \varepsilon_r)\Delta(P, h).$$

Let $\widehat{\boldsymbol{\beta}}$ denote the hyperplane associated with the smallest upper bound encountered so far in the search (assuming the trimming parameter h^-). Given a cell C, we assert that C can be killed if

$$\Delta^-(C) \;>\; \Delta_{\widehat{\boldsymbol{\beta}}}(P, h^-)/(1 + \varepsilon_r). \tag{1}$$

The reason is that for any $\boldsymbol{\beta}$ in such a cell, we have $\Delta_{\widehat{\boldsymbol{\beta}}}(P, h^-) < (1+\varepsilon_r)\Delta_{\boldsymbol{\beta}}(P, h)$. Thus, C cannot provide a solution whose cost is so low that it would contradict the hypothesis that $\widehat{\boldsymbol{\beta}}$ is a valid hybrid approximation. Therefore, it is safe to eliminate C from further consideration. (Note that future iterations might change $\widehat{\boldsymbol{\beta}}$, but only in a manner than would decrease $\Delta_{\widehat{\boldsymbol{\beta}}}(P, h^-)$. Thus, the decision to kill a cell never needs to be reconsidered.)

It is not hard to show that whenever the ratio between a cell's upper bound and lower bound becomes smaller than $(1+\varepsilon_r)$, the cell will be killed. This is because $\widehat{\boldsymbol{\beta}}$ was selected from the processed cell having the smallest value of Δ^+, and so such a cell satisfies

$$\Delta^-(C) \;>\; \Delta^+(C)/(1+\varepsilon_r) \;\geq\; \Delta_{\widehat{\boldsymbol{\beta}}}(P, h^-)/(1+\varepsilon_r).$$

This implies that C satisfies the condition in Eq. (1) for being killed. It follows that the algorithm will terminate once all cells have been subdivided to such a small size that this condition holds.

Cell processing order. An important element in the design of an efficient geometric branch-and-bound algorithm is the order in which active cells are selected for processing. When a cell is selected for processing, there are two desirable outcomes we might hope for. First, the representative hyperplane from this cell will have a lower LTS cost than the best hyperplane $\widehat{\boldsymbol{\beta}}$ seen so far. This will bring us closer to the optimum LTS cost, and it has the benefit that future cells are more likely to be killed by the condition of Eq. (1). Second, the lower bound of this cell will be so high that the cell will be killed, thus reducing the number of active cells that need to be considered. This raises the question of whether there are easily computable properties of the active cells that are highly correlated with either of these desired outcomes. We considered the following potential criteria for selecting the next cell:

(1) *Max-samples*: Select the active cell that contains the largest number of randomly sampled elemental fits, that is, the cell C that maximizes $|S(C)|$.

(2) *Min-lower-bound*: Select the active cell having the smallest lower bound, $\Delta^-(C)$.

(3) *Min-upper-bound*: Select the active cell having the smallest lower bound, $\Delta^+(C)$.

(4) *Oldest-cell*: Select the active cell that has been waiting the longest to be processed.

Based on our experience, none of these criteria alone is the best choice throughout the entire search. At the start of the algorithm, when many cells have a large number of samples, criterion (1) tends to work well because it favors cells that are representative of typical elemental fits. But as the algorithm proceeds, and cells are further subdivided, the number of samples per cell decreases. In such cases, this criteria cannot distinguish one cell from another. Criteria (2) and (3) are generally good in these middle phases of the algorithm. But when these two criteria are used exclusively, cells that are far from the LTS optimum are never processed. Adding criterion (4) helps remedy this unbalance.

Our approach to selecting the next active cell employs an adaptive strategy. The algorithm assigns a weight to each of the four criteria. Initially, all the criteria are given the same weight. At the start of each stage, the algorithm selects the next criteria randomly based on these weights. That is, if the current weights are denoted $w_1, \ldots, w_4$, criterion i is selected with probability

$w_i/(w_1 + \cdots + w_4)$. We select the next cell using this criterion. After processing this cell, we either reward or penalize this criterion depending on the outcome. First, we compute the ratio between the cell's new lower bound and the best LTS cost seen so far, that is, $\rho^- = \Delta^-(C)/\Delta_{\widehat{\boldsymbol{\beta}}}(P, h^-)$. Observe that ρ^- is nonnegative and increases as the lower bound approaches the current best LTS cost. With probability $\min(1, \rho^-)$ we increase the current criteria's weight by 50%, and otherwise we decrease it by 10%. Second, we compute the inverse of the ratio between the cell's new upper bound and the best LTS cost seen so far, that is, $\rho^+ = \Delta_{\widehat{\boldsymbol{\beta}}}(P, h^-)/\Delta^+(C)$. Again, ρ^+ is nonnegative and increases as the upper bound approaches the best LTS cost. With probability $\min(1, \rho^+)$ we increase the current criteria's weight by 50%, and otherwise we decrease it by 10%.

The complete algorithm. The algorithm begins by generating the initial sample S_0 of random elemental fits and the initial cell C_0 as the smallest bounding hyperrectangle containing this cell. The initial set of active cells is $\{C_0\}$. We then repeat the following stages until this set is empty. First, the above cell-selection strategy is applied to select and remove the next cell C from this set. By the subdivision process, we split this cell into two children cells C_0 and C_1. The set of samples $S(C)$ is then partitioned among these two cells as $S(C_0)$ and $S(C_1)$, respectively. Next, for each of these children, the lower and upper bounds are computed as described earlier. If the upper bound cost is smaller than the current best LTS cost, then we update the current best LTS fit $\widehat{\boldsymbol{\beta}}$ and its associated cost. For each child cell, we test whether it can be killed by applying the condition of Eq. (1). If the cell is not killed, it is added to the list of active cells. In either case, the selection criteria that was used to determine this cell is rewarded or penalized, as described above. On termination, we output the current best fit $\widehat{\boldsymbol{\beta}}$ and its associated cost.

By the remarks made earlier regarding when cells are killed, it follows that on termination the resulting hyperplane $\widehat{\boldsymbol{\beta}}$ is a valid $(\varepsilon_r, \varepsilon_q)$-hybrid approximation to the optimal hyperplane whose slope coefficients lying within the initial cell.

Unfortunately, it is not easy to provide a good asymptotic bound on the algorithm's overall running time. Unlike Fast-LTS, which always runs for a fixed number of iterations irrespective of the structure of the data set, the branch-and-bound algorithm adapts its behavior in accordance with the structural properties of the point set and the desired accuracy of the final result. As we shall see in Section 5, the algorithm terminates very rapidly for well-conditioned inputs, but it can take much longer when the data are poorly conditioned.

Even though we cannot bound the total number of stages, we can bound the running time of each stage. In the next section we will show that the upper and lower bounds, $\Delta^+(C)$ and $\Delta^-(C)$, can each be computed in $O(n \log n)$ time, where n is the number of points. Otherwise, the most time consuming part of each stage is the time needed to compute the next active cell. If m denotes the maximum number of active cells at any time, and we simply store them in a list, the running time of each stage is $O(m + n \log n)$. (Through the use of more sophisticated data structures, it is possible to reduce the running time to $O(\log m + n \log n)$, but since we expect m to be smaller than n, we did not bother to implement this.)

4 Computing Upper and Lower Bounds

In this section we describe how to compute the upper and lower bounds for a given cell C in the geometric branch-and-bound algorithm described in the previous section. Recall that P and h

denote the point set and trimming parameter, respectively, and that a hyperplane is represented as a vector of coefficients $\boldsymbol{\beta} = (\beta_1, \ldots, \beta_d)$ in $\mathbb{R}^d$, but our solution space stores only the slope coefficients $(\beta_1, \ldots, \beta_{d-1})$. The cell C is represented by a pair of vectors $\boldsymbol{\beta}^-, \boldsymbol{\beta}^+ \in \mathbb{R}^{d-1}$, and consists of the Cartesian product of intervals $\prod_{i=1}^{d-1}[\beta_i^-, \beta_i^+]$, which we denote by $[\boldsymbol{\beta}^-, \boldsymbol{\beta}^+]$. Let $\Delta_C(P,h) = \min_{\boldsymbol{\beta} \in C} \Delta_{\boldsymbol{\beta}}(P,h)$ denote the smallest LTS cost of any point of C. Our objective is to compute upper and lower bounds on this quantity.

In the previous section we explained how the algorithm samples a representative vector of slope coefficients from C. To compute the cell's upper bound, $\Delta^+(C)$, we compute the value of the y-intercept coefficient that, when combined with the representative vector of slope coefficients, produces the hyperplane that minimizes the LTS cost. It is straightforward to show that this can be reduced to solving a 1-dimensional LTS problem, which can then be solved in $O(n \log n)$ time [21]. We will present the complete algorithm, since it will be illustrative when we generalize this to the more complex problem of computing the cell's lower bound.

Recall from Section 3 that the trimming parameter is h^- when computing the upper bound, but we will refer to it as h in this section to simplify the notation. Let $p_i = (\boldsymbol{x}_i, y_i)$ denote the ith point of P, where $\boldsymbol{x}_i \in \mathbb{R}^{d-1}$ and $y_i \in \mathbb{R}$. The squared residual of p_i with respect to a hyperplane $\boldsymbol{\beta} = (\beta_1, \ldots, \beta_d)$, which we denote by $r_i^2(\boldsymbol{\beta})$, is

$$r_i^2(\boldsymbol{\beta}) \;=\; \left(y_i - \left(\sum\nolimits_{j=1}^{d-1} \beta_j x_{i,j} + \beta_d\right)\right)^2 \;=\; \left(\beta_d - \left(y_i - \sum\nolimits_{j=1}^{d-1} \beta_j x_{i,j}\right)\right)^2. \qquad (2)$$

Let $b_i = y_i - \sum_{j=1}^{d-1} \beta_j x_{i,j}$. We can visualize b_i as the intersection of y-axis and the hyperplane passing through p_i whose slope coefficients match $\boldsymbol{\beta}$ (see Fig. 4(a)). Let $B = \{b_1, \ldots, b_n\}$ denote this set of intercepts. For any hyperplane $\boldsymbol{\beta}$, the squared distance $(b_i - \beta_d)^2$ between intercepts is clearly equal to $r_i^2(\boldsymbol{\beta})$. Therefore, the desired intercept β_d of the LTS hyperplane whose slope coefficients match $\boldsymbol{\beta}$'s is the point on the y-axis that minimizes the sum of squared distances to its h closest points in B. That is, computing β_d reduces to solving the (1-dimensional) LTS problem on the n-element set B.

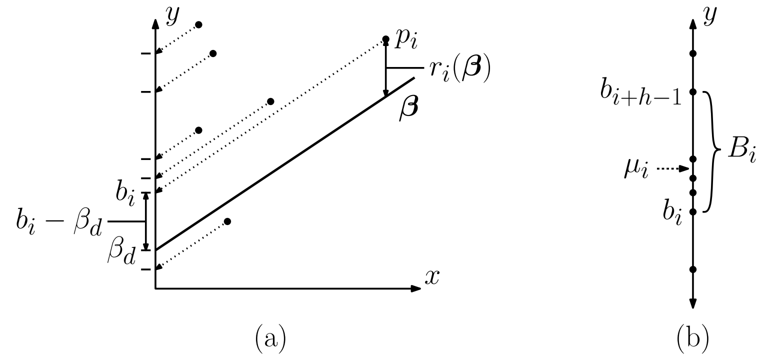


Fig. 4: Computing the optimum y-intercept for a given slope $\boldsymbol{\beta}$: (a) projecting the points and (b) the subset $\{b_i, \ldots, b_{i+h-1}\}$.

Before presenting the algorithm for the 1-dimensional LTS problem, we begin with a few observations. First, let us assume that the points of B are sorted in nondecreasing order and have been renumbered so that $b_1 \leq \cdots \leq b_n$. Clearly, the h-element subset B that minimizes the sum of squared distances to any point on the y-axis consists of h consecutive points of B. For $1 \leq i \leq n-h+1$, define $B_i = \{b_i, \ldots, b_{i+h-1}\}$ (see Fig. 4(b)). The desired upper bound is just the minimum among these $n-h+1$ least-squares costs. This can be computed easily by brute force in $O(hn) = O(n^2)$ time, but we will show that it can be solved by an incremental approach in $O(n)$ time.

The point that minimizes the sum of squared deviates within each subset B_i is just the mean of the subset, which we denote by μ_i. The least-squares cost is the subset's standard deviation, which we denote by σ_i. Define $\textsc{sum}(i) = \sum_{k=i}^{i+h-1} b_k$ and $\textsc{ssq}(i) = \sum_{k=i}^{i+h-1} b_k^2$. Given these, it well known that we can compute the mean and standard deviation as

$$\mu_i \;=\; \frac{\textsc{sum}(i)}{h} \qquad \text{and} \qquad \sigma_i^2 \;=\; \left(\frac{\textsc{ssq}(i) - (\textsc{sum}(i)^2/h)}{h-1}\right)^{1/2}. \tag{3}$$

Thus, it suffices to show how to compute $\textsc{sum}(i)$ and $\textsc{ssq}(i)$, for $1 \leq i \leq n-h+1$. We begin by computing the values of $\textsc{sum}(1)$ and $\textsc{ssq}(1)$ in $O(h)$ time by brute force. As we increment the value of i, we can update the quantities of interest in $O(1)$ time each. In particular,

$$\textsc{sum}(i+1) \;\leftarrow\; \textsc{sum}(i) + (b_{i+h} - b_i) \qquad \text{and} \qquad \textsc{ssq}(i+1) \;\leftarrow\; \textsc{ssq}(i) + (b_{i+h}^2 - b_i^2).$$

Thus, given the initial $O(n \log n)$ time to sort the points and the $O(h)$ time to compute $\textsc{sum}(1)$ and $\textsc{ssq}(1)$, the remainder of the computation runs in constant time for each i. Therefore, the overall running time is $O(n \log n + h + (n-h+1)) = O(n \log n)$. The final LTS cost is just the minimum of the σ_i's.

Next, we will show how to generalize this to the more complex task of computing the lower bound, $\Delta^-(C)$. Recall that the objective is to compute a lower bound on the LTS cost of *any* hyperplane $\boldsymbol{\beta}$ whose slope components lie within the $(d-1)$-dimensional hyperrectangle $[\boldsymbol{\beta}^-, \boldsymbol{\beta}^+]$. We will demonstrate that this can be reduced to the problem of solving a variant of the 1-dimensional LTS problem over a collection of n intervals, which we call the *interval LTS problem*. We will present an $O(n \log n)$ time algorithm for this problem.

Let $(\boldsymbol{x}_i, y_i)$ denote the coordinates of $p_i \in P$, where $\boldsymbol{x}_i \in \mathbb{R}^{d-1}$ and $y_i \in \mathbb{R}$. For any hyperplane $\boldsymbol{\beta}$, recall the formula of Eq. (2) for the squared residual $r_i^2(\boldsymbol{\beta})$. We seek the value of β_d that minimizes the sum of the h smallest squared residuals subject to the constraint that $\boldsymbol{\beta}$'s slope coefficients lie within $[\boldsymbol{\beta}^-, \boldsymbol{\beta}^+]$. Although we do not know the exact values of the these slope coefficients, we do have bounds on them. Using the fact that $\beta_j^- \leq \beta_j \leq \beta_j^+$, for $1 \leq j \leq d-1$, we can derive upper and lower bounds on the second term in the squared residual formula (Eq. (2)) by a straightforward application of interval arithmetic [13]. In particular, for $1 \leq i \leq n$,

$$b_i^+ \;=\; y_i - \sum_{j=1}^{d-1} \beta'_j x_{i,j}, \quad \text{where } \beta'_j = \begin{cases} \beta_j^- & \text{if } x_{i,j} \geq 0, \\ \beta_j^+ & \text{if } x_{i,j} < 0. \end{cases} \tag{4}$$

$$b_i^- \;=\; y_i - \sum_{j=1}^{d-1} \beta''_j x_{i,j}, \quad \text{where } \beta''_j = \begin{cases} \beta_j^+ & \text{if } x_{i,j} \geq 0, \\ \beta_j^- & \text{if } x_{i,j} < 0. \end{cases} \tag{5}$$

These quantities are analogous to the values b_i used in the upper bound, subject to the uncertainty in the slope coefficients. It is easy to verify that $b_i^- \leq b_i^+$, and for any $\boldsymbol{\beta}$ whose slope coefficients lie within $[\boldsymbol{\beta}^-, \boldsymbol{\beta}^+]$, the value of $r_i^2(\boldsymbol{\beta})$ is of the form $(\beta_d - b_i)^2$, for some $b_i \in [b_i^-, b_i^+]$. Analogous to the case of the upper bound computation, this is equivalent to saying that any hyperplane passing through p_i along the direction of $\boldsymbol{\beta}$ intersects the y-axis at a point in the interval $[b_i^-, b_i^+]$ (see Fig. 5). For the purposes of obtaining a lower bound on the LTS cost, we may take b_i to be the closest point in $[b_i^-, b_i^+]$ to the hypothesized intercept β_d. Thus, we have reduced our lower bound problem to computing the value of β_d that minimizes the sum of the smallest h squared distances to a collection of n intervals. This is a generalization of the 1-dimensional LTS problem, but where instead of points, we now have intervals.

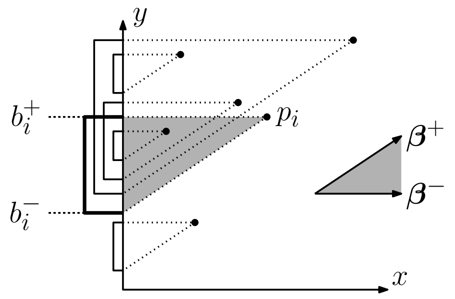


Fig. 5: Reducing the lower bound to the interval LTS problem.

More formally, we define the *interval LTS problem* as follows. Given a point b and a closed interval define the *distance* from b to this interval to be the minimum distance from b to any point of the interval. (The distance is zero if b is contained within the interval.) Given a set B of n nonempty, closed intervals on the real line and a trimming parameter h, for any real b, define $r_{[i]}(b, B)$ to be the distance from b to the ith closest interval of B. Also, define

$$\Delta_b(B, h) \;=\; \left(\frac{1}{h-1} \sum_{i=1}^{h} r_{[i]}^2(b, B) \right)^{1/2}.$$

The interval LTS problem is that of computing the minimum value of $\Delta_b(B, h)$, over all reals b, which we denote by $\Delta(B, h)$. Summarizing the presentation to this point, we obtain the following reduction.

Lemma 3 *Consider an n-element point set P in $\mathbb{R}^d$, a trimming parameter h, and a cell C defined by the slope bounds $\boldsymbol{\beta}^-, \boldsymbol{\beta}^+ \in \mathbb{R}^{d-1}$. Let B denote the set of n intervals $[b_i^-, b_i^+]$ defined in Eqs. (4) and (5) above. Then for any $\boldsymbol{\beta} \in C$, $\Delta(B, h) \leq \Delta_{\boldsymbol{\beta}}(P, h)$.*

The rest of this section will be devoted to giving an $O(n \log n)$ time algorithm that solves the interval LTS problem. Our approach is a generalization of the algorithm for the upper-bound processing. First, we will identify a collection of $O(n)$ subsets of intervals of size h, such that the one with the lowest cost will be the solution to the interval LTS problem. Second, we will show how to compute the LTS costs of these subsets efficiently through an incremental approach. To avoid discussion of messy degenerate cases, we will make the general-position assumption that the interval endpoints of B are distinct. This can always be achieved through an infinitesimal perturbation of the endpoint coordinates.

Recall that in the upper-bound algorithm, we computed the LTS cost of each h consecutive points. In order to generalize this concept to the interval case, we first sort the left endpoints B in nondecreasing order, letting $b^-_{[j]}$ denote the jth smallest left endpoint. Similarly, we sort the right endpoints, letting $b^+_{[i]}$ denote the ith smallest right endpoint. Define I_i to be the (possibly empty) interval $\left[b^+_{[i]}, b^-_{[i+h-1]}\right]$, and define B_i to be the (possibly empty) subset of intervals of B whose right endpoints are at least $b^+_{[i]}$, and whose left endpoints are at most $b^-_{[i+h-1]}$. To avoid future ambiguity with the term "interval," we will refer to any interval formed from the endpoints of B as a *span*, and each interval I_i is called an *h-span* (see Fig. 6). We next prove a technical result about the sets B_i.

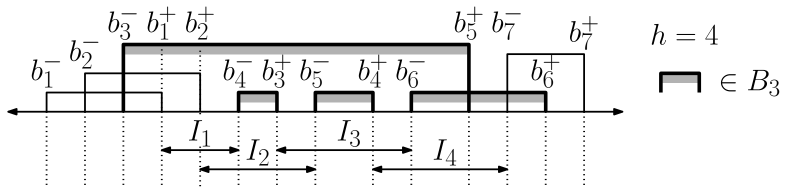


Fig. 6: For $h = 4$, the h-spans I_i. The intervals of the subset B_3 corresponding to $I_3 = \left[b^+_{[3]}, b^-_{[6]}\right]$ are highlighted.

Lemma 4 *Let (B, h) be an instance of the interval LTS problem, and let B_i be the subsets of B defined above, for $1 \le i \le n-h+1$. If for any i, $b^+_{[i]} > b^-_{[i+h-1]}$, then $\Delta(B, h) = 0$. Otherwise, each set B_i consists of exactly h intervals of B.*

Proof: Observe that (by our general-position assumption) $i-1$ intervals of B lie strictly to the left of $b^+_{[i]}$, and $n-(i+h-1)$ intervals lie strictly to the right of $b^-_{[i+h-1]}$. If $b^+_{[i]} > b^-_{[i+h-1]}$, let k denote the number of intervals of B that contain the span $\left[b^-_{[i+h-1]}, b^+_{[i]}\right]$. Every interval of B is either among the $i-1$ intervals to the left of $b^+_{[i]}$, and/or the $n-(i+h-1)$ intervals that lie to the right of $b^-_{[i+h-1]}$, or the k that contain $\left[b^-_{[i+h-1]}, b^+_{[i]}\right]$. Therefore,

$$n \;\le\; (i-1) + (n-(i+h-1)) + k \;\le\; n-h+k,$$

from which we conclude that $k \ge h$. Thus, every point of the span $\left[b^-_{[i+h-1]}, b^+_{[i]}\right]$ is contained within h intervals of B. This implies that the distance from any such point to all of its h closest intervals is zero. Therefore, $\Delta(B_i, h) = 0$, and so $\Delta(B, h) = 0$.

On the other hand, if $b^+_{[i]} \le b^-_{[i+h-1]}$, then the $i-1$ intervals of B to the left of $b^+_{[i]}$ are disjoint from the $n-(i+h-1)$ intervals to the right of $b^-_{[i+h-1]}$. Since the remaining n intervals of B are in B_i, it follows that $|B_i| = n-(i-1)-(n-(i+h-1)) = h$, as desired. $\Box$

Henceforth, let us assume that $b^+_{[i]} > b^-_{[i+h-1]}$ for all i, since if we ever detect that this is not the case, we may immediately report that $\Delta(B, h)$ is zero and terminate the algorithm. Intuitively, the subsets B_i are chosen to be the "tightest" subsets of B having h elements. Next, we prove formally that for the purposes of solving the interval LTS problem, it suffices to consider just these subsets. For $1 \le i \le n-h+1$, define $\Delta(B_i, h)$ to be the LTS cost of the interval LTS problem on only the h intervals of B_i.

Lemma 5 *Given an instance (B, h) of the interval LTS problem, $\Delta(B, h) = \Delta(B_i, h)$ for some i, where $1 \leq i \leq n - h + 1$.*

Proof: Let B' denote the subset of B of size h that achieves the minimum LTS cost. Suppose towards a contradiction that $\Delta(B', h) < \min_i \Delta(B_i, h)$. Let $b^+_{[i]}$ and $b^-_{[j]}$ denote the leftmost right endpoint and rightmost left endpoint in B', respectively. Since the span from $b^+_{[i]}$ to $b^-_{[j]}$ must overlap at least h intervals of B, by the same reasoning as in Lemma 4, we have $j \geq i + h - 1$. Further, we may assume that $j > i + h - 1$, for otherwise B' would be equal to B_i. Thus, B' spans at least $h + 1$ intervals, which implies that there exists at least one "unused" interval of B that is in B_i but not in B'. Let I denote any such interval (see Fig. 7(a)).

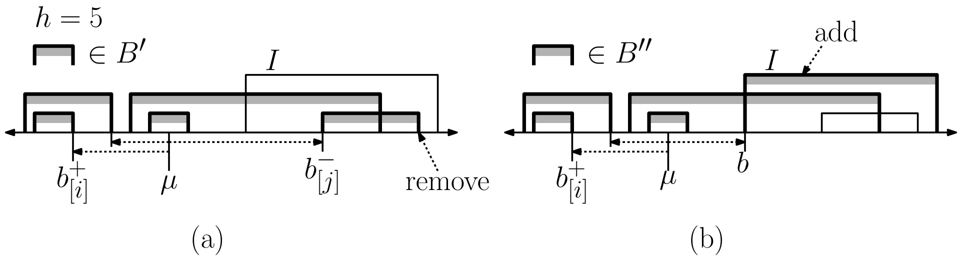


Fig. 7: Proof of Lemma 5. By replacing the interval whose left endpoint is anchored to $b^-[j]$ with the unused interval I anchored to b, we decrease the LTS cost.

First, we assert that $b^+_{[i]} < b^-_{[j]}$. To see why, observe that otherwise, $b^+_{[i]}$ is contained within $h+1$ intervals (by the same reasoning as in Lemma 4), implying that $\Delta(B_i, h) = 0$, which would violate our hypothesis that none of the B_i's is optimal. Given this assertion, let μ denote the point that minimizes the sum of squared distances to the intervals of B' (see Fig. 7(a)). Clearly, $b^+_{[i]} \leq \mu \leq b^-_{[j]}$. By left-right symmetry, we may assume without loss of generality that μ is closer to $b^+_{[i]}$ than it is to $b^-_{[j]}$. (More specifically, if we negate all the interval endpoints, we may apply the proof with the roles of $b^+_{[i]}$ and $b^-_{[j]}$ reversed.) Because $b^-_{[j]}$ is the rightmost left endpoint in B', the distance from μ to $b^-_{[j]}$ is the largest among all the intervals of B whose closest endpoint to μ lies in the span $[b^+_{[i]}, b^-_{[j]}]$, and in particular this is true for the interval I. Consider the set B'' formed by taking B' and replacing the interval anchored at $b^-_{[j]}$ with I (see Fig. 7(b)). Since I is closer to μ than $b^-_{[j]}$ is, the LTS cost of B'' is smaller than the LTS cost of B'. This contradicts our hypothesis that B' achieves the minimum LTS cost. $\square$

From the above lemma, it follows that in order to solve the interval LTS problem, it suffices to compute the LTS cost of each of the subsets B_i, for $1 \leq i \leq n - h + 1$. Just as we did in the upper bound computation, we will adopt an incremental approach. Recall that $\Delta(B_i, h)$ denotes the interval LTS cost of B_i, and let μ_i denote the point that minimizes the sum of squared distances from itself to all of the intervals of B_i. Our approach will be to compute the initial values, μ_1 and $\Delta(B_1, h)$, explicitly by brute force in $O(h)$ time. Then, for i running from 2 up to $n - h + 1$, we will show how to update the subsequent values μ_i and $\Delta(B_i, h)$, each in constant time.

In the upper bound algorithm, we observed that the value that minimizes the sum of squared distances to a set of numbers is just the mean of the set. However, generalizing this simple observations to a set of intervals is less obvious. Given an arbitrary interval $[b^-, b^+]$ of B, the function that maps any point x on the real line to its squared distance to this interval is clearly convex. (It is not strictly convex because the function is zero for all points that lie within the interval.) Since $\Delta(B_i, h)$ is the minimum of the sum of h such functions, and by our assumption that no h intervals of B contain in a single point, it follows that this function is strictly convex, and hence μ_i is its unique local minimum. Given an initial estimate on the location of μ_i, we can exploit convexity to determine the direction in which to move. As the algorithm transitions from B_{i-1} to B_i, we remove one interval from the left (the one anchored at $b^+_{[i-1]}$) and add one interval to the right (the one anchored at $b^-_{[i+h-1]}$). Since we remove an interval from the left end and add one on the right end, it follows that $\mu_i \geq \mu_{i-1}$. Thus, the search for μ_i proceeds monotonically to the right.

To make this more formal, let $\{b_1, \ldots, b_{2n}\}$ denote the sorted sequence of the interval endpoints of B in nondecreasing order. This implicitly defines $2n - 1$ intervals of the form $[b_{k-1}, b_k]$, for $1 < k \leq 2n$ where μ_i might lie. Again, to avoid ambiguity with the term "interval," we refer to these intervals as *segments* (see Fig. 8(a)). All the points within the interior of any given segment have the property that they lie to the left/right/contained within the same intervals of B. Our algorithm operates by maintaining three indices, i, j, and k. We will set $j = i + h - 1$ so that $I_i = \left[b^+_{[i]}, b^-_{[j]}\right]$ is the current h-span of interest. The index k specifies the *current segment*, $[b_k, b_{k+1}]$, which represents the hypothesized segment that contains μ_i. The algorithm repeatedly increases k as long as μ_i is determined to lie to the right of b_{k+1}.

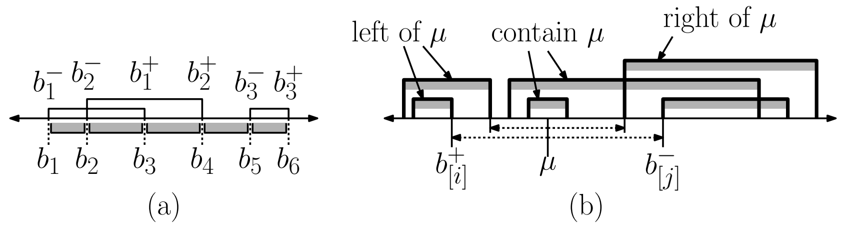


Fig. 8: Segments and contributions: (a) The sorted endpoints $\langle b_1, \ldots, b_{2n}\rangle$ and the associated segments (shaded), (b) the mean μ_i and the distance contributions from the intervals of B_i.

How do we determine whether the current segment contains μ_i? First, we classify the every interval of B_i as lying to the left, right, or containing the segment's interior. The intervals of B_i that contain the segment's interior contribute zero to the squared distance, and so they may be ignored. For those intervals that lie entirely to the segment's left (resp., right), the interval's right (resp., left) endpoint determines the squared distance (see Fig. 8(b)). Let us call this endpoint the *relevant endpoint* of the associated interval. As in the computation of the upper bound, we will maintain two quantities SUM and SSQ, which will be updated throughout the algorithm. The first stores the sum of the relevant endpoints and the second stores the sum of squares of the relevant endpoints. As in Eq. (3), the value μ_i and the LTS cost $\Delta(B_i, h) = \sigma_i$ will be derived from these quantities.

Each time we advance the current segment by incrementing k, we are now either entering an interval of B (if b_k is a left endpoint) or leaving an interval (if b_k is a right endpoint). In the first case the interval we are entering was contributing its left endpoint to (SUM and SSQ) and is now not making a contribution (see Fig. 9(a)). In the second case, the interval we are leaving was not contributing and is now contributing its right endpoint (see Fig. 9(b)).

Throughout, the algorithm maintains Δ_{best}, which stores the minimum LTS cost of any B_i

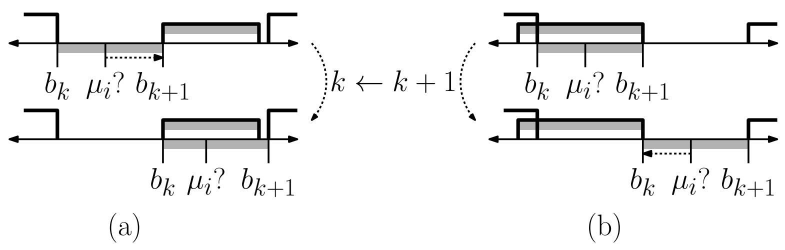


Fig. 9: Contribution updates when advancing the current segment.

encountered thus far. We can now present the complete algorithm.

```
(1) [Initializations:]
    (a) [Sort:] Sort the left endpoints of $B$ as $\langle b^-_{[1]}, \ldots, b^-_{[n]} \rangle$, the right endpoints as $\langle b^+_{[1]}, \ldots, b^+_{[n]} \rangle$,
        and all the endpoints as $\langle b_1, \ldots, b_{2n} \rangle$.
    (b) [Initialize costs:] Set SUM $\leftarrow \sum_{1 \le j \le h} b^-_{[j]}$, SSQ $\leftarrow \sum_{1 \le j \le h} (b^-_{[j]})^2$, and $\Delta_{\text{best}} \leftarrow +\infty$.
    (c) [Initialize indices:] Let $i \leftarrow k \leftarrow 1$ and $j \leftarrow h$.
(2) [Main loop:] While $i \le n - h - 1$ do:
    (a) [Check for $h$-fold interval overlap:] If $b^+[i] \ge b^-[j]$, set $\Delta_{\text{best}} \leftarrow 0$ and return.
    (b) [Update $\mu$:] Recalling Eq. (3), set $\mu \leftarrow$ SUM$/h$.
    (c) [Find the segment that contains $\mu$:] While $b_{k+1} < \mu$ do:
        (i) [Advance to the next segment:] Set $k \leftarrow k + 1$.
        (ii) [Entering an interval?] If $b_k$ is the left endpoint of some interval of $B$, set SUM $\leftarrow$
             SUM $- b_k$ and SSQ $\leftarrow$ SSQ $- (b_k)^2$ (see Fig. 9(a))
        (iii) [Exiting an interval?] Otherwise, $b_k$ is the right endpoint of some interval of $B$. Set
              SUM $\leftarrow$ SUM $+ b_k$ and SSQ $\leftarrow$ SSQ $+ (b_k)^2$ (see Fig. 9(b))
        (iv) [Update $\mu$:] Set $\mu \leftarrow$ SUM$/h$.
    (d) [Update LTS cost:] Recalling Eq. (3), set $\sigma \leftarrow \left( \frac{\text{SSQ} - (\text{SUM}^2/h)}{h-1} \right)^{1/2}$. If $\sigma < \Delta_{\text{best}}$ then
        set $\Delta_{\text{best}} \leftarrow \sigma$.
    (e) [Remove contribution of leftmost interval $b^+_{[i]}$:] SUM $\leftarrow$ SUM $- b^+_{[i]}$ and SSQ $\leftarrow$ SSQ $- (b^+_{[i]})^2$.
    (f) [Advance to next subset:] Set $i \leftarrow i + 1$ and $j \leftarrow j + 1$.
    (g) [Add contribution of rightmost interval $b^-_{[j]}$:] SUM $\leftarrow$ SUM $+ b^-_{[j]}$ and SSQ $\leftarrow$ SSQ $+ (b^-_{[j]})^2$.
(3) Return $\Delta_{\text{best}}$ as the final LTS cost
```

The algorithm's correctness has already been justified. To establish the algorithm's running time, observe that Step (1a) takes $O(n \log n)$ time, and Step (1b) takes $O(h)$ time. All the other steps take only constant time. Each time the loop of Step (2c) is executed, the value of k is increased. Since k cannot go beyond the last segment (since clearly $\mu \le b_{2n}$), the total number of iterations of this loop throughout the entire algorithm is at most $2n$. Since the loop of Step (2) is repeated at most $n - h + 1$ times, the overall running time is $O(n \log n + h + 2n + (n - h - 1)) = O(n \log n)$. In summary we have the following result, which together with Lemma 3 proves that the LTS lower bound can be computed for each cell in $O(n \log n)$ time.

Theorem 2 *Given a collection B of n intervals on the real line and a trimming parameter h, it is possible to solve the interval LTS problem on B in $O(n \log n)$ time.*

5 Empirical Analysis

As mentioned in the introduction, while Fast-LTS is efficient in practice, it does not provide guarantees on the accuracy of its output. In contrast, on termination, Adaptive-LTS provides guarantees the accuracy of its results (assuming that the optimum is contained within the initial cell). In this section we show that when presented with inputs of low dimension (that is, having a small number of independent variables), Adaptive-LTS performs quite efficiently and can often provide good bounds on the accuracy of the final result. We will demonstrate this empirically on a number of synthetically generated distributions and one actual data set, which was derived from an application in astronomy.

Before presenting our results, let us remark on the structure that is common to all our experiments. We implemented both Rouseeuw and van Driessen's Fast-LTS and our Adaptive-LTS in C++ (compiled by g++ 4.5.2 with optimization level "-O3" and running on a dual-core Intel Pentium-D processor under Ubuntu Linux 11.04). In all experiments but one (shown in Fig. 20 below), we let the algorithm choose the initial cell bounds.

Both Fast-LTS and Adaptive-LTS operate in a series of stages. Each stage of our implementation of Fast-LTS consists of a single random elemental fit followed by two C-steps. (This is the same number used by Rousseeuw and van Driessen in [22].) After each stage we output the LTS cost of the resulting fit. Each experiment consisted of 500 such stages (the default number of stages for FastLTS). Our plots for Fast-LTS show, for each stage, the LTS cost of the current fit and the minimum LTS cost among all the fits seen so far. After these stages, Fast-LTS takes the ten best fits and runs a large number of C-steps on each. Because we are primarily interested in the convergence properties of both algorithms, we have omitted these final C-steps in our experiments. (But this could easily be added to both algorithms.)

For Adaptive-LTS, each stage consists of the processing of a single cell. Recall that this involves sampling a hyperplane from the current cell to which two C-steps are then applied. In addition, a lower bound is computed for the current cell. After each stage, we output the LTS-cost of the current fitting hyperplane and the minimum lower bound among all active cells at this point of the search. Although Adaptive-LTS has a termination condition, for the sake of comparison with FastLTS we disabled the termination condition and instead ran the algorithm for 500 stages.

5.1 Synthetically Generated Data

For these experiments, we generated a data set consisting of 1000 points in $\mathbb{R}^d$, for $d \in \{2, 3\}$. In order to simulate point sets that contain outliers, each data set consisted of the union of points drawn from two or more distributions. One of these, the *inlier distribution*, contains points that lie close to a randomly generated hyperplane. The others, the *outlier distributions*, contain points that are drawn from some other distribution. We have aimed to generate data sets with various degrees of numerical conditioning.

HYPERPLANE+UNIFORM (2-dimensional): Our first experiment involved a 2-dimensional, well-conditioned distribution, consisting of 1000 points. First, a line of the form $y = \beta_1 x + \beta_2$ was generated, where β_1 was sampled uniformly from $[-0.25, +0.25]$, and β_2 was sampled uniformly from $[-1, +1]$. Next, 550 points (55% inliers) were generated with the x-coordinate sampled uniformly from $[-1, +1]$, and the y-coordinates generated by computing the value of the line at these x-coordinates and adding a Gaussian deviate with mean 0 and standard deviation 0.01. The remaining 450 points (45% outliers) were sampled uniformly from the square $[-1, +1]^2$. Because the inliers were drawn from a hyperplane (actually a line in this case) and the outliers were drawn from a uniform distribution, we call this distribution HYPERPLANE+UNIFORM (see Fig. 10).

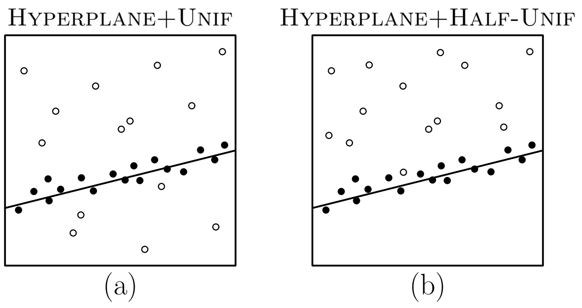
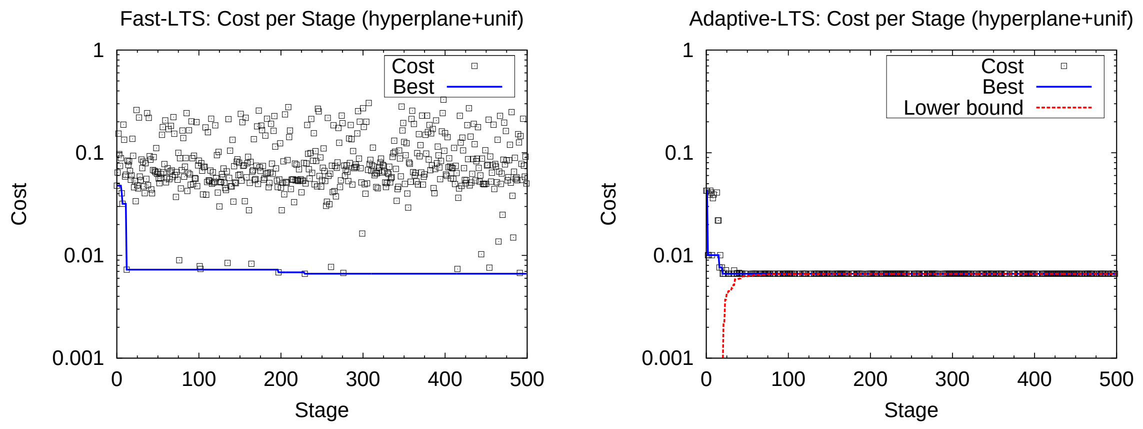


Fig. 10: The HYPERPLANE+UNIFORM and HYPERPLANE+HALF-UNIF distributions.

We ran both Fast-LTS and Adaptive-LTS on the resulting data set for 500 stages. Although in most of our experiments, we set the trimming parameter to 50%, to make this instance particularly easy to solve, we ran both algorithms with a relatively low trimming parameter of $h = 0.1$ (that is, 10% outliers). In Fig. 11(a) and (b) we show the results for Fast-LTS and Adaptive-LTS, respectively, where the x-axis indicates the stage number and the y-axis indicates the LTS-cost. (Note that the y-axis is on a logarithmic scale.) Each (small square) point of each plot indicates the LTS-cost of the sampled hyperplane. The upper (solid blue or "Best") curve indicates the minimum LTS-cost of any hyperplane seen so far. The lower (broken red or "Lower bound") of Fig. 11(b) indicates the minimum lower bound of any active cell. The optimum LTS-cost lies somewhere between these two curves, and therefore, the ratio between the current best and current lower bound limits the maximum relative error that would result by terminating the algorithm and outputting the current best fit.

As mentioned earlier, this is a well-conditioned distribution, and therefore it not surprising that both algorithms rapidly converge to a solution that is nearly optimal. Given only information on the best LTS cost, a user of Fast-LTS would not know when to terminate the search. In contrast, a user of Adaptive-LTS would know that after just 75 iterations, the relative difference between the best upper and lower bounds is smaller than 1%. Thus, terminating the algorithm at this point would imply an approximate error of at most 1%. It is also interesting to note that Fast-LTS generates elemental fits at random, and hence the pattern of plotted points remains consistently random throughout all 500 stages. In contrast, the sampled hyperplanes generated by Adaptive-LTS shows signs of converging to a subregion of the configuration space where the most promising solutions reside.



(a) (b)

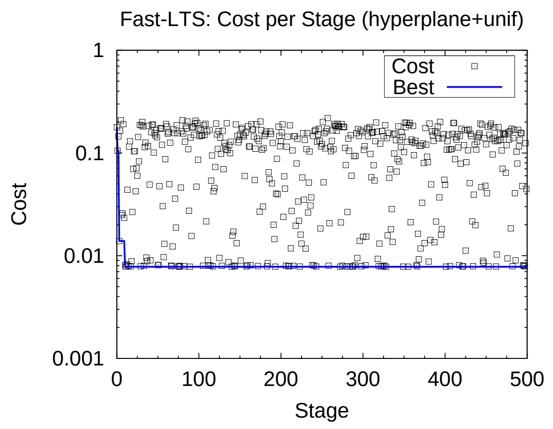
Fig. 11: LTS cost versus stage number for the HYPERPLANE+UNIFORM distribution ($d = 2$, $h = 0.1$) for (a): Fast-LTS and (b): Adaptive-LTS.

HYPERPLANE+UNIFORM (3-dimensional): Our second experiment involved the same distribution, but in $\mathbb{R}^3$ and using a larger value of h. First, a plane of the form $y = \beta_1 x_1 + \beta_2 x_2 + \beta_3$ was generated, where β_1 and β_2 were sampled uniformly from $[-0.25, +0.25]$, and β_2 was sampled uniformly from $[-1, +1]$. As before, 550 points (55% inliers) were generated with the x_1- and x_2-coordinates sampled uniformly from $[-1, +1]$, and the y-coordinates generated by computing the value of the plane at these x-coordinates and adding a 3-dimensional deviate whose coordinates are independent Gaussians of mean 0 and standard deviation 0.01. The remaining 450 points (45% outliers) were sampled uniformly from the cube $[-1, +1]^3$.

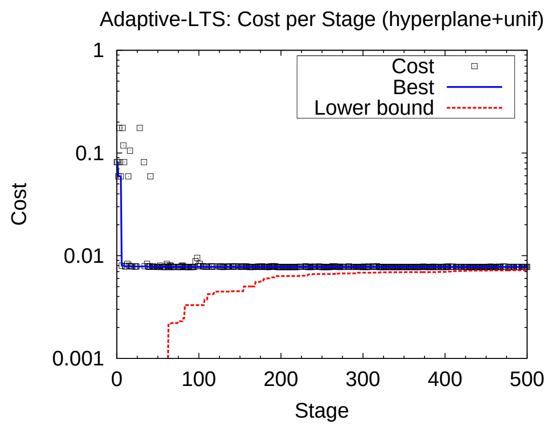
We ran both Fast-LTS and Adaptive-LTS on the data set for 500 stages with $h = 0.5$. In Fig. 12(a) and (b) we show the results for Fast-LTS and Adaptive-LTS, respectively. Again, both algorithms converge rapidly to a solution that is nearly optimal. However, as in the previous experiment, a user of Adaptive-LTS could use the ratio between the best upper and lower bounds to limit the maximum error in the LTS cost. For example, after 200 stages the relative error is within 10%, and after 300 stages it is within 5%. Observe that the rate of convergence is slower than in the earlier 2-dimensional experiment. This is likely due to the increase in the dimension (which results in searching a larger solution space) and the increase in the trimming parameter (which forces the algorithm to find a hyperplane that fits a larger fraction of the data).

HYPERPLANE+HALF-UNIF: This involved a data set consisting of 1000 points in $\mathbb{R}^3$, in which the outlier distribution was more skewed. The inliers were generated in the same manner as in the previous experiment. The outliers were sampled uniformly from the portion of the 3-dimensional hypercube $[-1, +1]^3$ that lies above the plane (see Fig. 10(b)). As before, we ran both Fast-LTS and Adaptive-LTS on the data set for 500 stages with $h = 0.5$. In Fig. 13(a) and (b) we show the results for Fast-LTS and Adaptive-LTS, respectively. The convergence properties of the two algorithms is similar to the previous experiment. After 275 stages of Adaptive-LTS, the relative error is within 10% and after 500 stages it is within 5%.

FLAT+SPHERE: For our final synthetic experiment, we designed a rather pathological distribution

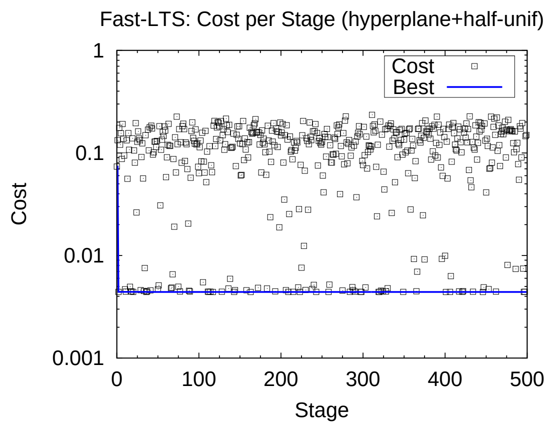


(a)

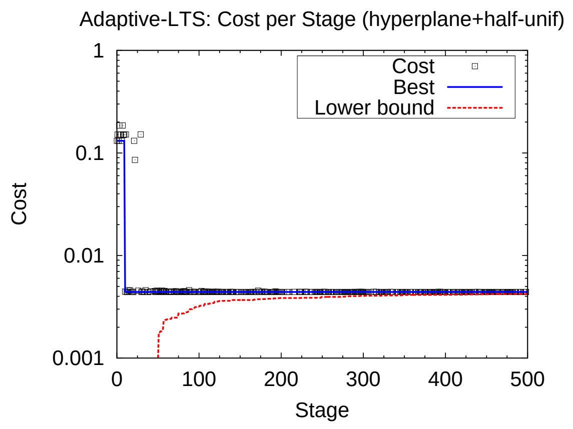


(b)

Fig. 12: LTS cost versus stage number for the HYPERPLANE+UNIFORM distribution ($d = 3$, $h = 0.5$) for (a): Fast-LTS and (b): Adaptive-LTS.



(a)



(b)

Fig. 13: LTS cost versus stage number for the HYPERPLANE+HALF-UNIF distribution ($d = 3$, $h = 0.5$) for (a): Fast-LTS and (b): Adaptive-LTS.

with the intention of challenging both algorithms. The inlier distribution was chosen so that almost all the inliers are degenerate (thus resulting in many unstable elemental fits) and the remaining few inliers are a huge distance away (thus penalizing any inaccurate elemental fits).

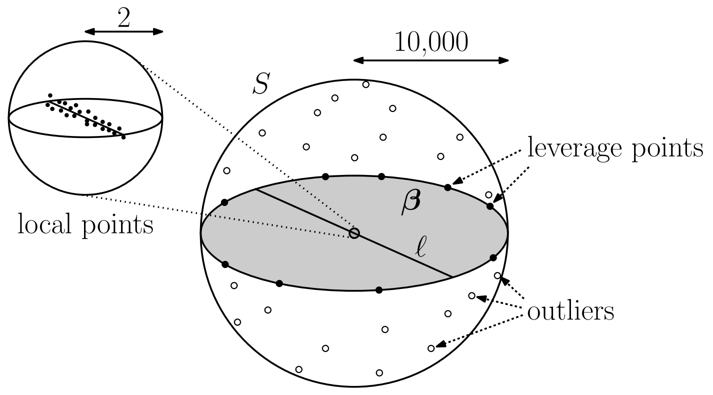
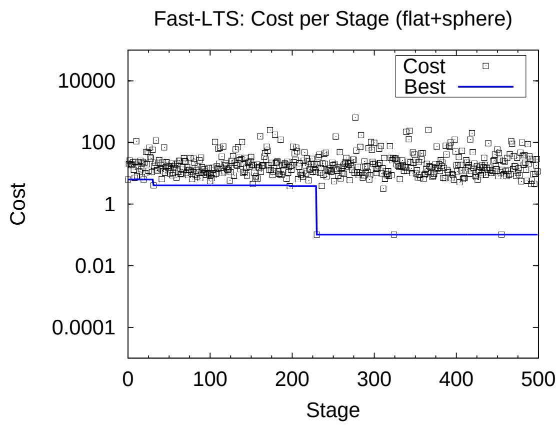


Fig. 14: The FLAT+SPHERE distribution.

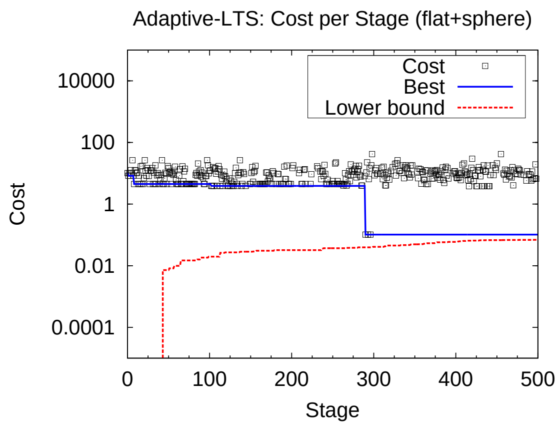
The point set consisted of 1000 points in $\mathbb{R}^3$ with 500 inliers and 500 outliers. Let S be a large sphere centered at the origin with radius 10,000, let $\boldsymbol{\beta}$ be plane passing through the origin, and let ℓ be a line passing through the origin that lies on $\boldsymbol{\beta}$ (see Fig. 14). The inliers were sampled from two distributions. First, 490 *local points* were generated uniformly along a line segment of length two centered at the origin and lying on ℓ, where each point was perturbed by a randomly oriented vector whose length was drawn from a Gaussian distribution with mean zero and standard deviation 0.10. The remaining 10 inliers, called *leverage points*, were sampled uniformly from the equatorial circle where $\boldsymbol{\beta}$ intersects S. We set the trimming parameter to $h = 0.5$, implying that exactly 500 points are used in the computation of the LTS cost. Finally, the outliers consisted of 500 points that were sampled uniformly from S.

To see why this distribution is particularly difficult, observe that barring lucky coincidences, the only way to obtain a low-cost LTS fit is to combine all the local points with all the leverage points to obtain a fit that lies very close to $\boldsymbol{\beta}$. Thus, any elemental fit that involves even one outlier is unlikely to provide a good fit. Because of their degenerate arrangement along ℓ, any random sample of inliers that fails to include at least one leverage point is unlikely to lie close to $\boldsymbol{\beta}$. The probability of sampling three inliers such that at least one is a leverage point is roughly $(500/1000)^3 \cdot 10/500 = 0.025$. Note that by decreasing the fraction of leverage points relative to the total number of inliers, we can make this probability of a useful elemental fit arbitrarily small. This point set clearly fails both of the criteria given in Section 2 for well-conditioned point sets, since the vast majority of inliers are degenerately positioned, and there are a nontrivial number of leverage points.

Our experiments bear out the problems of this poor numerical conditioning (see Fig. 15). Both algorithms cast about rather aimlessly until somewhere between stages 200–300, where they each succeed in sampling a suitable fit. This experiment demonstrates the principal advantage of Adaptive-LTS over Fast-LTS. A user of Fast-LTS who saw only the results of the first 200 iterations might be tempted to think that the algorithm had converged to an optimal LTS cost of roughly 3.8, rather than the final cost of roughly 0.102. Terminating the algorithm prior to stage 200 would have resulted in a relative error of over 3000%. In contrast, a user of Adaptive-LTS would know by



(a)



(b)

Fig. 15: LTS cost versus stage number for the FLAT+SPHERE distribution ($d = 4$, $h = 0.5$) for (a): Fast-LTS and (b): Adaptive-LTS.

stage 500 that the relative error in the final LTS cost is less than 50%. (Although it is not evident from our plots, after roughly 1500 stages the lower bound increases to the point that it can be inferred that the approximation error is less than 10%, and after roughly 2000 stages it is less than 5%. Note that the convergence is due to improvements in the lower bound. The upper bound did not change in later stages.)

Execution Times: So far we have analyzed only the LTS costs generated by the two algorithms. An important question is how the performance of Adaptive-LTS compares with Fast-LTS. In Table 1 we summarize the execution times and LTS costs for both of these algorithms for 500 stages. In all cases, both algorithms generated essentially the same fitting hyperplane and, hence, achieved the same LTS cost. While the execution time of Adaptive-LTS was consistently higher than that of Fast-LTS, the difference is not very large. As can be seen from the table, there is only one instance (HYPERPLANE+UNIFORM in 2D) where Adaptive-LTS required more than twice the execution time of Fast-LTS, and even in this case, the ratio between the two execution times is only slightly greater than three.

Table 1: Summary of execution times and LTS costs for the synthetic experiments for 500 iterations of each algorithm.

Experiment				Fast-LTS		Adaptive-LTS	
Distribution	d	h	Fig.	Time (sec)	LTS Cost	Time (sec)	LTS Cost
HYPERPLANE+UNIFORM	2	0.1	11	0.14	0.00660	0.44	0.00660
HYPERPLANE+UNIFORM	3	0.5	12	0.47	0.00776	0.83	0.00776
HYPERPLANE+HALF-UNIF	3	0.5	13	0.48	0.00440	0.73	0.00440
FLAT+SPHERE	3	0.5	15	0.81	0.10220	1.11	0.10220

5.2 DPOSS Data Set

Our second experiment involved a set of points from the Digitized Palomar Sky Survey (DPOSS), from the the California Institute of Technology [2]. The data set consisted of 132,402 points in $\mathbb{R}^6$, from which we sampled 10,000 at random for each of our experiments. Of the six coordinates, we considered the problem of estimating the first coordinate MAperF, which measures the object's overall brightness in the F spectral band, as a function of one or more of the coordinates csfF, csfJ, csfN, which measure the stellar quality of the object in the spectral bands F, J, and N, respectively. Fig. 16 shows a scatter plot of MAperF versus csfF, and also shows the LTS fit (which was obtained by both our algorithm and FastLTS) and an ordinary least square (OLS) fit. We used the same experimental setup as in the synthetic experiments, by running both FastLTS and AdaptiveLTS for 500 stages.

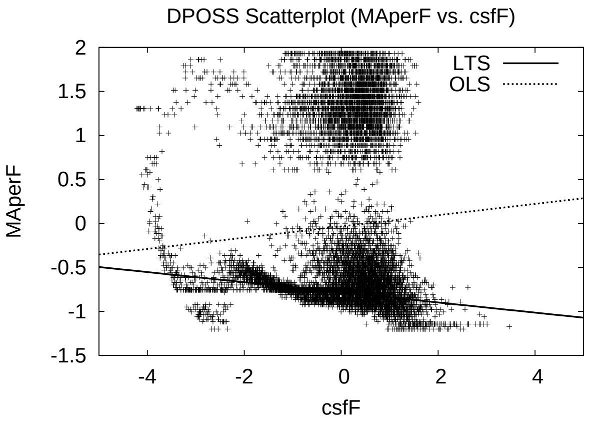
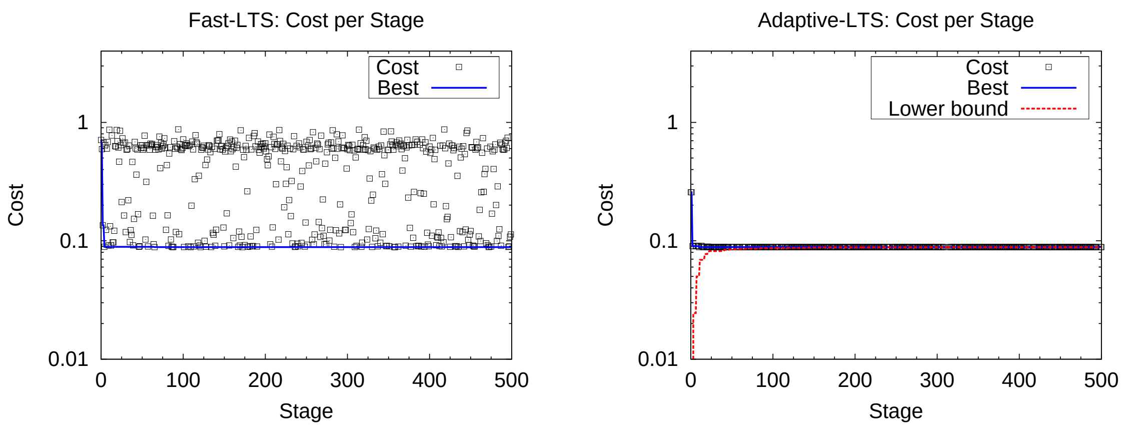


Fig. 16: The DPOSS data set (MAperF vs. csfF).

In the first experiment, we considered a 2-dimensional instance of estimating MAperF as a function of csfF (see Fig. 17). Both algorithms rapidly converged to essentially the same solution (shown in Fig. 16). Because it provides a lower bound, a user of AdaptiveLTS would know after 50 stages that the relative error in the LTS cost of this solution is less than 5%.

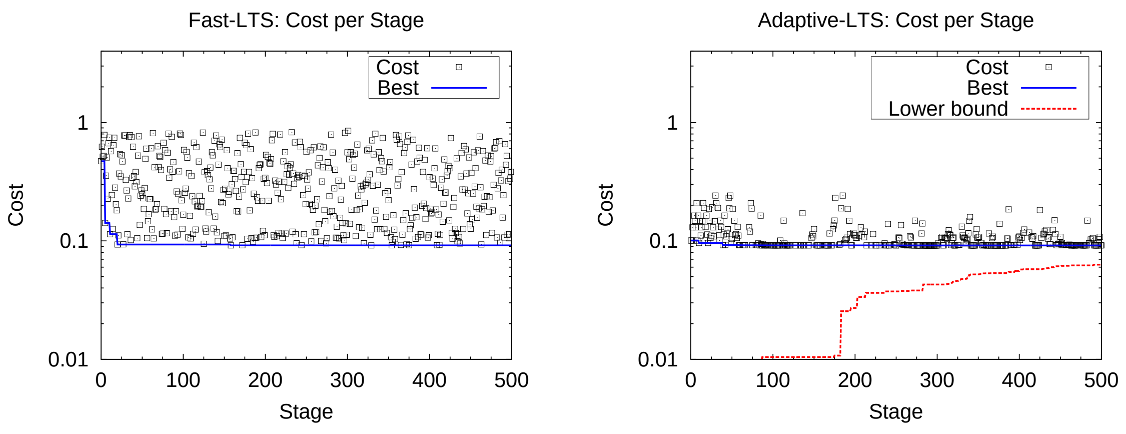
Our next experiment considered a 3-dimensional instance of estimating MAperF as a function of both csfF and csfJ (see Fig. 18). Again, both algorithms rapidly converged to essentially the same solution. Compared to the 2-dimensional example, it takes Adaptive LTS substantially longer to obtain a good lower bound. This is in part because the solution space is of higher dimension, and hence more time is required to search the space. After 500 stages the relative error in the LTS cost is less than 40%. (Although it is not evident from the plots, after roughly 800 stages the lower bound increases to the point that it can be inferred that the approximation error is less than 10%, and after roughly 1400 stages it is less than 5%. As in the synthetic experiments, the convergence is due to improvements in the lower bound. The upper bound did not change in later stages.)

Our final experiment demonstrates one of the practical limitations of AdaptiveLTS. We considered a 4-dimensional instance of estimating MAperF as a function of csfF, csfJ, and csfN (see Fig. 19). Again, both algorithms rapidly converged to essentially the same solution. However, the higher dimensional solution space takes much more time to search. After 500 stages, the lower bound is still zero and hence does not even appear on the plot. Even after 10,000 stages the lower



(a) (b)

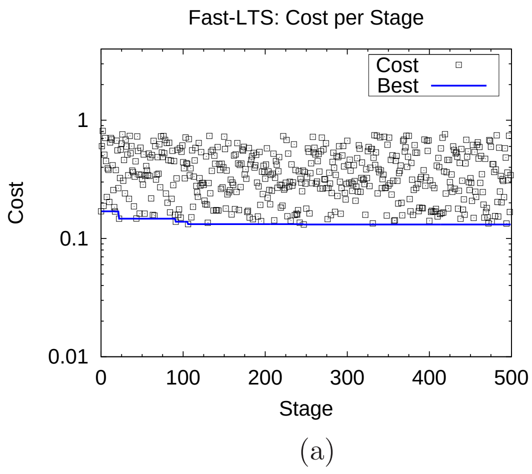
Fig. 17: LTS cost versus stage number for estimating MAperF as function of csfF in the DPOSS data set ($d = 2$) for (a): Fast-LTS and (b): Adaptive-LTS.



(a) (b)

Fig. 18: LTS cost versus stage number for the DPOSS data set ($d = 3$) for (a): Fast-LTS and (b): Adaptive-LTS.

bound provides an approximation error bound of only about 25%. Thus, even though both Fast-LTS and Adaptive-LTS find the same solution fairly soon, it takes much more time to establish a guarantee on the quality of this solution.



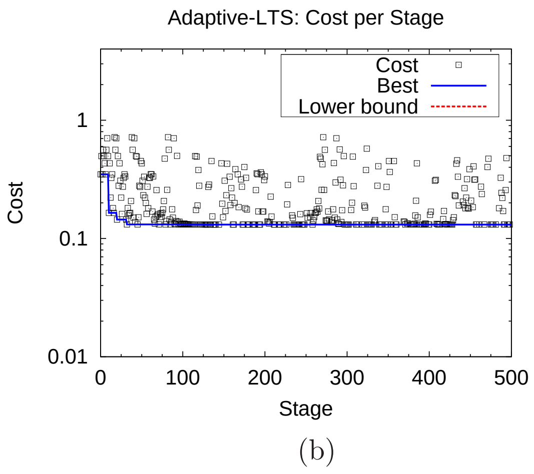


Fig. 19: LTS cost versus stage number for the DPOSS data set ($d = 4$) for (a): Fast-LTS and (b): Adaptive-LTS.

A user can improve the algorithm's speed of convergence if there is *a priori* information that can be used to reduce the size of the initial cell. For example, in Fig. 20, we repeat the above 4-dimensional DPOSS experiment, but rather than generating the initial cell automatically, we set it to $(-0.1, -0.1, -0.1) \times (+0.1, +0.1, +0.1)$ (which we verified contains the LTS-plane computed by both Fast-LTS and Adaptive-LTS). In this case, after 500 iterations the approximation error is roughly 30%.

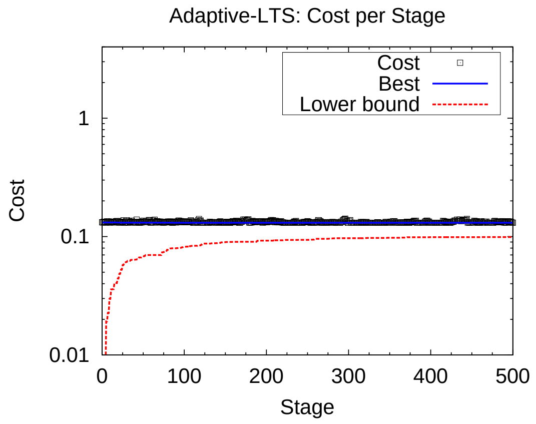


Fig. 20: The same 4-dimensional data set used in Fig. 19, but with the smaller initial cell of $(\pm 0.1, \pm 0.1, \pm 0.1)$.

As in our synthetic experiments, we also compared the relative performance of Adaptive-LTS and Fast-LTS. In Table 2 we summarize the execution times and LTS costs for both of these algorithms for 500 stages. Both algorithms generated essentially the same fitting hyperplane and, hence achieved the same LTS cost. Because of its higher overhead, Adaptive-LTS did require more execution time for the same number of stages, but in all instances the running time was less than 50% greater than Fast-LTS.

Table 2: Summary of execution times and LTS costs for the DPOSS experiments for 500 iterations of each algorithm.

DPOSS			Fast-LTS		Adaptive-LTS	
d	h	Fig.	Time (sec)	LTS Cost	Time (sec)	LTS Cost
2	0.5	17	5.02	0.0884	7.31	0.0884
3	0.5	18	5.77	0.0915	7.40	0.0915
4	0.5	19	7.72	0.1308	8.54	0.1311
4	0.5	20	7.63	0.1308	10.40	0.1308

6 Concluding Remarks

In this paper we have presented two results related to the computation of the linear least trimmed squares estimator. First, we introduced a measure of the numerical condition of a point set. We showed that if a point set is well conditioned, then it is possible to bound the accuracy (as a function of the conditioning parameters) of the LTS fit resulting from a sufficiently large number of random elemental fits. Second, we presented an approximation algorithm for LTS, called Adaptive-LTS. Given a point set, a trimming parameter, and bounds on the maximum and minimum slope coefficients, this algorithm computes a hybrid approximation to the optimum LTS fit assuming the slope coefficients are drawn from these bounds. We implemented this algorithm and presented empirical evidence on a variety of data sets of this algorithm's efficiency and effectiveness. In contrast to existing practical approaches, this algorithm computes a lower bound on the optimum LTS cost. Therefore when the algorithm terminates it provides an upper bound on the approximation error.

There are a number of possible directions for future research. First, our analysis of well-conditioned point sets considered only the results of random elemental fits, but it ignored the effect of possible C-steps. It would be interesting to consider the effect of the numeric condition on the convergence rate of the C-steps. Second, an obvious weakness of our Adaptive-LTS algorithm is its reliance on the requirement that the initial bounds on the slope coefficients be given. (The program can estimate these bounds from random elemental fits, but we cannot guarantee that the optimum fit lies within these bounds.) It would be nice to have the algorithm compute the initial bounds in such a manner that the optimum LTS cost is guaranteed to lie within them. Finally, although we showed that each stage of the algorithm runs in $O(m + n \log n)$ (where n is the number of points and m is the number of active cells), but we do not have good bounds on the number of stages until termination. Deriving asymptotic time bounds on the overall running time of the algorithm would be useful.

Finally, we would like to thank Peter Rousseeuw for providing us with the DPOSS data set.

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