

On Computing Geometric Estimators of Location

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Abstract

Let S be a data set of n points in R^d , and $\hat{\mu}$ be a point in R^d which “best” describes S . Since the term “best” is subjective, there exist several definitions for finding $\hat{\mu}$. However, it is generally agreed that such a definition, or *estimator of location*, should have certain statistical properties which make it *robust*. Most estimators of location assign a *depth* value to any point in R^d and define $\hat{\mu}$ to be a point with maximum depth. Here, new results are presented concerning the computational complexity of estimators of location. We prove that in R^2 the computation of *simplicial* and *halfspace* depth of a point requires $\Omega(n \log n)$ time, which matches the upper bound complexities of algorithms by Rousseeuw and Ruts. Our lower bounds also apply to two sign tests, that of Hodges and that of Oja and Nyblom. In addition, we propose algorithms which reduce the time complexity of calculating the points with greatest *Oja* and *simplicial* depth. Our fastest algorithms use $O(n^3 \log n)$ and $O(n^4)$ time respectively, compared to the algorithms of Rousseeuw and Ruts which use $O(n^5 \log n)$ time. One of our algorithms may also be used to find a point with minimum weighted sum of distances to a set of n lines in $O(n^2)$ time. This point is called the *Fermat-Torricelli point of n lines* by Roy Barbara, whose algorithm uses $O(n^3)$ time. Finally, we propose a new estimator which arises from the notion of *hyperplane depth* recently defined by Rousseeuw and Hubert.

Résumé

Que S soit un ensemble de n points en R^d , et que $\hat{\mu}$ soit un point en R^d qui décrit S le mieux. Comme le terme “mieux” est subjectif, il existe plusieurs définitions pour trouver $\hat{\mu}$. Cependant, il est généralement convenu qu’une telle définition, ou *estimateur d’emplacement*, devrait avoir certaines propriétés statistiques qui la fait *robuste*. La plupart des estimateurs d’emplacement assignent une valeur de profondeur à n’importe quel point en R^d et ils définissent $\hat{\mu}$ comme un point avec une profondeur maximum. Ici, de nouveaux résultats sont présentés concernant la complexité informatique d’estimateurs d’emplacement. Nous prouvons qu’en R^2 le calcul de la profondeur *simpliciale* et *halfspace* d’un point nécessite un temps $\Omega(n \log n)$, qui égale aux bornes supérieures des complexités des algorithmes par Rousseeuw et Ruts. Nos bornes inférieures s’appliquent aussi à deux *sign tests*, celui de Hodges et celui d’Oja et Nyblom. De plus, nous proposons des algorithmes qui réduisent le temps informatique de calculer les points avec la meilleure profondeur Oja et simpliciale. Nos algorithmes les plus rapides utilisent le temps $O(n^3 \log n)$ et $O(n^4)$ respectivement, comparés aux algorithmes de Rousseeuw et Ruts qui utilisent le temps $O(n^5 \log n)$. Un de nos algorithmes pourrait être utilisé pour trouver un point avec une somme minimum de distances d’un ensemble de n lignes en temps $O(n^2)$. Ce point est nommé le *point Fermat-Torricelli de n lignes* par Roy Barbara, dont l’algorithme utilise le temps $O(n^3)$. Enfin, nous proposons un nouveau estimateur, qui surgit de la notion de *profondeur hyperplane* récemment défini par Rousseeuw et Hubert.

Statement of Originality

Except for the introduction, the appendix, and results whose authors have been cited where first introduced, all elements of this thesis are original contributions to knowledge. Assistance has been received only where mentioned in the acknowledgements.

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While working on this thesis, I received a great amount of help from Dr. Toussaint and from Mike Soss. Despite their busy schedule, they were always willing to give me advice. The three of us worked together to obtain the results presented in chapter 4. These results also appear in the form of a technical report [AST01]. We worked together with Carmen Cortes and Paco Gomez to obtain the results presented in chapter 3, which may also be found in [ACG⁺01].

I thank my family in Greece for always encouraging me, and my family in Canada for giving me a home away from home. I am also extremely fortunate to have met Erin, who made the past few years of hard work bearable.

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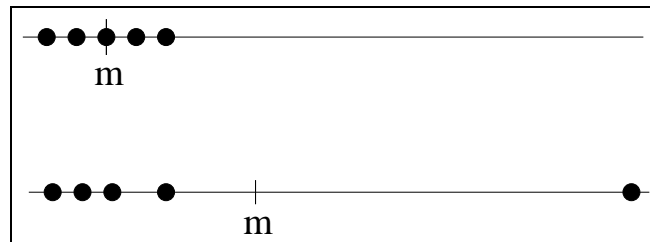
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Chapter 1

Introduction

Consider the following problem: you are given a set of data points whose underlying probability distribution is unknown, or non-parametric and unimodal. The task is to estimate a point (location) which best describes the set. When dealing with such a problem, it is important to consider the issue of *robustness*: how much does the answer change if some of the data is perturbed? How easy is it to create a data set for which an estimator yields an absurd answer? As an example of a non-robust estimator (which also shows why the problem is not trivial), take the mean of the set of points: if one point is moved far from the rest, the mean will follow (see figure 1.1). To be literally extreme, if we move the “corrupt” point to infinity, the mean will also go to infinity. This example indicates that robustness is particularly important when there is a possibility that our data set contains “contaminated” or “corrupt” data. It is also important when we simply do not want some data to have more importance than others. If we take the mean as an estimator, outlying points carry more weight than points near the mean. In figure 1.1, deleting the outlying point would have a greater impact on the location of the mean than deleting a point in the dense region.

As mentioned above, a single point is enough to greatly influence the mean of a data set. By contrast, at least half of the points in a set must be moved to infinity

Figure 1.1: The mean (m) is not a robust estimator.

in order to force the median to do the same. This suggests a measure of robustness for estimators of location [Sma90]:

- The *breakdown point* is the proportion of data which must be moved to infinity so that the estimator will do the same.

Rousseeuw and Lopuhaa [RL91] discussed the breakdown point of various estimators. They gave credit to Hodges [Hod67] and Hampel [Ham68] for introducing the concept. Lopuhaa [Lop92] stated that it was Donoho and Huber [DH83] who suggested the definition given above, which is intended for finite data sets. Donoho and Gasko [DG92] also provided many results concerning the breakdown point, some of which are mentioned in chapter 2.

In R^1 (in a univariate data set) the median has a breakdown point of $\frac{1}{2}$ and the mean has a breakdown point of $\frac{1}{n}$, where n is the number of data points. It has been shown [RL91] that the maximum breakdown point for any estimator is $\frac{1}{2}$, so in R^1 the median excels according to this robustness criterion. In fact, Bassett [Bas91] proved that in R^1 the median is the only estimator which possesses the properties of equivariance, maximum breakdown, and monotonicity (the median never moves in the opposite direction of a perturbation).

Measures of robustness typically used in R^2 or higher include invariance to certain types of transformations of the data. For example, given a set of points in the plane, we would not want our estimator to be affected by the choice of coordinate axes

(including origin, direction and scale). An estimator is *invariant to affine transformations* of the data set if its position relative to the data is not affected by displacement, rotation, scaling or shearing of the coordinate system.

We have already seen that the high breakdown point of the median in R^1 is a reason for choosing it over the mean as an estimator of location. The breakdown point of the mean is $\frac{1}{n}$ in all dimensions, as you may visualize in R^2 or R^3 . If we attempt to make a similar statement about the median, we immediately face a problem: what is the median of a multivariate data set? This question has been asked by mathematicians for at least a century, and the answer is still not clear. There is more than one way to describe the univariate median, and therefore there are many multivariate generalizations which reduce to the well known results of R^1 .

Clearly, we cannot generalize the R^1 median to higher dimensions by arbitrarily selecting a direction in high-dimensional space. Some people suggest combining various medians taken in different directions. In 1902, Hayford suggested the *vector-of-medians* of orthogonal coordinates [Hay02, Sma90]. This involves selecting an orthogonal coordinate system and computing the univariate median along each axis. This is similar to finding the multivariate mean, and works well for other problems such as finding derivatives of functions (gradients). Unfortunately, as Hayford was aware, the vector-of-medians depends on the choice of orthogonal directions. You may verify this easily using a set of three non-collinear points. In fact, as Rousseeuw [Rou85] pointed out, this method may yield a median which is outside the convex hull¹ of the data. Mood [Moo41] also proposed a joint distribution of unidimensional medians and used integration to find the multivariate median.

Soon after Hayford's median definition, Weber [Web09] proposed a new location estimator. Weber's estimator is the point which minimizes the sum of distances to

¹The convex hull of n points in R^2 is the convex polygon with smallest perimeter that encloses the data.

all data points. This definition holds for the univariate median, so Weber's estimator may be used as a multivariate median definition. A special case of the Weber problem had already been posed in the 17th century, but outside of the context of location estimators, by Fermat and Torricelli (see [Ros30]). In the 1920's the problem was rediscovered independently by Gini and Galvani [GG29], Eells [Eel30], and Griffin [Gri27]. This estimator may be found in the literature under a variety of other names, such as the L_1 median [Sma90], or the mediancentre [Gow74]. Some properties of this multivariate median are discussed in section 2.1.

In 1929 Hotelling [Hot29] described the univariate median as the point which minimizes the maximum number of data points on one of its sides. This notion was generalized to higher dimensions many years later by Tukey [Tuk75]. The Tukey median, or *halfspace* median, is perhaps the most widely studied and used multivariate median in recent years, and is discussed in section 2.2.

A very intuitive definition for the univariate median is to continuously remove pairs of extreme data points. A generalization of this notion appeared by Shamos [Sha76] and by Barnett [Bar76], although Shamos stated that the idea originally belongs to Tukey. *Convex hull peeling* iteratively removes convex hull layers of points until a convex set remains. Convex hull peeling and the related method of ellipsoid peeling are discussed in section 2.3.

In 1983, Oja [Oja83] introduced a definition for the multivariate median which generalizes the notion that the univariate median is the point with minimum sum of distances to all data points. However, Oja measured distance as one-dimensional volume. Thus the Oja median is a point for which the total volume of simplices² formed by the point and appropriate subsets of the data set is minimum. Section 2.4 contains a more detailed discussion.

In 1990, Liu [Liu90] proposed yet another multivariate definition, generalizing the

²A simplex is a line segment in R^1 , a triangle in R^2 , a tetrahedron in R^3 , etc.

fact that the univariate median is the point contained in the most intervals between pairs of data points. In higher dimensions, intervals (segments) are replaced by simplices. This method is discussed in section 2.5.

Gil, Steiger and Wigderson [GSW92] compared robustness and computational aspects of certain medians, although they imposed the restriction that the median must be one of the data points. They proposed a new definition for the multivariate median: for every data point, take the vector sum of all unit vectors to other data points. The median is any data point for which the length of the vector sum is less than or equal to one. The authors noted that the univariate median satisfies this condition, and claimed that their median is “unique”. Their definition seems strange in R^2 , since one can imagine a symmetric convex set of data for which the length of the vector sum is greater than one for all data points. It would make more sense to consider all points in R^2 as candidates for the median.

Another reason for using the median in R^1 is that it provides a method of ranking data. This concept can be generalized for the Oja, Liu and Tukey medians, as well as for convex hull peeling. Each of these medians maximizes/minimizes a certain *depth* function, and any point in R^d can be assigned a depth according to the particular function.

Recently a new significant notion of multivariate depth was proposed by Rousseeuw and Hubert [RH99a]. The *hyperplane depth* of a point with respect to a set of hyperplanes is the minimum number of hyperplanes that a ray extending from that point must cross. In R^1 this defines the median of n points, although a multivariate median definition related to hyperplane depth has yet to be proposed. We attempt to make such a definition in section 2.6, where hyperplane depth is discussed in more detail.

We mention certain other estimators of location, which are not necessarily generalizations of the univariate median, such as *minimal volume ellipsoid covering* by Rousseeuw [Rou85]. This estimator is the center of a minimum volume ellipsoid

which contains roughly half of the data. It is invariant to affine transformations and has a 50% breakdown point for a data set in general position³. Rousseeuw also described another estimator with the same properties, introduced independently by Stahel [Sta81] and Donoho [Don82]. Their method involves finding a projection for each data point x in which x is most outlying. They then compute a weighted mean based on the results. Toussaint and Poulsen [TP79] proposed successive pruning of the *minimum spanning tree (MST)* of n points as a method of determining their center. To construct a *MST*, we connect certain data points with edges so that there exists a path between any two points and the sum of all edge lengths is minimized. This method seems to work well in general, although certain patterns of points may cause the location of the center to seem unnatural. Another graph-based approach was suggested by Green [Gre81]. Green proposed constructing a graph joining points adjacent in the *Delaunay triangulation* of the data set. Two data points $\{a, b\}$ in R^2 are adjacent if there exists a point in R^2 for which the closest data points are a and b . The Delaunay depth of a data point is the number of edges on the shortest path from the point to the convex hull. In general, the center of a graph has also been considered to be the set of points for which the maximum path length to reach another point is minimized [Har69].

Several other estimators which are based more on statistical methods exist. For example, *M-Estimators*, *L-Estimators* and *R-Estimators* were discussed by Huber [Hub72].

Robust estimators of location have been used for data description, multivariate confidence regions, p -values, quality indices, and control charts (see [RR96]). Applications of depth include hypothesis testing, graphical display [MRR⁺01] and even voting theory [RR99]. Halfspace, hyperplane and simplicial depth are also closely related to regression [RR99]. For a recent account of statistical uses of depth, see [LPS99].

³A data set is in *general position* if no three points are collinear. Occasionally this is extended to denote sets where no four points are co-circular.

For a more detailed introduction to robust estimators of location, we suggest a classic paper by Small [Sma90]. Finally, more links between computational geometry and statistics have been made by Shamos [Sha76].

The main focus of this thesis is on the computation of certain estimators of location. When describing the asymptotic computational complexity of algorithms and problems with respect to the size of input n , we will use the “universally accepted” notation of Knuth (see [Knu76, PS85]). Thus for some function $f(n)$ and for large enough n , we say that $O(f(n))$ is at most a (positive) constant factor of $f(n)$, $\Omega(f(n))$ is at least a constant factor of $f(n)$, and $\Theta(f(n))$ is both $O(f(n))$ and $\Omega(f(n))$. Upper bounds for the time and space used by *algorithms* will be in the *real RAM* model of computation (see [PS85]). According to this model, only arithmetic operations ($+$, $-$, \times , $/$) and comparisons are allowed, for real numbers of infinite precision (occasionally this is extended to include certain functions such as trigonometric, exponential, k -th root, etc). Each operation costs one unit of time. The same applies for storing and retrieving each real number, where the storage of a number also requires a unit of space. Lower bounds for the worst case complexity of algorithms *or* problems will be in the *algebraic decision tree* model (see [PS85]). A (binary) algebraic decision tree represents the set of possible sequences of operations made by a RAM algorithm, where the root of the tree represents the first operation performed and each leaf represents a possible output. Any path from the root to a leaf in the tree also represents the time for a specific sequence of operations. The worst case performance of an *algorithm* is specified by the longest path from the root to some leaf. Obtaining lower bounds for the time complexity of *problems* typically involves determining the path length size that an algebraic decision tree must have for the tree to be able to produce the desired output for any possible input. For example, it can be shown (see [CLR90]) that any algebraic decision tree which is capable of sorting n real numbers based on comparisons alone must have a path with

length $\Omega(n \log n)$, and therefore *any* RAM algorithm restricted to comparisons must take $\Omega(n \log n)$ time in the worst case to sort n real numbers. For a discussion on the connection between the RAM and algebraic decision tree models, see [PS80].

The univariate median of n points is easily computed in $O(n \log n)$ time by sorting the points. An optimal $O(n)$ time method was proposed by Blum et al [BFP⁺73]. Many undergraduate introductory texts to data structures and algorithms describe this algorithm as well as several techniques for sorting (e.g. [CLR90]).

In chapter 2, some of the most popular multivariate medians are discussed, including breakdown properties and computational issues. We also define a new median which adapts the notion of hyperplane depth to a set of points in R^d . In chapter 3 we describe how to compute halfspace and simplicial depth in $O(n \log n)$ time. Our descriptions are simplified versions of the algorithms of Rousseeuw and Ruts [RR96]. Similar algorithms have been proposed by Khuller and Mitchell [KM89], and also by Gil, Steiger and Wigderson [GSW92]. We match the upper bounds of the simplicial and halfspace depth algorithms by proving that these problems require $\Omega(n \log n)$ time. Our lower bounds also apply to the sign tests of Hodges [Hod55] and of Oja and Nyblom [ON89]. These tests are used to determine if there is a statistically significant difference between two distributions of n points.

In chapter 4 we present our algorithms for computing the simplicial and Oja medians. The Oja median is found using $O(n^3 \log n)$ time and $O(n^2)$ space. The simplicial median is found in $O(n^4 \log n)$ time and $O(n^2)$ space, *or* $O(n^4)$ time and space. Thus we improve the time complexity for computing both medians. The fastest algorithms to date were by Rousseeuw and Ruts [RR96] and used $O(n^5 \log n)$ time and $O(n)$ space. In the same section, we show that the point with minimum weighted sum of distances to n lines, also known as the *Fermat-Torricelli point of n lines*, can be computed in $O(n^2)$ time and $O(n)$ space. We therefore improve an algorithm suggested by Roy Barbara [Bar00] which uses $O(n^3)$ time and $O(n)$ space.

Chapter 2

Multivariate Medians

To set the stage for the new results obtained in this thesis, in this chapter some of the main multivariate medians are reviewed, including robustness and computational complexity issues.

2.1 The L1 Median

Note: The median definition described below has been proposed independently by several scientists and therefore is known under several names in the literature. We will use the “neutral” term *L1 median*, which is also used by Small [Sma90].

In 1909 Alfred Weber published his *theory on the location of industries* [Web09]. As a solution to a transportation cost minimization problem, Weber considered the point which minimizes the sum of Euclidean distances to all points in a given data set. In R^1 the median is such a point, so Weber’s solution can be used as a generalization of the univariate median. The solution to Weber’s problem, will be referred to in this section as the *L1 median*. Both Weber and Georg Pick, who wrote the mathematical appendix in Weber’s book, were not able to find a solution for a set of more than three points in the plane. In the 1920’s, the same definition was rediscovered independently

by other researchers, who were primarily interested in finding the centers of population groups. Eells [Eel30] pointed out that for years the U.S. Census Bureau had been using the mean to compute the center of the U.S. population. Apparently they thought that the mean is the location which minimizes the sum of distances to all points in a set. In 1927, Griffin [Gri27] independently made the same observation, based on some earlier work by Eells. According to Ross [Ros30], Eells had discovered the error in 1926, but publication was delayed for bureaucratic reasons. Ross also printed a section of a paper by Gini and Galvani [GG29], translated from Italian to English. Gini and Galvani proposed the use of the $L1$ median and argued its superiority over the mean and the vector-of-medians approach (such as Hayford's).

None of the authors mentioned above were able to propose a method for computing the $L1$ median for sets of more than three points, even though the solution for three points had been known since the 17th century. According to Ross [Ros30] and Groß and Stempel [GS98], Pierre de Fermat first posed the problem of computing the point with minimum sum of distances to the vertices of a given triangle. Fermat discussed this problem with Evangelista Torricelli, who later computed the solution (see also [dF34] and [LV19]). Hence the $L1$ median for $n > 3$ is often referred to as the *generalized Fermat-Torricelli point*.

Scates [Sca33] suggested that the location of the $L1$ median for $n > 3$ cannot be computed exactly. At the same time, Galvani [Gal33] proved that the solution is a unique point in R^2 and higher dimensions. All algorithms to this date involve gradients or iterations and only find an approximate solution. One of the first such algorithms was by Gower [Gow74], who referred to the $L1$ median as the *mediancentre*. Groß and Stempel [GS98] discussed iteration and gradient methods for computing the $L1$ median.

The $L1$ median is known to be invariant to rotations of the data, but not to changes in scale. Another interesting property of the $L1$ median is that any measurement X

of the data set can be moved along the vector from the median to X without changing the location of the median [GG29]. The breakdown point of the $L1$ median has been found to be $\frac{1}{2}$ [Rou85]. This is evident in R^1 by noticing that if we place just over half of the data at one point, then the median will always stay there (figure 2.1). This idea can be extended to any data set within a bounded region. When just under half of the data is moved to infinity, the median remains in the vicinity of the majority of the data, since the bounded region resembles a point from infinity.

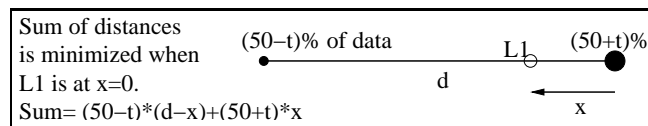


Figure 2.1: The breakdown point of the $L1$ median is $\frac{1}{2}$.

2.2 The Halfspace Median

In 1929, Hotelling [Hot29](see also [Sma90]) introduced his interpretation of the univariate median, while considering the problem of two competing ice-cream vendors on a one-dimensional beach. Hotelling claimed that the optimal location for the first vendor to arrive would be the location which minimized the maximum number of people on one side. This location happens to coincide with the univariate median. Tukey [Tuk75] is credited for generalizing this notion. The multivariate median based on this concept is usually referred to as the *Tukey* or *halfspace* median. Donoho and Gasko [DG92] were actually the first to define the multivariate halfspace median, since Tukey was primarily concerned with depth.

In order to define the multivariate halfspace median it is easier in fact to first consider the notion of *halfspace depth* for a query point θ with respect to a set S of n points in R^d . For each closed halfspace that contains θ , count the number of points

in S which are in the halfspace. Take the minimum number found over all halfspaces to be the depth of θ . For example in R^2 , place a line through θ so that the number of points on one side of the line is minimized (see figure 2.2). The halfspace median of a data set is any point in R^d which has maximum halfspace depth.

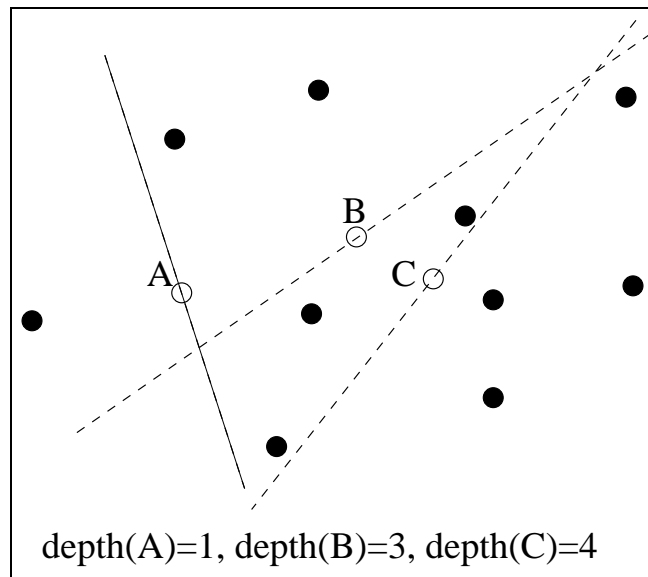


Figure 2.2: The halfspace depth of some points.

The halfspace median is generally not a unique point. However the set of points of maximal depth is guaranteed to be a closed, bounded convex set. The median is invariant to affine transformations, and can have a breakdown point between $\frac{1}{d+1}$ and $\frac{1}{3}$. If the data set is in general position, maximum depth is bounded below by $\lceil \frac{n}{d+1} \rceil$ and above by $\lceil \frac{n}{2} \rceil$ (see [DG92]).

Notice that any point outside of the convex hull of S has depth zero. To find the region of maximum depth in R^2 , we can use the fact that its boundaries are segments of lines passing through pairs of data points. In other words, the vertices of the desired region must be intersection points of lines through pairs of data points. There are $O(n^4)$ intersection points, and it is a straightforward task to find the depth of a query point in $O(n^2)$ time (for each line defined by the query point and a data point,

count the number of data points above and below the line). Thus in $O(n^6)$ time, we can find the intersection points of maximum depth. An improvement upon this was made by Rousseeuw and Ruts [RR96], who showed how to compute the halfspace depth of a point in $O(n \log n)$ time (see chapter 3). Their algorithm therefore uses $O(n^5 \log n)$ time to compute the deepest point. Later they also gave a more complicated $O(n^2 \log n)$ version and provided implementations [RR98]. They seemed to be unaware that before this, Matoušek [Mat91] had presented an $O(n \log^5 n)$ algorithm for computing the halfspace median. Matoušek showed how to compute any point with depth greater than some constant k in $O(n \log^4 n)$ time and then used a binary search on k to find the median. Recently Matoušek's algorithm was improved by Langerman and Steiger [LS00], whose algorithm computes the median in $O(n \log^4 n)$ time. A further improvement to $O(n \log^3 n)$ is to appear in Langerman's Ph.D. thesis [Lan01]. A recent implementation by Miller et al [MRR⁺01] uses $O(n^2)$ time and space to find all depth contours, after which it is easy to compute the median. They claim that Matoušek's algorithm is too complicated for practical purposes.

Another interesting location based on halfspace depth is the *centerpoint*, which is a point with depth at least $\lceil \frac{n}{d+1} \rceil$. Gill, Steiger and Wigderson [GSW92] stated that the centerpoint could be used as a multivariate median since it coincides with the median in R^1 . Edelsbrunner [Ede87] showed that a centerpoint can be found for any data set. The number $\lceil \frac{n}{d+1} \rceil$ arises from Helly's theorem (see [RH99a] for a more detailed account). Cole, Sharir and Yap [CSY87] were able to compute the centerpoint in $O(n \log^5 n)$ time. Matoušek improved this result by setting k equal to $\lceil \frac{n}{d+1} \rceil$ in his algorithm, thus obtaining the centerpoint in $O(n \log^4 n)$ time. Finally, Jadhav and Mukhopadhyay [JM94] gave an $O(n)$ algorithm to compute the centerpoint.

2.3 Convex Hull Peeling and Related Methods

Perhaps the most intuitive visual interpretation of the univariate median is the idea of peeling away outlying data: we throw out the smallest and largest values recursively, until we are left with one or two. We can easily generalize this idea to higher dimensions. One way is to iteratively peel away convex hull layers of the data set, until a convex set remains (figure 2.3). As in the univariate case, if more than one point remains, we take the mean. Most of the credit for introducing this concept is given to Shamos [Sha76] and Barnett [Bar76]. However, Shamos stated that the idea originally belongs to Tukey.

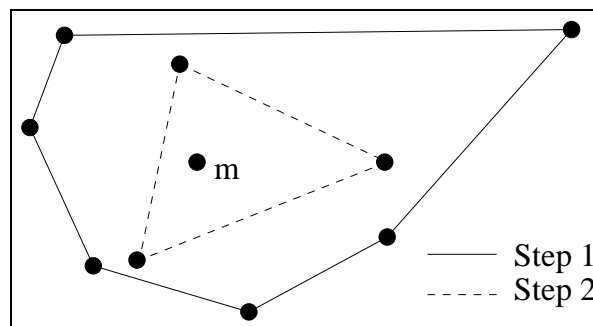


Figure 2.3: Multivariate median (m) via convex hull peeling.

Even a naive algorithm for convex hull peeling should not take longer than $O(n^2 \log n)$ time in R^2 . The convex hull may be computed in $O(n \log n)$ time [Gra72]. Matching lower bounds have been found in several models of computation (see [Avis82, Yao81]). In the worst case it is possible that only three data points will be removed in each iteration, which leads to $O(n)$ convex hull calculations. The task can be done easily in $O(n^2)$ time by slightly modifying the Jarvis “gift-wrapping” convex hull algorithm [Jar73]. This algorithm takes $O(hn)$ time to compute the convex hull, where h is the number of vertices on the hull. Once the hull is computed, the modified algorithm continues with the remaining points. This modification was first proposed

by Shamos [Sha76]. Later Overmars and van Leeuwen [OvL81] designed a data structure which maintains the convex hull of a set of points after the insertion/deletion of arbitrary points, with a cost of $O(\log^2 n)$ time per insertion/deletion. This provides an $O(n \log^2 n)$ time method for convex hull peeling. Finally, Chazelle [Cha85] improved this result by ignoring insertions and taking advantage of the structure in the sequence of deletions in convex hull peeling. Chazelle's algorithm uses $O(n \log n)$ time to compute all convex layers and the depth of any point.

A technique similar to convex hull peeling was proposed by Titterton [Tit78]. He proposed iteratively peeling minimum volume ellipsoids containing the data set. Both methods of peeling data can have very low breakdown points. Donoho and Gasko [DG92] proved that the breakdown point of these methods cannot exceed $\frac{1}{d+1}$ in R^d and stated that the breakdown point seems to always approach 0 as n approaches infinity. In figure 2.4 we show how the breakdown point can approach 0 for a specific configuration of points. There is only one point inside the convex hull so it is the median. It can be moved an arbitrary distance to the right, as long as its nearest neighbor is moved by the same amount.

Another ellipsoid method was proposed by Rousseeuw [Rou85]. His median is the center of the minimum volume ellipsoid that covers approximately half of the data points. Rousseeuw proves that this estimator is invariant under affine transformations and has a 50% breakdown point for data in general position.

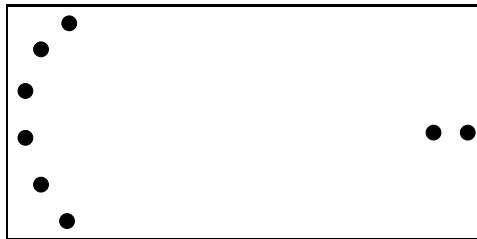


Figure 2.4: Example of how the breakdown point of convex hull peeling can be made to approach zero.

2.4 The Oja Simplex Median

Consider $d+1$ points in R^d . These points form a simplex, which has a d -dimensional volume. For example, in R^3 four points form a tetrahedron, and in R^2 three points form a triangle whose area is “2-dimensional volume”. Now consider a data set in R^d for which we seek the median. Oja proposed the following measure for a query point θ in R^d [Oja83] (see figure 2.5):

- for every subset of d points from the data set, form a simplex with θ .
- sum together the volumes of all such simplices.

We can call this sum *Oja depth*. The Oja simplex median is any point $\hat{\mu}$ in R^d with minimum Oja depth.

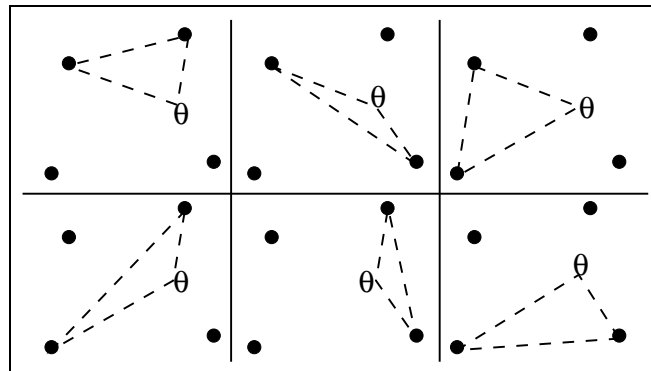


Figure 2.5: The simplices considered for a candidate Oja median (θ) in R^2 . ($n = 4$)

Since one-dimensional volume is length, the Oja median reduces to the standard univariate median. In R^1 , the Oja median minimizes the sum of distances to all data points, as does the $L1$ median. Unlike the $L1$ median, the Oja median is not guaranteed to be a unique point in higher dimensions. However Oja mentions (without proof) that the points of maximum depth form a convex set and that to compute such a point in R^2 it suffices to consider only intersection points of lines formed by pairs

of data points. We prove these properties in chapter 4. An important feature of the Oja median is that it is invariant to affine transformations. However, data sets may be constructed for which the breakdown point approaches zero. Notice that if the data does not “span” the dimension of the space that it is in (ex: data on a line in R^2 or data on a plane in R^3 , then it is possible to find simplices with zero volume even at infinity. This seems like an unrealistic case for any application though. A nicer example for R^2 is given by Niinimaa, Oja and Tableman [NOT90], although the example used resembles a bimodal distribution and the corrupted points cannot be moved in arbitrary directions.

The straightforward method of calculating the Oja median is to compute the depth of each intersection point. In R^2 this can be done in $O(n^6)$ time: for each of the $O(n^4)$ intersection points there are $O(n^2)$ triangles for which the area must be computed, and the area of a triangle can be computed in constant time. The same upper bound holds for an algorithm of Niinimaa, Oja and Nyblom [NON92]. The algorithm selects a line between two data points and computes the gradient of Oja depth at each intersection point along the line until one such point is found to be a minimum. A new line from this point is then selected, and the procedure is repeated. The gradient is computed in $O(n^2)$ time and it is possible that all intersection points will be visited. Rousseeuw and Ruts [RR96] provided a technique for computing the Oja gradient in $O(n \log n)$ time and stated that the same algorithm can be used to find the median in $O(n^5 \log n)$ time. In chapter 4 we propose an algorithm which computes the Oja median in $O(n^3 \log n)$ time.

2.5 The Simplicial Median

Another interpretation of the univariate median is that it is the point which lies inside the greatest number of intervals constructed from the data points. Liu generalized this idea as follows [Liu90]: the simplicial median in R^d is a point in R^d which is contained

in the most simplices formed by subsets of $d+1$ data points. An example for R^2 with $n = 4$ is shown in figure 2.6. The simplicial depth of a point in R^d is the number of simplices which contain the point. Liu's original definition involves closed simplices, although later in [Liu95] she repeats the definition using open simplices. Unless mentioned otherwise, when we refer to simplicial depth or the simplicial median, we will use the original definition (a point on the boundary of a simplex is inside the simplex).

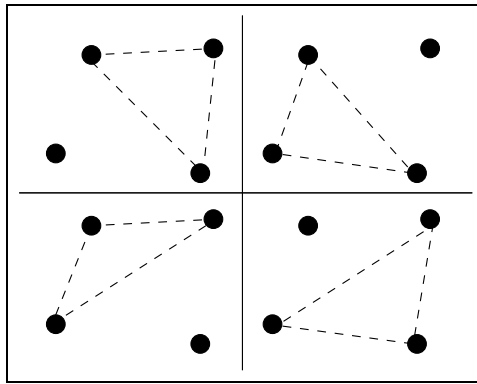


Figure 2.6: The simplices considered for the simplicial median in R^2 . ($n = 4$)

Liu showed that the simplicial median is invariant to affine transformations. However, not much information is known about the breakdown point. Gil, Steiger and Wigderson [GSW92] constructed a set of points for which the *data point* of maximum simplicial depth could be moved arbitrarily far away with only a few corrupting points. This does not necessarily imply anything for the simplicial median of Liu.

Although Liu was the first to define simplicial depth and introduce the notion to the statistical community, this concept had already been considered before. Boros and Füredi [BF84] proved that for a set of n points in general position in R^2 there always exists a point contained in at least $\frac{n^3}{27} + O(n^2)$ open triangles formed by the points. This implies that the depth of the simplicial median in R^2 is $\Theta(n^3)$. Bárány [Bár82]

showed that in R^d there always exists a point contained in

$$\frac{1}{(d+1)^{d+1}} \binom{n}{d+1} + O(n^d)$$

simplices.

A straightforward method of finding the simplicial median in R^2 is to partition the plane into cells which have segments between points as boundaries (figure 2.7 has cells A-I).

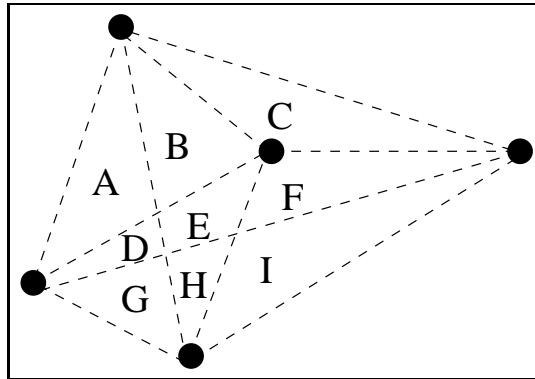


Figure 2.7: Data splits the plane into cells A-I.

First, notice that every point within a given cell has equal depth. Furthermore, a point on a boundary between two cells must have depth at least as much as any adjacent interior point. Similarly, an intersection point (where more than two cells meet) must have depth at least as much as any adjacent boundary point. Therefore by determining how many triangles contain each intersection point we can find the simplicial median.

If a set of n line segments has k intersection points, they can be reported in $O(n \log n + k)$ time and $O(n)$ space with a line sweeping technique of Balaban [Bal95]. In the case of simplicial depth, we have $O(n^2)$ line segments formed between pairs of data points, and unfortunately k is $\Theta(n^4)$ [SW94]. Thus the algorithm of Balaban

takes $O(n^4)$ time and $O(n^2)$ space for our purposes, so it is better to use brute-force to compute each intersection point. The total time for this is $O(n^4)$ and the space used is $O(n)$. Since there are $O(n^3)$ triangles formed by n points, a brute-force calculation of the simplicial median uses $O(n^7)$ time and $O(n)$ space. Khuller and Mitchell [KM89] proposed an $O(n \log n)$ time algorithm to compute the number of triangles formed by triples of a data set which contain a query point in R^2 . Their algorithm came just before Liu's definition. Gil, Steiger and Wigderson [GSW92] independently proposed the same algorithm and considered the simplicial median to be the *data point* with maximum depth. A third version of this algorithm appeared later, but also independently, by Rousseeuw and Ruts [RR96]. We describe the technique and provide a matching lower bound for this problem in chapter 3. Rousseeuw and Ruts were the first to point out that by computing the depth of each intersection point, the simplicial median may be found in $O(n^5 \log n)$ time. In Chapter 4 we propose algorithms which further reduce this time complexity. We compute the simplicial median in $O(n^4 \log n)$ time using $O(n^2)$ space, *or* in $O(n^4)$ time and space.

For R^3 Gil, Steiger and Wigderson [GSW92] proposed an algorithm to compute the simplicial depth of a point in $O(n^2)$. Cheng and Ouyang [CO98] discovered a slight flaw in this algorithm and provided a corrected version. They also provided a $O(n^4)$ time algorithm for R^4 and commented that for higher dimensions the brute-force algorithm becomes better. They mention that an algorithm suggested by Rousseeuw and Ruts [RR96] for higher dimensions seems to have some discrepancies.

2.6 Hyperplane Depth and a New Median

The most recent notion of depth for a point in R^d is by Rousseeuw and Hubert [RH99a], although their definition of depth is not with respect to a set of points. They defined the *hyperplane depth* of a point θ with respect to a set of n hyperplanes to be the minimum number of hyperplanes that a ray emanating from θ must cross. An example

for R^2 is given in figure 2.8.

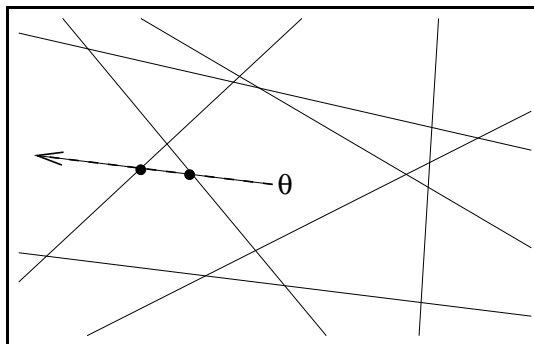


Figure 2.8: Hyperplane depth in R^2 : the depth of θ is the minimum number of lines crossed by a ray from θ .

The authors remarked that the point with maximum hyperplane depth (which they call the *hyperplane median*) can be seen as the “deepest” or “most central” point in the arrangement of hyperplanes. They proved that in R^1 such a point is in fact the median. They conjectured that in R^d there always exists a point with depth greater than $\lceil \frac{n}{d+1} \rceil$ and proved this for $d = 1$ and $d = 2$. They provided an $O(n)$ time algorithm to compute such a point in R^2 . Furthermore they showed that maximum hyperplane depth cannot be greater than $\lfloor \frac{n+d}{2} \rfloor$ if the hyperplanes are in general position (no two hyperplanes parallel and no $d + 1$ hyperplanes concurrent), and that the hyperplane median is invariant to affine transformations.

Langerman and Steiger [LS00] provided an $O(n \log n)$ time algorithm to compute the hyperplane median of n hyperplanes in R^2 . If a query point is on a hyperplane, Langerman and Steiger do not count this plane as crossing a ray from the query point. They also provided a matching lower bound and mentioned previous results such as an $O(n^3)$ time algorithm by Rousseeuw and Hubert [RH99b] and an $O(n \log^2 n)$ time algorithm by van Kreveld et al [vKMR⁺99]. Amenta et al [ABET00] proposed an $O(n^d)$ time algorithm which constructs the arrangement¹ of the n hyperplanes and

¹For details concerning the arrangement of n lines, see appendix A.

uses a breadth first search to locate the hyperplane median in R^d . They also proved the conjecture of Rousseeuw and Hubert.

Although hyperplane depth is equivalent to the median in R^1 , no generalization has been made for the multivariate median of a set of points in R^d . The concept of a ray intersecting a minimum number of hyperplanes may be used as follows: given a set S of n points in R^d , construct the set H of hyperplanes formed by subsets of d points in S . Find the point μ with maximum hyperplane depth with respect to H . The point μ can be called the H -median of S . The algorithm of Langerman and Steiger would compute the bivariate H -median in $O(n^2 \log n)$ time, since there are $O(n^2)$ hyperplanes in R^2 for a set of n points. It makes sense that for a given point p we should consider that a ray from p does not cross hyperplanes containing p . Otherwise, even the points on the convex hull of the data set would have significant depth.

Chapter 3

Algorithms and Lower Bounds for Depth in R^2

In this chapter, some recent and new results concerning the depth of a query point in R^2 are presented. In section 3.1 we describe simplified versions of the algorithms of Rousseeuw and Ruts [RR96] for computing halfspace and simplicial depth in $O(n \log n)$ time. Their simplicial depth algorithm is practically the same as those by Khuller and Mitchell [KM89], and by Gil, Steiger and Wigderson [GSW92]. In section 3.2 we prove that the computation of halfspace and simplicial depth requires $\Omega(n \log n)$ time, which matches the upper bounds of these algorithms. Finally in section 3.3 we show that our lower bounds also apply for the sign tests of Hodges [Hod55] and of Oja and Nyblom [ON89].

3.1 Algorithms for the Depth of a Point in R^2

3.1.1 Halfspace Depth Calculation

Suppose we have a data set S of n points, and a point θ for which we want to compute halfspace depth. First, note that it suffices to consider only halfspaces determined

by lines through θ , as mentioned in section 2.2. If any element in S coincides with θ we can ignore it and increment the depth value when we are finished. Sort S radially about θ and construct a directed line L through θ and some point s in S . For example, in figure 3.1 L is directed from θ to point 1. Let L_f be the halfline on L that extends from θ and crosses s (shown thicker in figure 3.1). Count the number of points on or to the left of L , excluding points on L_f . This represents the points in the closed halfspace defined by a line rotated slightly counterclockwise from L . Rotate L counterclockwise until it encounters a new point. Notice that it is possible for L to rotate through an angle of zero. If the next encounter is on L_f , we know that the current halfspace to the left of L will have one less point. Otherwise, we know that the current halfspace will gain one point. We update the minimum value found every time L changes direction (if there are no two points collinear with θ this will happen every time). The process ends when L has performed one full cycle. The overall running time is dominated by the sorting step, so it is $O(n \log n)$.

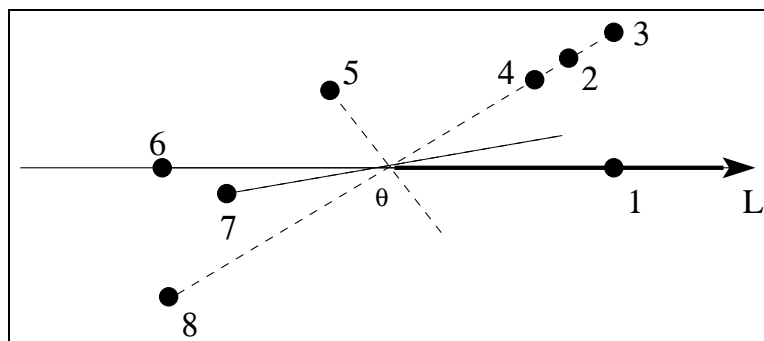


Figure 3.1: Sorting technique for depth computation.

In the example of figure 3.1, L initially contains points 6 and 1. The initial halfspace contains points 2 through 6, so the initial minimum is five. When L is rotated it first encounters point 7, which is not on L_f . Thus the new halfspace contains six points and the minimum is still five. After the next rotation, L will contain points 2,3,4 and 8. The minimum value will be updated only after all of

these points are processed. The minimum will become four, corresponding to points 5 through 8. By continuing this process we find that the halfspace depth of θ is equal to two, and is found when L_f crosses point 7.

3.1.2 Simplicial Depth Calculation

To find the simplicial depth of θ with respect to S we can compute the number of triangles formed by triples of points in S which do *not* contain θ and subtract this number from the total number of triangles. We will use the fact that the three vertices of a triangle which does not contain θ must lie in an open halfspace determined by a line through θ .

The algorithm for simplicial depth relies on the same technique used for halfspace depth. Consider any open halfspace determined by a line through θ . Any triangle formed by points in that halfspace cannot contain θ . All that is required to compute the simplicial depth of θ is to enumerate all such triangles and subtract them from the total number which is $\binom{n}{3}$.

Sort S radially about θ , breaking ties by placing points furthest from θ first. For each point s_i ($1 \leq i \leq n$) that is met by the line L we compute h_i : the number of points which are between θ and s_i or strictly to the left of L . These points are colored black in the example of figure 3.2.

The number of triangles whose *first* vertex is s_i and which do not contain θ is $\binom{h_i}{2}$. By proceeding in this way we are sure that every triangle is counted once. The quantity h is updated in the same way as in the previous section.

The simplicial depth of θ is

$$\binom{n}{3} - \sum_{i=1}^n \binom{h_i}{2}$$

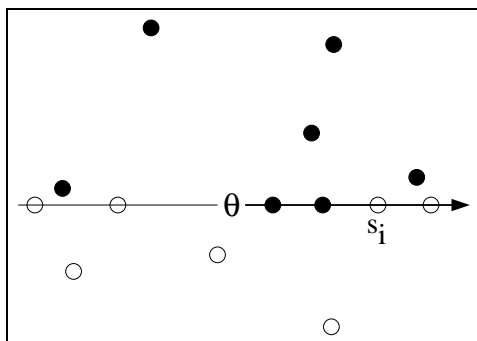


Figure 3.2: Simplicial depth calculation: s_i is the *first* vertex for any triangle formed by s_i and two black points.

where $\binom{p}{q}$ is zero if $p < q$.

The complexity is identical to that of calculating halfspace depth.

3.2 Lower Bounds for Computing the Depth of a Point in R^2

In this section we prove that computing simplicial and halfspace depths requires $\Omega(n \log n)$ time.

3.2.1 Halfspace Depth Lower Bound

We show that finding halfspace depth allows us to answer the question of *Set Equality*, which has an $\Omega(n \log n)$ lower bound in the algebraic decision tree model of computation [BO83]:

- **Set Equality:** Given two sets $A = \{a_1, a_2, \dots, a_n\}$ and $B = \{b_1, b_2, \dots, b_n\}$, is $A = B$?

Lemma 3.1 Let $S = \{s_1, s_2, \dots, s_{2n}\}$ be a set of $2n$ points in the plane radially sorted around the point $\theta \notin S$. Then the halfspace depth of θ is n if and only if s_i, θ, s_{n+i} are collinear, with θ between s_i and s_{n+i} , for all $1 \leq i \leq n$.

Proof. Suppose that s_i, θ, s_{n+i} are collinear, with θ between s_i and s_{n+i} , for all $1 \leq i \leq n$. Then for any line L through θ , the points s_i and s_{n+i} either lie on opposite sides of L , or they both lie on L (see figure 3.3a). Since we have n such pairs of $\{s_i, s_{n+i}\}$, each closed halfspace determined by a line through θ contains at least n points of S . The minimum of n is achieved by selecting a line which does not touch any points of S .

Now suppose that s_i, θ, s_{n+i} are not collinear or that θ is not between s_i and s_{n+i} for some $1 \leq i \leq n$. Then since the angle $\angle s_i \theta s_{n+i} < 2\pi$, it is possible to draw a line L through θ such that s_i and s_{n+i} are on the same side of L . Therefore all s_j for $i \leq j \leq n+i$ are strictly on one side of L . Since there are at least $n+1$ points strictly on one side of L , there are at most $n-1$ points on the other side or on the line. Thus the halfspace depth of θ is at most $n-1$ (see figure 3.3b).

□

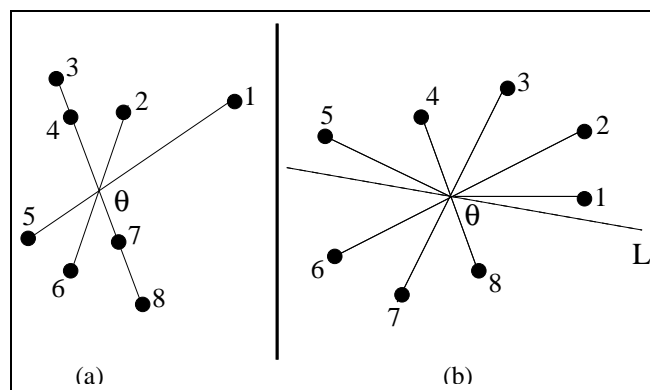


Figure 3.3: Halfspace depth depends on angular symmetry.

Theorem 3.2 *Halfspace depth* requires $\Omega(n \log n)$ time in the worst case.

Proof. We reduce *Set Equality* to halfspace depth. Let $A = \{a_1, a_2, \dots, a_n\}$ and $B = \{b_1, b_2, \dots, b_n\}$ be two sets of real numbers. For every i ($1 \leq i \leq n$) construct the points $(a_i, 1)$ and $(-b_i, -1)$ in the plane¹. Thus we have a set S of $2n$ points, and we select $(0, 0)$ as the query point θ (see figure 3.4). Considering the elements of S in radially sorted order about θ , the elements of A correspond to the points $s_1 \dots s_n$, and the elements of B correspond to $s_{n+1} \dots s_{2n}$. The only computation is the construction of S , which can be performed in linear time. Suppose we now find the halfspace depth of θ . If it is n , we know that s_i, θ, s_{n+i} are collinear for all $1 \leq i \leq n$, by lemma 3.1. Therefore $A = B$. Again, by lemma 3.1, if the depth of θ is not equal to n , we cannot have n pairs of points which are reflections of each other through θ , so $A \neq B$. Therefore by finding halfspace depth, we can answer the question of Set Equality.

□

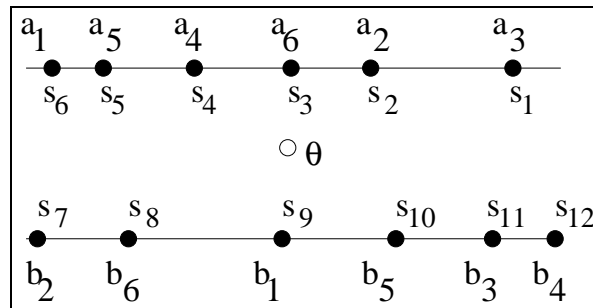


Figure 3.4: *Set equality* of sets A and B can be reduced to halfspace depth of set S .

¹If non-degenerate points are desired, we can instead construct the points (ia_i, i) and $(-ib_i, -i)$.

3.2.2 Simplicial Depth Lower Bound

We show that finding simplicial depth allows us to answer the question of *Element Uniqueness*, which has an $\Omega(n \log n)$ lower bound in the algebraic decision tree model of computation [BO83]:

- **Element Uniqueness:** Given a set $A = \{a_1, a_2, \dots, a_n\}$, is there a pair $i \neq j$ such that $a_i = a_j$?

Theorem 3.3 *Simplicial depth* requires $\Omega(n \log n)$ time in the worst case.

Proof. We reduce *Element Uniqueness* to simplicial depth. Let $A = \{a_1, a_2, \dots, a_n\}$ be a set of real numbers, for $n \geq 3$. For every a_i where $1 \leq i \leq n$ construct the points $(a_i, 1)$ and $(-a_i, -1)$ which are reflections of each other through $(0,0)$. Thus we have a set S of $2n$ points. s_i and s_{n+i} are reflections of each other through the origin, which we select as the query point θ .

Suppose s_i is a unique element in S . Then the quantity h_i , as defined in section 3.1.2, must equal $n - 1$, since h_i includes all points $s_{i+1}, \dots, s_{n+i-1}$ (see figure 3.5a). Thus if no element is duplicated in S , the simplicial depth of θ with respect to S must be

$$D = \binom{2n}{3} - \sum_{i=1}^{2n} \binom{n-1}{2}.$$

Now suppose $s_i = s_{i+1}$ for some i . Then $h_{i+1} < n - 1$, since h_{i+1} includes at most the points $s_{i+2}, \dots, s_{n+i-1}$. It does not include the reflection of s_i (see figure 3.5b). Thus if some element is duplicated in S , the simplicial depth of θ with respect to S is strictly higher than if S has no repeated elements. Therefore by finding simplicial depth, we can answer the question of Element Uniqueness: the elements of A are unique if and only if the depth of $(0,0)$ with respect to S is D . The only computations

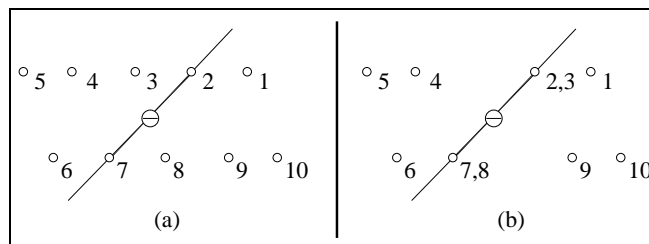


Figure 3.5: Simplicial depth lower bound: (a) h_2 contains s_3, s_4, s_5, s_6 . — (b) h_3 contains s_4, s_5, s_6 but not s_7 .

in the reduction are the construction of S and the computation of D , which can be performed in linear time.

□

3.3 Ramifications

In this section we show that the lower bounds developed in section 3.2 may be applied to the bivariate sign tests of Hodges [Hod55] and of Oja and Nyblom [ON89]. Sign tests are used to determine if there is a statistically significant difference in the two distributions of n pairs of data points.

3.3.1 The Bivariate Hodges Sign Test

The Hodges sign test is conducted as follows: Given a direction d and a set of n vectors formed by n pairs of points, project each vector onto d and count the number of projections which have the same direction as d . We call such vectors *positive* (see figure 3.6a).

The output of the test is the maximum number of positive vectors found over all directions. Rousseeuw and Ruts [RH99b] mention that halfspace depth is related to the Hodges sign test. We briefly explain how: first, shift every vector to the origin.

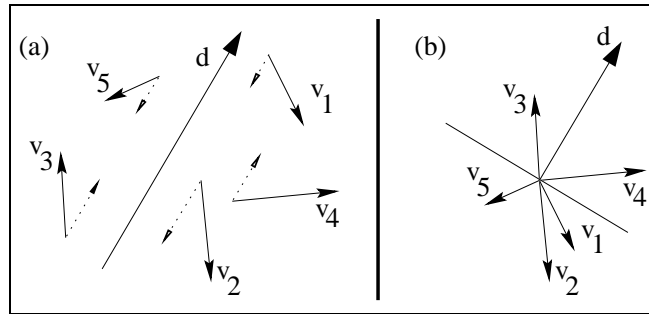


Figure 3.6: v_3 and v_4 are *positive* vectors with respect to direction d .

This does not influence any directions, so the output of the test is unaffected. Now notice that for a given direction d the number of positive vectors is determined by a halfspace orthogonal to d (figure 3.6b). It is now clear that the maximum number of positive vectors over all directions is the complement of the halfspace depth of the origin.

Theorem 3.4 *The bivariate Hodges sign test requires $\Omega(n \log n)$ time in the worst case.*

Proof. The halfspace depth of a query point θ with respect to a data set of n points may be determined by constructing n vectors (from θ to each data point) in linear time and applying the Hodges sign test to these vectors.

□

3.3.2 The Bivariate Oja-Nyblom Sign Test

Given a data set of n points, the sign test of Oja and Nyblom involves computing the number of triples of points, each of which has the property that it falls on the same side of some line through the origin. Rousseeuw and Ruts [RR96] mention that their methods, described in section 3.1, may be used to compute this sign test. The relation to the problem of computing simplicial depth is clear.

Theorem 3.5 *The Oja-Nyblom sign test requires $\Omega(n \log n)$ time in the worst case.*

Proof. The simplicial depth of a query point θ with respect to a data set of n points may be determined by applying the Oja-Nyblom sign test to the data, taking θ as the origin.

□

Chapter 4

New Median Algorithms

In this chapter we present new algorithms for computing two bivariate medians. In section 4.1 we present our algorithms for the Oja median. Algorithm *Oja-1* has a time complexity of $O(n^3 \log n)$ and uses $O(n^2)$ space. Our gradient descent algorithm, *Oja-2*, uses $O(n^4)$ time and $O(n^2)$ space. It may be also be used to find the Fermat-Torricelli points of n lines in $O(n^2)$ time and $O(n)$ space. In section 4.2 we present our algorithm for computing the simplicial median, which uses $O(n^4 \log n)$ time and $O(n^2)$ space *or* $O(n^4)$ time and space. As mentioned in chapter 2, our algorithms for computing the Oja and simplicial medians improve the time complexity of the algorithms by Rousseeuw and Ruts which use $O(n^5 \log n)$ time. Our algorithm for computing the Fermat-Torricelli points of n lines improves the one by Barbara which uses $O(n^3)$ time.

4.1 Oja Median Algorithms

4.1.1 Properties of the Oja Median in R^2

Some properties of the Oja median in R^2 are first stated and proved. Let L be the set of lines formed by each pair of points in a data set S . Note that by “Oja median”

we mean one point for which Oja depth is minimum. If other such points exist it is an easy matter to find them, as should be apparent after the proof of lemma 4.4.

Lemma 4.1 *The Oja depth of a point θ with respect to S can be expressed as a weighted sum of the distances from θ to each line in L .*

Proof. By definition, Oja depth is the sum of the areas of all triangles (θ, s_i, s_j) , where $1 \leq i < j \leq n$. The area of each triangle may be expressed as $\frac{1}{2}bh$, where b is the distance from s_i to s_j and h is the orthogonal distance from the point θ to the line $\overline{s_i s_j}$.

□

Lemma 4.2 *The Oja median must be on one of the intersection points of the lines in L .*

Proof. Each cell formed by the arrangement of lines in L can be considered to be a linear program¹, where the feasible region is determined by the edges of the cell, and the function to be minimized is the weighted sum of lemma 4.1. Therefore if the median is located within a given cell, it must be on one of its vertices. The median cannot be at infinity (as part of an open cell) since the Oja depth would be infinite, as is apparent by lemma 4.1.

□

Lemma 4.3 *The Oja depth along any line ℓ in the plane varies in a piecewise-linear manner, with inflection points occurring only where ℓ crosses lines in L .*

Proof. The rate of change of Oja depth is constant along ℓ within any cell of the arrangement of lines, since the cell represents a linear program. As ℓ crosses from one

¹For an introduction to linear programming, see [Chv83].

cell to the next, it crosses from one linear program to another. The transition occurs at the common edge of two cells, which is on a line in L .

□

Lemma 4.4 *The Oja depth along a line ℓ has only one local minimum, from which the rate of change of Oja depth increases monotonically in both directions.*

Proof. Suppose that the Oja depth is decreasing as we move along ℓ in some direction, and that along this direction we encounter line m which is a member of L . This encounter does not affect the contribution of any other line in L to Oja depth. Since crossing m can only increase m 's contribution to Oja depth, the result is that Oja depth cannot decrease at a faster rate. Since Oja depth decreases from infinity as we approach the members of L from either direction on ℓ , the lemma follows by induction. The local minimum can be a point or a segment between two intersection points.

□

In figure 4.1 we illustrate lemma 4.4. If Oja depth $f(\ell)$ is decreasing along ℓ as we approach m , the situation of figure 4.1 cannot exist.

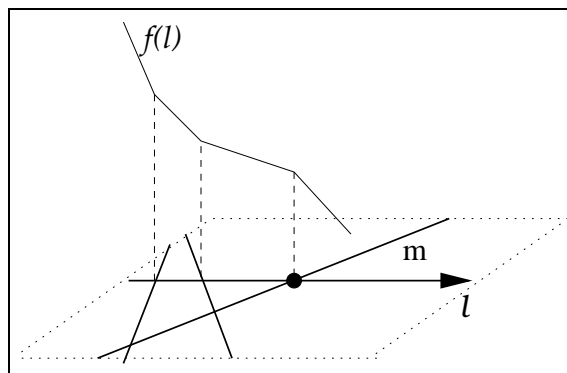


Figure 4.1: Oja depth $f(\ell)$ cannot decrease at a faster rate when crossing m .

Corollary 4.5 *The Oja depth function is convex.*

Proof. A bivariate function f is convex if, for every $x_1, x_2 \in R^2$ and every α , $0 \leq \alpha \leq 1$, there holds

$$f(\alpha x_1 + (1 - \alpha)x_2) \leq \alpha f(x_1) + (1 - \alpha)f(x_2).$$

By lemma 4.4, the above property holds for Oja depth.

□

Corollary 4.6 *The points in R^2 with minimum Oja depth form a convex polygon with $O(n)$ vertices on its boundary.*

Proof. Since the Oja depth function is a convex polyhedron, the minimum value must be at a vertex, a line segment or a face of the polyhedron, all of which are convex. If we project these objects back onto the plane, we obtain an intersection point, a boundary segment on a cell, or a single cell in the arrangement of L . Every data point can contribute at most two lines to the boundary of a cell, so every cell has $O(n)$ segments on its boundary. Thus the number of intersection points with minimum Oja depth is $O(n)$.

□

Lemma 4.7 *If the Oja depth decreases along two directions u and v from a point p , then it must also decrease in all directions between u and v (within the acute angle).*

Proof. All points along u or v from p have depth less than the depth at p . Between any point along u and any point along v we can form a line, along which the depth cannot have a local maximum, by lemma 4.4. Therefore the depth along this line and between the two points cannot be greater than the depth of both points, which implies that the depth cannot be greater than the depth at p . This also implies that

from any point p , the directions in which depth increases must span at least 180° . Otherwise Oja depth would decrease in all directions from p , which contradicts the fact that there can be no local maximum.

□

Lemma 4.8 *The Oja depth of a point θ may be found in $O(n \log n)$ time.*

Proof. Sort the data points $\{s_1 \dots s_n\}$ radially about θ . We wish to sum the areas of all triangles with vertices (θ, s_i, s_j) . Let v_i be the vector from θ to s_i . We can ensure that the area of each triangle is computed once by considering only the triangles for which the cross product $v_i \times v_j$ is positive. This is similar to the enumeration of triangles for the calculation of simplicial depth. Figure 4.2 illustrates the triangles considered for $i = 1$.

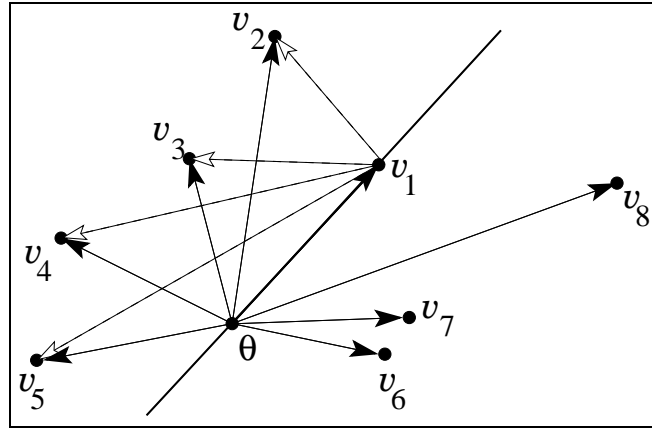


Figure 4.2: Oja depth calculation: the triangles considered for v_1 .

The cumulative areas of these triangles is the length of

$$\frac{1}{2}v_1 \times v_2 + \frac{1}{2}v_1 \times v_3 + \frac{1}{2}v_1 \times v_4 + \frac{1}{2}v_1 \times v_5.$$

In general, if k triangles are associated with vector v_i , the sum of areas A_i is

$$A_i = \sum_{j=i+1}^{i+k} \frac{1}{2}|v_i \times v_j|$$

where j is taken modulo n . Using a basic cross-product relation we get

$$A_i = \frac{1}{2}v_i \times (v_{i+1} + v_{i+2} + \cdots + v_{i+k}). \quad (4.1)$$

A_1 may be computed in $O(n)$ time. Now we proceed through the sorted list of vectors, as in the halfspace depth calculation. Every time we encounter a vector, we add it or subtract it from the vector sum in equation 4.1, in the same way that we updated the contents of each halfspace. Since each vector will be added and subtracted once, this process takes $O(n)$ time to compute all remaining A_i . Therefore the time complexity of this procedure is dominated by the initial sorting step.

□

We can use figure 4.2 to give an example of the above procedure. Initially we have $A_1 = \frac{1}{2}v_1 \times V$, where V is the vector sum of v_2, v_3, v_4, v_5 . When we sweep a line through the vectors in a counterclockwise direction, we first encounter v_2 . Thus we subtract v_2 from V and compute $A_2 = \frac{1}{2}v_2 \times V$. When we reach v_4 , V will be equal to v_5 . After v_4 the rotating line will cross v_6 and v_7 , which are added to V . Therefore $A_5 = \frac{1}{2}v_5 \times (v_6 + v_7)$.

Lemma 4.9 *The minimum Oja depth along any line ℓ may be found in $O(n^2)$ time.*

Proof. Compute the intersection points of ℓ with all lines of L in $O(n^2)$ time. For each line t in L consider the vector v between the two points that determine t . Compute w , the magnitude of this vector's orthogonal component to ℓ . This corresponds to a weight for the intersecting point of t and ℓ (see figure 4.3). The area of the triangle formed by the two points of t and a point p on ℓ is equal to the distance from p to the intersection point multiplied by its weight. Thus for any point on ℓ , Oja depth equals a weighted sum of distances to all intersection points on ℓ . In other words, the minimum Oja depth along ℓ is equal to the weighted univariate median of

$O(n^2)$ points. This may be computed in $O(n^2)$ time with a slight modification of the univariate median algorithm of Blum et al [BFP⁺73] mentioned in the introduction (chapter 1).

□

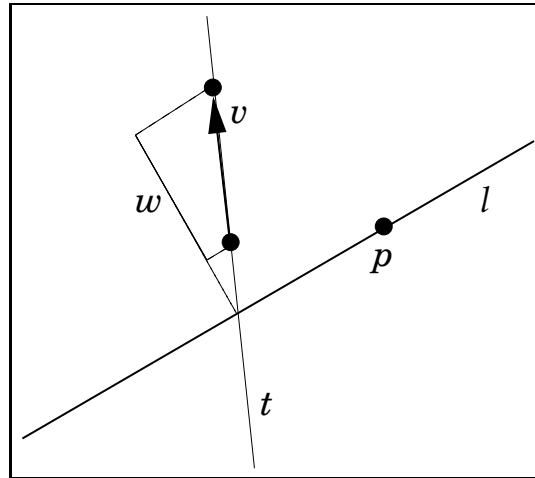


Figure 4.3: Calculating Oja depth on a line.

Note that as with the univariate median, the minimum Oja depth along a line may be computed by first sorting all the intersection points. This would increase the complexity by a factor of $\log n$.

4.1.2 The two Algorithms

Algorithm *Oja-1*

For each point s_i in S do the following:

1. Sort radially the lines determined by s_i and every other point of S .
2. Perform a binary search on the sorted lines: each step consists of computing the point d with minimum depth along one line, determining which side of that line

contains directions where the depth does not increase from d , and proceeding in that region of space.

3. If a line is found where depth only increases from d , halt and return d .

In figure 4.4, suppose we have sorted all lines from s_i to other data points. We start the binary search with lines a and b which split the plane into four quadrants containing roughly the same number of lines. Now after computing the minimum Oja depth on a and b , we restrict the location of the Oja median to one quadrant. If it is the upper-left quadrant, we continue the binary search by selecting line c , which again splits the remaining list of lines evenly.

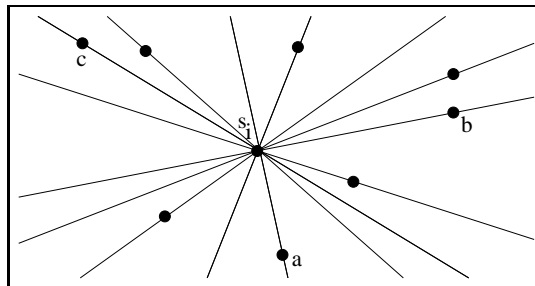


Figure 4.4: Algorithm *Oja-1*: For each data point s_i perform a binary search on the lines to other data points.

Theorem 4.10 *Algorithm Oja-1 computes the bivariate Oja median of n points in $O(n^3 \log n)$ time and $O(n^2)$ space.*

Proof. Binary search is made possible by lemma 4.7, which implies that for a point with minimum depth along a line, the depth must increase in all directions of at least one side of the line. The region in which to proceed may be found by using the gradient of the Oja depth function, which can be computed in $O(n^2)$ time by Niinimaa, Oja and Nyblom [NON92] or in $O(n \log n)$ time by Rousseeuw and Ruts [RR96]. Thus the

complexity of one step in the binary search is dominated by calculating the minimum depth on a line, which takes $O(n^2)$ time by lemma 4.9. The binary search continuously shrinks a wedge in the plane where the Oja median may be found, or in other words expands the region where the median cannot be found. Since by lemma 4.2 the median must be located on one of the lines in L , there must exist a data point for which this wedge will shrink to a single line. The minimum depth along this line is the Oja median. $O(n^2) * O(\log n)$ time suffices for one data point. Thus the total complexity for step 2 is $O(n^3 \log n)$. This dominates the time complexity of this algorithm since step 1 takes $O(n^2 \log n)$ time by brute force or $O(n^2)$ with a method described in Appendix A. The amount of space used is $O(n^2)$ for step 1.

□

Algorithm *Oja-2*

Choose any line in L and label it as ℓ .

1. Find the point p with minimum Oja depth on ℓ .
2. Find the intersecting line at p which has the steepest rate of change of Oja depth (this is done in a similar way to finding which region to proceed in during algorithm *Oja-1*). If the steepest slope is not negative then stop. Otherwise, label the line with steepest slope as ℓ and go to step 1.

Theorem 4.11 *Algorithm Oja-2 computes the bivariate Oja median of n points in $O(n^4)$ time and $O(n^2)$ space.*

Proof. Due to lemma 4.7 we know that once the region on one side of a line is rejected, the line will never be re-visited by a gradient descent. Since the function is convex, the descent must succeed after visiting $O(n^2)$ lines. By lemma 4.9, $O(n^2)$ time suffices

for step 1. Thus the total complexity amounts to $O(n^4)$. Only one line is processed at a time, so the space used is $O(n^2)$.

□

Note that we could also simply find the minimum depth on each of the $O(n^2)$ lines without using a gradient descent. The complexity would only differ by a constant factor.

4.1.3 The Fermat-Torricelli Points of n Lines

In section 4.1.1, lemmas 4.1 and 4.2 imply that the Oja median is a Fermat-Torricelli point of L . However we cannot use algorithm *Oja-1* for any set of lines, since this algorithm relies on the fact that a large number of lines pass through each point in S . Instead algorithm *Oja-2* may be used since it assumes nothing about the position of the lines. Therefore we have the following theorem:

Theorem 4.12 *The Fermat-Torricelli points of n lines may be computed in $O(n^2)$ time and $O(n)$ space, using algorithm *Oja-2*.*

4.2 Simplicial Median Algorithm

Let S be a data set of n points in R^2 , and I be the set of line *segments* formed between every pair of points in S .

Lemma 4.13 *To find a point with maximum simplicial depth it suffices to consider the intersection points of segments in I .*

Proof. Consider the arrangement of cells whose boundaries are segments in I . All points in the interior of a given cell must have equal simplicial depth. Any point on the boundary of this cell must have depth at least equal to points in the interior.

Finally, any vertex of the cell must have depth at least equal to any point on an adjacent boundary. These vertices are the intersection points of segments in I .

□

To simplify the description of our algorithm for computing the simplicial median, assume that S is in general position, in the sense that no three points are collinear. Later we explain how this assumption may be removed, if desired, without influencing the time or space complexity.

Algorithm *Simp-Med*

1. Calculate the simplicial depth of every data point in S .
2. Compute the number of points which are strictly to one side of each segment in I (each side separately).
3. For every segment ℓ in I ,
 - (a) compute and sort the intersection points of all other segments with ℓ , if there are any.
 - (b) let MAX be the greatest depth among the endpoints of ℓ .
 - (c) if there exist other intersection points on ℓ , calculate the simplicial depth d of the intersection point adjacent to one of the endpoints. Update MAX (if $MAX < d$, $MAX \leftarrow d$).
 - (d) continue through the sorted list: every time an intersecting line is left behind, subtract from d the number of points strictly behind the line. Every time a line is encountered, add to d the number of points strictly ahead of that line. Update MAX after encountering each intersection.
4. Exit with the greatest MAX value found over all segments, and the associated intersection point.

Figure 4.5 illustrates the logic behind step 3 of algorithm *Simp-Med*. Once we know the depth of an intersection point (step 3c), we can compute all other depths along the given segment, each in constant time. Each intersecting segment forms a triangle with every point strictly to one side. Thus every time we encounter a segment, we enter as many triangles as there are points on the other side of this segment. Every time we leave a segment behind, we exit triangles formed by that segment and each point on the other side. So in figure 4.5, suppose we are moving from left to right along the current line segment, and just before encountering segment t , we have some value $d = 10$. Upon encountering t , we can see that we are now inside three new triangles: one for each point to the right of t . As soon as we move to the right of t , we will no longer be inside five triangles. So on t , $d = 13$, and immediately after, $d = 8$.

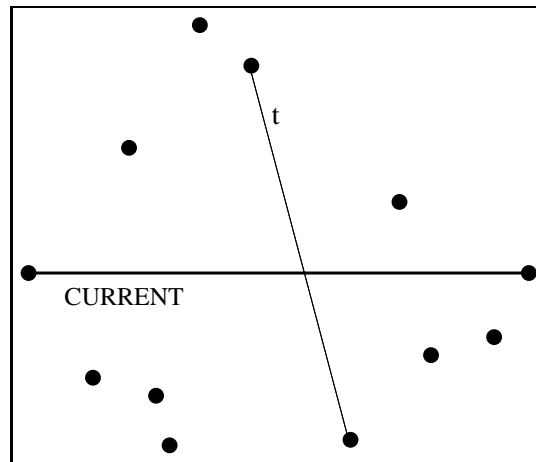


Figure 4.5: Algorithm *Simp-Med*: the current line segment traversed, and an intersecting segment t .

In case we have multiple segments intersecting the current line at the same point, we may form a temporary list of these segments. When the last one is encountered, we process the list: First we add the points to the right of each line, then we subtract all the points to the left of each line.

Theorem 4.14 *Algorithm Simp-Med computes the bivariate simplicial median of n points in $O(n^4 \log n)$ time and $O(n^2)$ space or alternatively in $O(n^4)$ time and space.*

Proof. All intersection points are checked, so by lemma 4.13 a point of maximum simplicial depth is found. Step 1 takes $O(n^2 \log n)$ time in total since the calculation of simplicial depth for a point takes $O(n \log n)$ time with the algorithm of Rousseeuw and Ruts [RR96]. Step 2 is straightforward to do in $O(n^3)$ time by brute force. Step 3a takes $O(n^2 \log n)$, 3b is constant, 3c is $O(n \log n)$, and 3d takes $O(n^2)$ time. Thus step 3 takes $O(n^4 \log n)$ once run for every segment, and dominates the time complexity of this algorithm. The space used is $O(n^2)$ for steps 2 and 3a. If we compute the arrangement² of I in $O(n^4)$ time and space as preprocessing, then step 3a is no longer necessary. In this case, the preprocessing step would dominate the complexity of the algorithm.

□

We note that certain steps of algorithm *Simp-Med* may be performed more efficiently, without improving the asymptotic complexity overall (apart from some constant factor). For example take step 2 where we count the number of points on each side of every line segment. The problem of counting or reporting the points to one side of a query line has been the focus of extensive research in the past. Of course, this problem is of interest only when several queries are made. Typically some form of preprocessing takes place which allows each query to be answered in less than the brute-force $O(n)$ time. Chazelle, Guibas and Lee [CGL85] compute the convex layers of the given data set as a preprocessing step (in $O(n \log n)$ time using Chazelle's algorithm mentioned in chapter 2). Then they report every point on one side of a query line in $O(k + \log n)$ time, where k is the number of points reported. Since we only need to *count* the points in step 2, we describe only the relevant portions of their

²This concept is described in Appendix A.

algorithm. A given query line is tested for intersection with every convex layer. This may be done in $O(\log v_i)$ time for layer i which has v_i vertices, by performing a binary search on the edges of the layer. If the line and convex layer intersect, it is an easy matter to count the number of points on each side of the query line in constant time. This is done by considering the indices of the layer's segments which intersect the query line. We see that the time complexity $T(n)$ depends on the number of convex layers k :

$$T(n) = \sum_{i=1}^k O(\log v_i)$$

where $\sum_{i=1}^k v_i = n$. If there is one layer, $T(n)$ becomes $O(\log n)$, but if there are $O(n)$ layers, $T(n)$ is $O(n)$. The expected number of convex hull layers for a uniform distribution of data points in a convex area is $\Omega(n^{\frac{2}{3}})$ and $O(n^{\frac{2}{3}} \log^{\frac{1}{3}} n)$ [Dev01]. In the case that the lower bound is achieved, $T(n)$ is $O(n^{\frac{2}{3}} \log n)$. The algorithm of Edelsbrunner and Welzl [EW86] uses $O(n \log n)$ preprocessing time and then takes $O(k + n^{0.695})$ time for each query. However, in this algorithm if points are only *counted* the time complexity reduces to $O(n^{0.695})$. The total space used is $O(n)$. Agarwal and Erickson [AE98] provide an extensive survey on this problem and similar topics, including a discussion of lower bounds and time-space tradeoffs. Since step 2 of algorithm *Simp-Med* performs $O(n^2)$ queries, the algorithm of Chazelle, Guibas and Lee takes $O(n^3)$ time in the worst case, but will have a better time complexity than the brute-force method for some data distributions. The algorithm of Edelsbrunner and Welzl takes $O(n^{2.695})$ time for step 2. By taking advantage of the structure of the lines in this problem, we can further reduce this time complexity. This is done by using a procedure similar to that mentioned in section 3.1.1. For every data point, we essentially compute halfspace depth, but store the points counted for every halfplane considered. Therefore step 2 can be performed in $O(n^2 \log n)$ time. Furthermore, it is possible to sort all points about each point in $O(n^2)$ time (see [LC85, Ede87] or Appendix A), so the halfspace depth procedure then takes only $O(n)$ time per data

point. This means that the time complexity of step 2 reduces to $O(n^2)$. The same applies for computing the simplicial depth of all data points in step 1.

Finally we explain how the general position assumption may be removed. Steps 1 and 2 are not affected. While performing step 3a for some line ℓ , if we encounter an intersection point which happens to be a data point, we can simply stop processing ℓ and go to the next segment. We may do this because the intersecting data point will form segments with both endpoints of ℓ , so all points on ℓ will be processed anyway. This leaves one more case to consider. Suppose that if we extend an intersecting segment t we will find c collinear points. We can determine this easily since we know the number of points strictly to the side of t . It follows that we must also have more intersecting segments collinear with t . If there are m such segments, then we claim that on this intersection point we are inside $\frac{m(c-2)}{2}$ triangles, apart from those considered by the regular algorithm. We arrive at this number from the following argument: With the endpoints of an intersecting segment and one of the other c points, we can form a triangle containing the intersection point. Therefore using the two endpoints we can form $c - 2$ such triangles. Suppose that x is the third point for one of these triangles. Then x and one of the endpoints will form another intersecting segment. So the same triangle will be counted exactly one more time when the other segment is processed. Therefore we have $c - 2$ triangles counted for each of the m segments, and we multiply by a factor of $\frac{1}{2}$ to avoid counting each triangle twice.

Chapter 5

Conclusion

We have presented an overview of several estimators of location, including an account of recent developments on robustness and computational complexity issues. Emphasis was given to estimators which have a geometrical aspect to them. The most important elements of this thesis were the new results obtained concerning bivariate depths and estimators of location.

We have defined a new median for n points in any dimension, by adapting the hyperplane depth of Rousseeuw and Hubert to a set of points. Properties of this median may be studied easily through simulations in the near future, since relatively fast algorithms for hyperplane depth already exist.

We have proved that the computation of simplicial or halfspace depth for one point in R^2 requires $\Omega(n \log n)$ time. Thus we have matched the upper bound complexity of the algorithms of Rousseeuw and Ruts. In addition, we have shown that the computation of the bivariate sign tests of Hodges and of Oja and Nyblom require $\Omega(n \log n)$ time. Recently we learned that a different lower bound proof for halfspace depth was obtained independently by Langerman and Steiger [LS00].

We have reduced the complexity of calculating the Oja and simplicial medians. The Oja median may be computed in $O(n^3 \log n)$ time and $O(n^2)$ space. The simplicial

median may be computed in $O(n^4 \log n)$ time with $O(n^2)$ space, or alternatively, in $O(n^4)$ time and space. This improves the results of Rousseeuw and Ruts, whose algorithms compute each median in $O(n^5 \log n)$ time. Our algorithm *Oja-2* may be used to compute the Fermat-Torricelli points of n lines in $O(n^2)$ time and $O(n)$ space, thus improving the algorithm of Barbara which takes $O(n^3)$ time. Furthermore, our proof that the solution must be on an intersection point is much shorter.

This research has left certain open problems, which we list below:

Conjecture 5.1 *The computation of Oja depth requires $\Omega(n \log n)$ time.*

Open Problem 5.2 *Prove conjecture 5.1, or disprove it by providing a procedure faster than that described in lemma 4.8.*

Open Problem 5.3 *What are the highest attainable lower bounds for computing the halfspace, simplicial, Oja and H -medians in R^2 ?*

As mentioned in section 2.6 the algorithm of Langerman and Steiger may be used to compute the bivariate H -median of n points in $O(n^2 \log n)$ time. However, their algorithm was designed to work for arbitrarily placed hyperplanes, whereas the hyperplanes considered for the H -median have some structure.

Open Problem 5.4 *Can the $O(n^2 \log n)$ time algorithm for computing the H -median be improved?*

Open Problem 5.5 *What are the breakdown points of the simplicial and H -medians?*

Since the submission of this thesis, some of the results obtained have been improved [ALST01]. The Oja median may be computed in $O(n \log^3 n)$ time and $O(n)$ space, and the Fermat-Torricelli points of n lines may be computed in $O(n)$ time and space. We are optimistic that in the near future we will also be able to improve our algorithm for the simplicial median, and we intend to study the alternate definition involving open simplices.

Appendix A

Arrangements of Lines

Consider a set L of n lines in the plane. As we can see in figure A.1, L splits the plane into convex cells, line segments and intersection points. This partition of the plane is known as an *arrangement* of lines. In computational geometry it is often convenient to use the structure of arrangements as opposed to dealing with each line separately. Examples of applications are given in [O'R95]. We say that we have *constructed the arrangement* of L if:

- for every line ℓ in L we have a sorted list of all intersection points on ℓ .
- for every intersection point we have a radially sorted list of all lines intersecting the point.

An arrangement of n lines may be constructed in $\Theta(n^2)$ time and space. This result was first obtained by Chazelle, Guibas and Lee [CGL85], and by Edelsbrunner, O'Rourke and Seidel [EOS86]. The proof of this result is described well in [O'R95]. The same algorithm may be used to construct an arrangement of line segments.

A nice application of arrangements is for sorting all points about every point in a data set in $O(n^2)$ time [LC85, Ede87]. This may be used in algorithms *Oja-1* and *Simp-Med*. We first briefly explain the concept of *duality*. Every point (a, b) in the

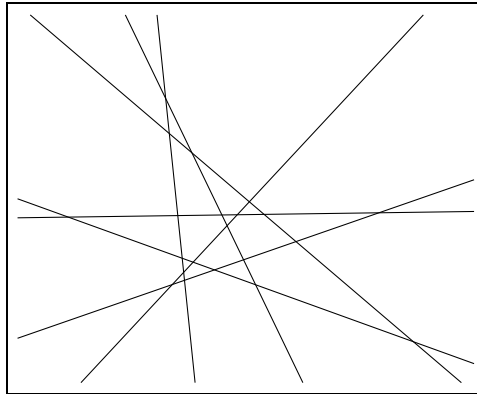


Figure A.1: An arrangement of lines.

plane may be mapped to a line $y = ax + b$ in a *dual plane*. On the other hand, lines in the plane are mapped to points in the dual. Other mappings exist and are described in [O'R95]. A set of n points in the plane will map to a set of n lines in the dual. Furthermore, the $O(n^2)$ lines between points in the plane map to the $O(n^2)$ intersection points of the lines in the dual. It is not too difficult to see that the radially sorted lines from a point p to all other points will map to a sorted set of intersection points on the dual line of p .

Given a set S of n points, construct the dual lines and compute their arrangement. Now for every point p in S , we wish to obtain a sorted list of the lines from p to other points in S . With figure A.2¹ we illustrate how this is done when p happens to be located on the origin. We have $S = \{a, b, c, d, e, f, g, h, p\}$, shown as black circles in the figure. Point p maps to the dual line $y = 0$. So we go to this line and find a sorted list of intersection points (shown as white circles). As we traverse this list from left to right, we map each intersecting line back to a point of S . Thus we enumerate the points of S in radially sorted order about p . Notice that there is one technicality: all dual lines with positive slopes map to points in S which are to the right of p , while

¹Figure A.2 was obtained by using an applet created by Fred Henle. See <http://www.cs.dartmouth.edu/~henle/Duality/Duality.html>.

dual lines with negative slopes map to points to the left of p . However we wish to manage this, it may be done in $O(n)$ time. Therefore this process takes $O(n^2)$ time for all points in S .

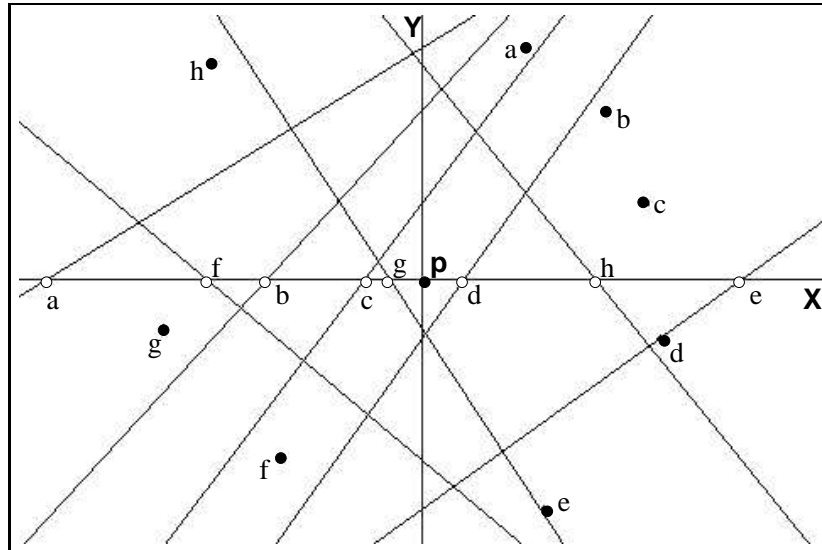


Figure A.2: A set of points and their dual lines.

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