Fitting a Graph to One-Dimensional Data*

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October 1, 2020

Abstract

Given n data points in \mathbb{R}^d , an appropriate edge-weighted graph connecting the data points finds application in solving clustering, classification, and regression problems. The graph proposed by Daitch, Kelner and Spielman (ICML 2009) can be computed by quadratic programming and hence in polynomial time. While a more efficient algorithm would be preferable, replacing quadratic programming is challenging even for the special case of points in one dimension. We develop a dynamic programming algorithm for this case that runs in $O(n^2)$ time.

1 Introduction

Many interesting data sets can be interpreted as point sets in \mathbb{R}^d , where the dimension d is the number of features of interest of each data point, and the coordinates are the values of each feature. Given such a data set, graph-based semi-supervised learning is a paradigm for making predictions on the unlabelled data using the proximity among the data points and possibly some labelled data (e.g. [3, 6, 9, 12, 14, 15, 16]). Classification, regression, and clustering are some popular applications. The graph has to be set up first in order to perform the subsequent processing. This requires the determination of the graph edges and the weights to be associated with the edges. For example, let w_{ij} denote the weight determined for the edge that connects two points p_i and p_j , and regression can be performed to predict function values f_i 's at the points p_i 's by minimizing $\sum_{i,j} w_{ij} (f_i - f_j)^2$, subject to fixing the subset of known f_i 's [3]. To allow efficient data analysis, it is important that the weighted graph is sparse.

The graph connectivity should satisfy the property that similar discrete samples are connected. To this end, different proximity graphs have been suggested for connecting proximal points. The kNN-graph connects each point to its k nearest neighbors. The ε -ball graph connects each point to all other points that are within a distance ε . After fixing the graph connectivity, edges to "near" points are given large weights and edges to "far away" points are given small weights. That is, the larger the weight of an edge between points p and q, the higher the influence of q on p and vice versa. It is thus inappropriate to use the Euclidean distances among the points as edge weights. Naively setting an edge weight as the reciprocal of the edge length does not work either because the influence of a point is required to fall much more rapidly as that point moves farther away. It has been proposed to associate a weight of $\exp(-\ell^2/2\sigma^2)$ to an edge of Euclidean length ℓ for some a priori determined parameter σ (e.g. [12]). A well-tuned

^{*}SWC is supported by Research Grants Council, Hong Kong, China (project no. 16203718). OC and TL were supported by ICT R&D program of MSIP/IITP [IITP-2015-0-00199]. A preliminary version appeared in Proceedings of the Canadian Conference on Computational Geometry, 2020 [2].

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 σ is important. A slight change in σ may greatly affect the processing outcomes as observed in some previous work (e.g. [14]). Several studies have found the kNN-graph and the ε -ball graphs to be inferior to other proximity graphs [3, 4, 15] for which both the graph connectivity and the edge weights are determined simultaneously by solving an optimization problem.

We consider the graph proposed by Daitch, Kelner, and Spielman [3]. It is provably sparse, and experiments have shown that it offers good performance in classification, clustering and regression. This graph is defined via quadratic optimization as follows: Let $P = \{p_1, p_2, \ldots, p_n\}$ be a set of n points in \mathbb{R}^d . We assign weights $w_{ij} \geq 0$ to each pair of points (p_i, p_j) , such that $w_{ij} = w_{ji}$ and $w_{ii} = 0$. These weights determine for each point p_i a vector \vec{v}_i , as follows:

$$\vec{v}_i = \sum_{j=1}^n w_{ij} (p_j - p_i).$$

Let v_i denote $\|\vec{v}_i\|$. The weights are chosen so as to minimize the sum

$$Q = \sum_{i=1}^{n} v_i^2,$$

under the constraint that the weights for each point add up to at least one (to prevent the trivial solution of $w_{ij} = 0$ for all i and j):

$$\sum_{j=1}^{n} w_{ij} \geqslant 1 \quad \text{for } 1 \leqslant i \leqslant n.$$

The resulting graph contains an edge connecting p_i and p_j if and only if $w_{ij} > 0$.

Daitch et al. [3] showed that there is an optimal solution where at most (d+1)n weights are non-zero. Moreover, in two dimensions, optimal weights can be chosen such that the graph is planar.

The optimal weights can be computed by quadratic programming. A quadratic programming problem with m variables can be solved in $\tilde{O}(m^3)$ time in the worst case [10]. In our case, there are n(n-1)/2 variables, which gives a worst-case running time of $\tilde{O}(n^6)$. Graphs based on optimizing other convex quality measures have also been considered [6, 15]. Our goal is to design an algorithm to compute the optimal weights in Daitch et al.'s formulation that is significantly faster than quadratic programming. Perhaps surprisingly, this problem is challenging even for points in one dimension, that is, when all points lie on a line. In this case, it is not difficult to show (Lemma 2.1) that there is an optimal solution such that $w_{ij} > 0$ if and only if p_i and p_j are consecutive.

Despite its simplicity, the one-dimensional problem can model the task of detecting change points and concept drift in a time series (e.g. [1, 5, 7, 8, 13]); for example, seasonal changes in sales figures and customer behavior. A time series of multi-dimensional data (z_1, z_2, \cdots) is given, and the problem is to decide the time steps t at which there is a "significant change" from z_{t-1} to z_t . Suppose that the "distance" between z_{t-1} and z_t can be computed according to some formula appropriate for the application (e.g. [5]). By forming a path graph with vertices corresponding to the data points and edge weights determined as mentioned previously, one can apply clustering algorithms (e.g. [3, 12]) to group "similar" vertices and detect the change points as the boundaries of adjacent clusters. This gives a potential application of the graph fitting problem in one dimension.

In general, although there are only n-1 variables in one dimension, the weights in an optimal solution do not seem to follow any simple pattern as we illustrate in the following two examples.

Some weights in an optimal solution can be arbitrarily high. Consider four points p_1, p_2, p_3, p_4 in left-to-right order such that $p_2 - p_1 = p_4 - p_3 = 1$ and $p_3 - p_2 = \varepsilon$. By symmetry, $w_{12} = w_{34}$, and so $v_1 = v_4 = w_{12}$. Since $w_{12} + w_{23} \ge 1$ and $w_{23} + w_{34} \ge 1$ are trivially satisfied by the requirement that $w_{12} = w_{34} \ge 1$, we can make v_2 zero by setting $w_{23} = w_{12}/\varepsilon$. In the optimal solution, $w_{12} = w_{34} = 1$ and $w_{23} = 1/\varepsilon$. So w_{23} can be arbitrarily large.

Given points p_1, \cdots, p_n in left-to-right order, it seems ideal to make v_i a zero vector. One can do this for $i \in [2, n-1]$ by setting $w_{i-1,i}/w_{i,i+1} = (p_{i+1}-p_i)/(p_i-p_{i-1})$, however, some of the constraints $w_i + w_{i+1} \geqslant 1$ may be violated. Even if we are lucky that for $i \in [2, n-1]$, we can set $w_{i-1,i}/w_{i,i+1} = (p_{i+1}-p_i)/(p_i-p_{i-1})$ without violating $w_i + w_{i+1} \geqslant 1$, the solution may not be optimal as we show below. Requiring $v_i = 0$ for $i \in [2, n-1]$ gives $v_1 = v_n = w_{12}(p_2-p_1)$. In general, we have $p_2 - p_1 \neq p_n - p_{n-1}$, so we can assume that $p_2 - p_1 > p_n - p_{n-1}$. Then, $w_{n-1,n} = w_{12}(p_2-p_1)/(p_n-p_{n-1}) > 1$ as $w_{12} \geqslant 1$. Since $w_{n-1,n} > 1$, one can decrease $w_{n-1,n}$ by a small quantity δ while keeping its value greater than 1. Both constraints $w_{n-1,n} \geqslant 1$ and $w_{n-2,n-1} + w_{n-1,n} \geqslant 1$ are still satisfied. Observe that v_n drops to $w_{12}(p_2-p_1) - \delta(p_n-p_{n-1})$ and v_{n-1} increases to $\delta(p_n-p_{n-1})$. Hence, $v_{n-1}^2 + v_n^2$ decreases by $2\delta w_{12}(p_2-p_1)(p_n-p_{n-1}) - 2\delta^2(p_n-p_{n-1})^2$, and so does Q. The original setting of the weights is thus not optimal. If $w_{n-3,n-2} + w_{n-2,n-1} > 1$, it will bring further benefit to decrease $w_{n-2,n-1}$ slightly so that v_{n-1} decreases slightly from $\delta(p_n-p_{n-1})$ and v_{n-1} increases slightly from zero. Intuitively, instead of concentrating $w_{12}(p_2-p_1)$ at v_n , it is better to distribute it over multiple points in order to decrease the sum of squares. But it does not seem easy to determine the best weights.

Although there are only n-1 variables in one dimension, quadratic programming still yields a running time of $\tilde{O}(n^3)$. We present a dynamic programming algorithm that computes the optimal weights in $O(n^2)$ time in the one-dimensional case. The intermediate solutions computed by the algorithm have an interesting structure where the derivative of the quality measure depends on the derivative of a subproblem's quality measure as well as the inverse of this derivative function. We have experimental evidence that explicitly representing the intermediate solutions may require exponential time and space, and so we develop an implicit representation that facilitates the dynamic programming algorithm.

2 A single-parameter quality measure function

We will assume that the points are given in sorted order, so that $p_1 < p_2 < p_3 < \cdots < p_n$. We first argue that the only weights that need to be non-zero are the weights between consecutive points, that is, weights of the form $w_{i,i+1}$.

Lemma 2.1. For d = 1, there is an optimal solution where only weights between consecutive points are non-zero.

Proof. For a solution S and $t \in \{1, 2, ..., n-1\}$, let $z_t(S)$ be the number of non-zero weights at distance t (that is, $z_t(S)$ is the cardinality of the set $\{i \mid w_{i,i+t} > 0 \text{ in } S\}$), and let $\mathbf{z}(S)$ be the vector

$$\mathbf{z}(S) = (z_{n-1}(S), z_{n-2}(S), \dots, z_3(S), z_2(S)).$$

Among all optimal solutions, that is, solutions minimizing the quality Q, let O be a solution that lexicographically minimizes $\mathbf{z}(O)$. We will show that $\mathbf{z}(O) = (0, \dots, 0)$.

Assume to the contrary that there is a weight $w_{i,k} > 0$ for some i < k-1 in O. Let j be an arbitrary index strictly between i and k. We construct a new optimal solution as follows: Let $a = p_j - p_i$, $b = p_k - p_j$, and $w = w_{i,k}$. In the new solution, we set $w_{i,k} = 0$, increase $w_{i,j}$ by $\frac{a+b}{a}w$, and increase $w_{j,k}$ by $\frac{a+b}{b}w$. Note that since a+b>a and a+b>b, the sum of weights at each vertex increases, and so the weight vector remains feasible. The value v_j changes by

 $-a \times \frac{a+b}{a}w + b \times \frac{a+b}{b}w = 0$; the value v_i changes by $-(a+b) \times w + a \times \frac{a+b}{a}w = 0$; the value v_k changes by $+(a+b) \times w - b \times \frac{a+b}{b}w = 0$. It follows that the new solution O' has the same quality as O, and is therefore also optimal. Since $\mathbf{z}(O')$ is lexicographically smaller than $\mathbf{z}(O)$, this is a contradiction to the choice of O.

To simplify the notation, we set $d_i = p_{i+1} - p_i$, for $1 \le i < n$; rename the weights as $w_i := w_{i,i+1}$, again for $1 \le i < n$; observe that

$$v_1 = w_1 d_1,$$

 $v_i = |w_i d_i - w_{i-1} d_{i-1}|$ for $2 \le i \le n - 1,$
 $v_n = w_{n-1} d_{n-1}.$

For $i \in [2, n-1]$, we introduce the quantity

$$Q_{i} = d_{i}^{2}w_{i}^{2} + \sum_{j=1}^{i} v_{j}^{2}$$

$$= d_{i}^{2}w_{i}^{2} + d_{1}^{2}w_{1}^{2} + \sum_{j=2}^{i} (d_{j}w_{j} - d_{j-1}w_{j-1})^{2},$$

and note that $Q_{n-1} = \sum_{i=1}^{n} v_i^2 = Q$. Thus, our goal is to choose the n-1 non-negative weights w_1, \ldots, w_{n-1} such that Q_{n-1} is minimized, under the constraints

$$w_1 \geqslant 1,$$

 $w_j + w_{j+1} \geqslant 1$ for $2 \leqslant j \leqslant n - 2,$
 $w_{n-1} \geqslant 1.$

The quantity Q_i depends on w_1, w_2, \ldots, w_i . We concentrate on w_i and consider the function

$$w_i \mapsto Q_i(w_i) = \min_{w_1, \dots, w_{i-1}} Q_i(w_1, w_2, \dots, w_{i-1}, w_i),$$

where the minimum is taken over all choices of w_1, \ldots, w_{i-1} that respect the constraints $w_1 \ge 1$ and $w_j + w_{j+1} \ge 1$ for $2 \le j \le i-1$. The function $Q_i(w_i)$ is defined on $[0, \infty)$.

We denote the derivative of the function $w_i \mapsto Q_i(w_i)$ by R_i . We will see shortly that R_i is a continuous, piecewise linear function. Since R_i is not differentiable everywhere, we define $S_i(x)$ to be the right derivative of R_i , that is

$$S_i(x) = \lim_{y \to x^+} R_i'(y).$$

The following result discusses R_i and S_i . The shorthand

$$\xi_i := 2d_i d_{i+1}$$
, for $1 \le i < n-1$,

will be convenient in its proof and the rest of the paper.

Theorem 2.1. The function R_i is strictly increasing, continuous, and piecewise linear on the range $[0, \infty)$. We have $R_i(0) < 0$, $S_i(x) \ge (2 + 2/i)d_i^2$ for all $x \ge 0$, and $R_i(x) = (2 + 2/i)d_i^2x$ for sufficiently large x > 0.

Proof. We prove all claims by induction over i. The base case is i = 2. Observe that

$$Q_2 = v_1^2 + v_2^2 + d_2^2 w_2^2 = 2d_1^2 w_1^2 - 2d_1 d_2 w_1 w_2 + 2d_2^2 w_2^2.$$

The derivative with respect to w_1 is

$$\frac{\partial}{\partial w_1} Q_2 = 4d_1^2 w_1 - 2d_1 d_2 w_2,\tag{1}$$

which implies that Q_2 is minimized for $w_1 = \frac{d_2}{2d_1}w_2$. This choice is feasible (with respect to the constraint $w_1 \geqslant 1$) when $w_2 \geqslant \frac{2d_1}{d_2}$. If $w_2 < \frac{2d_1}{d_2}$, then $\frac{\partial}{\partial w_1}Q_2$ is positive for all values of $w_1 \geqslant 1$, so the minimum occurs at $w_1 = 1$. It follows that

$$Q_2(w_2) = \begin{cases} \frac{3}{2} d_2^2 w_2^2 & \text{for } w_2 \geqslant \frac{2d_1}{d_2}, \\ 2d_2^2 w_2^2 - \xi_1 w_2 + 2d_1^2 & \text{otherwise,} \end{cases}$$

and so we have

$$R_2(w_2) = \begin{cases} 3d_2^2 w_2 & \text{for } w_2 \geqslant \frac{2d_1}{d_2}, \\ 4d_2^2 w_2 - \xi_1 & \text{otherwise.} \end{cases}$$
 (2)

In other words, R_2 is piecewise linear and has a single breakpoint at $\frac{2d_1}{d_2}$. The function R_2 is continuous because $3d_2^2w_2 = 4d_2^2w_2 - \xi_1$ when $w_2 = \frac{2d_1}{d_2}$. We have $R_2(0) = -\xi_1 < 0$, $S_2(x) \geqslant 3d_2^2$ for all $x \geqslant 0$, and $R_2(x) = 3d_2^2x$ for $x \geqslant \frac{2d_1}{d_2}$. The fact that $S_2(x) \geqslant 3d_2^2 > 0$ makes R_2 strictly increasing.

Consider now $i \ge 2$, assume that R_i and S_i satisfy the induction hypothesis, and consider Q_{i+1} . By definition, we have

$$Q_{i+1} = Q_i - \xi_i w_i w_{i+1} + 2d_{i+1}^2 w_{i+1}^2.$$
(3)

For a given value of $w_{i+1} \ge 0$, we need to find the value of w_i that will minimize Q_{i+1} . The derivative is

$$\frac{\partial}{\partial w_i}Q_{i+1} = R_i(w_i) - \xi_i w_{i+1}.$$

The minimum thus occurs when $R_i(w_i) = \xi_i w_{i+1}$.

Since R_i is a strictly increasing continuous function with $R_i(0) < 0$ and $\lim_{x \to \infty} R_i(x) = \infty$, for any given $w_{i+1} \ge 0$, there exists a unique value $w_i = R_i^{-1}(\xi_i w_{i+1})$. However, we also need to satisfy the constraint $w_i + w_{i+1} \ge 1$.

We first show that R_{i+1} is continuous and piecewise linear, and that $R_{i+1}(0) < 0$. We will distinguish two cases, based on the value of $w_i^{\circ} := R_i^{-1}(0)$.

Case 1: $w_i^{\circ} \geqslant 1$. This means that $R_i^{-1}(\xi_i w_{i+1}) \geqslant 1$ for any $w_{i+1} \geqslant 0$, and so the constraint of $w_i + w_{i+1} \geqslant 1$ is satisfied for the optimal choice of $w_i = R_i^{-1}(\xi_i w_{i+1})$. It follows that

$$Q_{i+1}(w_{i+1}) = Q_i(R_i^{-1}(\xi_i w_{i+1})) - \xi_i w_{i+1} R_i^{-1}(\xi_i w_{i+1}) + 2d_{i+1}^2 w_{i+1}^2.$$

The derivative R_{i+1} is therefore

$$R_{i+1}(w_{i+1}) = R_i(R_i^{-1}(\xi_i w_{i+1})) \frac{\xi_i}{R_i'(R_i^{-1}(\xi_i w_{i+1}))}$$

$$-\xi_i R_i^{-1}(\xi_i w_{i+1})$$

$$-\xi_i w_{i+1} \frac{\xi_i}{R_i'(R_i^{-1}(\xi_i w_{i+1}))}$$

$$+4d_{i+1}^2 w_{i+1}$$

$$=4d_{i+1}^2 w_{i+1} - \xi_i R_i^{-1}(\xi_i w_{i+1}).$$

$$(4)$$

Since R_i is continuous and piecewise linear, so is R_i^{-1} , and therefore R_{i+1} is continuous and piecewise linear. We have $R_{i+1}(0) = -\xi_i w_i^{\circ} < 0$.

Case 2: $w_i^{\circ} < 1$. Consider the function $x \mapsto f(x) = x + R_i(x)/\xi_i$. Since R_i is continuous and strictly increasing by the inductive assumption, so is the function f. Observe that $f(w_i^{\circ}) = w_i^{\circ} < 1$. As $w_i^{\circ} < 1$, we have $R_i(1) > R_i(w_i^{\circ}) = 0$, which implies that f(1) > 1. Thus, there exists a unique value $w_i^{\bowtie} \in (w_i^{\circ}, 1)$ such that $f(w_i^{\bowtie}) = w_i^{\bowtie} + R_i(w_i^{\bowtie})/\xi_i = 1$.

For $w_{i+1} \ge 1 - w_i^{\bowtie} = R_i(w_i^{\bowtie})/\xi_i$, we have $R_i^{-1}(\xi_i w_{i+1}) \ge w_i^{\bowtie}$, and so $R_i^{-1}(\xi_i w_{i+1}) + w_{i+1} \ge 1$. This implies that the constraint $w_i + w_{i+1} \ge 1$ is satisfied when $Q_{i+1}(w_{i+1})$ is minimized for the optimal choice of $w_i = R_i^{-1}(\xi_i w_{i+1})$. So R_{i+1} is as in (4) in Case 1.

the optimal choice of $w_i = R_i^{-1}(\xi_i w_{i+1})$. So R_{i+1} is as in (4) in Case 1. When $w_{i+1} < 1 - w_i^{\bowtie}$, the constraint $w_i + w_{i+1} \ge 1$ implies that $w_i \ge 1 - w_{i+1} > w_i^{\bowtie}$. For any $w_i > w_i^{\bowtie}$ we have $\frac{\partial}{\partial w_i} Q_{i+1} = R_i(w_i) - \xi_i w_{i+1} > R_i(w_i^{\bowtie}) - \xi_i (1 - w_i^{\bowtie}) = 0$. So Q_{i+1} is increasing, and the minimal value is obtained for the smallest feasible choice of w_i , that is, for $w_i = 1 - w_{i+1}$. It follows that

$$Q_{i+1}(w_{i+1}) = Q_i(1 - w_{i+1}) - \xi_i w_{i+1}(1 - w_{i+1})$$

$$+ 2d_{i+1}^2 w_{i+1}^2$$

$$= Q_i(1 - w_{i+1}) - \xi_i w_{i+1}$$

$$+ (\xi_i + 2d_{i+1}^2) w_{i+1}^2,$$

and so the derivative R_{i+1} is

$$R_{i+1}(w_{i+1}) = -R_i(1 - w_{i+1}) + (2\xi_i + 4d_{i+1}^2)w_{i+1} - \xi_i.$$
(5)

Combining (4) and (5), we have

• If $w_{i+1} < 1 - w_i^{\bowtie}$, then

$$R_{i+1}(w_{i+1}) = -R_i(1 - w_{i+1}) + (2\xi_i + 4d_{i+1}^2)w_{i+1} - \xi_i.$$
(6)

• If $w_{i+1} \geqslant 1 - w_i^{\bowtie}$, then

$$R_{i+1}(w_{i+1}) = 4d_{i+1}^2 w_{i+1} - \xi_i R_i^{-1}(\xi_i w_{i+1}).$$
(7)

For $w_{i+1} = 1 - w_i^{\bowtie}$, we have $R_i(1 - w_{i+1}) = R_i(w_i^{\bowtie}) = \xi_i(1 - w_i^{\bowtie})$ and $R_i^{-1}(\xi_i w_{i+1}) = R_i^{-1}(\xi_i(1 - w_i^{\bowtie})) = w_i^{\bowtie}$, and so both expressions have the same value:

$$-R_{i}(1-w_{i+1}) + (2\xi_{i} + 4d_{i+1}^{2})w_{i+1} - \xi_{i}$$

$$= \xi_{i}w_{i}^{\bowtie} - \xi_{i} + 2\xi_{i} - 2\xi_{i}w_{i}^{\bowtie} + 4d_{i+1}^{2}(1-w_{i}^{\bowtie}) - \xi_{i}$$

$$= 4d_{i+1}^{2}(1-w_{i}^{\bowtie}) - \xi_{i}w_{i}^{\bowtie}$$

$$= 4d_{i+1}^{2}(1-w_{i}^{\bowtie}) - \xi_{i}R_{i}^{-1}(\xi_{i}w_{i+1}).$$

Since R_i is continuous and piecewise linear, this implies that R_{i+1} is continuous and piecewise linear. We have $R_{i+1}(0) = -R_i(1) - \xi_i$. Since $w_i^{\circ} < 1$, we have $R_i(1) > R_i(w_i^{\circ}) = 0$, and so $R_{i+1}(0) < 0$.

Next, we show that $S_{i+1}(x) \ge (2+2/i+1)d_{i+1}^2$ for all $x \ge 0$, which implies that R_{i+1} is strictly increasing. If $w_i^{\circ} < 1$ and $x < 1 - w_i^{\bowtie}$, then by (6),

$$S_{i+1}(x) = S_i(1-x) + 2\xi_i + 4d_{i+1}^2$$

$$> 4d_{i+1}^2$$

$$> (2+2/i+1)d_{i+1}^2.$$

If $w_i^{\circ} \ge 1$ or $x > 1 - w_i^{\bowtie}$, we have by (4)and (7) that $R_{i+1}(x) = 4d_{i+1}^2 x - \xi_i R_i^{-1}(\xi_i x)$. By the inductive assumption that $S_i(x) \ge (2 + 2/i)d_i^2$ for all $x \ge 0$, we get $\frac{\partial}{\partial x} R_i^{-1}(x) \le 1/((2 + 2/i)d_i^2)$. It follows that

$$S_{i+1}(x) \geqslant 4d_{i+1}^2 - \frac{(2d_i d_{i+1})^2}{(2+2/i)d_i^2} = \left(4 - \frac{4}{2+2/i}\right)d_{i+1}^2$$
$$= \left(4 - \frac{2i}{i+1}\right)d_{i+1}^2$$
$$= \left(2 + \frac{2}{i+1}\right)d_{i+1}^2.$$

This establishes the lower bound on $S_{i+1}(x)$.

Finally, by the inductive assumption, when x is large enough, we have $R_i^{-1}(x) = x/((2+2/i)d_i^2)$, and so

$$R_{i+1}(x) = 4d_{i+1}^2 x - \frac{(2d_i d_{i+1})^2}{(2+2/i)d_i^2} x$$
$$= \left(2 + \frac{2}{i+1}\right) d_{i+1}^2 x,$$

completing the inductive step and therefore the proof.

3 The algorithm

Our algorithm progressively constructs a representation of the functions $R_2, R_3, \ldots, R_{n-1}$. The function representation supports the following three operations:

- Op 1: given x, return $R_i(x)$;
- Op 2: given y, return $R_i^{-1}(y)$;

• Op 3: given ξ , return x^{\bowtie} such that $x^{\bowtie} + \frac{R_i(x^{\bowtie})}{\xi} = 1$.

The proof of Theorem 2.1 gives the relation between R_{i+1} and R_i . This will allow us to construct the functions one by one—we discuss the detailed implementation in Sections 3.1 and 3.2 below.

Once all functions R_2, \ldots, R_{n-1} are constructed, the optimal weights $w_1, w_2, \ldots, w_{n-1}$ are computed from the R_i 's as follows. Recall that $Q = Q_{n-1}$, so w_{n-1} is the value minimizing $Q_{n-1}(w_{n-1})$ under the constraint $w_{n-1} \ge 1$. If $R_{n-1}^{-1}(0) \ge 1$, then $R_{n-1}^{-1}(0)$ is the optimal value for w_{n-1} ; otherwise, we set w_{n-1} to 1.

To obtain w_{n-2} , recall from (3) that $Q = Q_{n-1} = Q_{n-2}(w_{n-2}) - \xi_{n-2}w_{n-2}w_{n-1} + 2d_{n-1}^2w_{n-1}^2$. Since we have already determined the correct value of w_{n-1} , it remains to choose w_{n-2} so that Q_{n-1} is minimized. Since

$$\frac{\partial}{\partial w_{n-2}} Q_{n-1} = R_{n-2}(w_{n-2}) - \xi_{n-2} w_{n-1},$$

 Q_{n-1} is minimized when $R_{n-2}(w_{n-2}) = \xi_{n-2}w_{n-1}$, and so $w_{n-2} = R_{n-2}^{-1}(\xi_{n-2}w_{n-1})$. In general, for $i \in [2, n-2]$, we can obtain w_i from w_{i+1} by observing that

$$Q_{n-1} = Q_i(w_i) - \xi_i w_i w_{i+1} + g(w_{i+1}, \dots, w_{n-1}),$$

where g is function that only depends on w_{i+1}, \ldots, w_{n-1} . Taking the derivative again, we have

$$\frac{\partial}{\partial w_i} Q_{n-1} = R_i(w_i) - \xi_i w_{i+1},$$

so choosing $w_i = R_i^{-1}(\xi_i w_{i+1})$ minimizes Q_{n-1} . To also satisfy the constraint $w_i + w_{i+1} \ge 1$, we need to choose $w_i = \max\{R_i^{-1}(\xi_i w_{i+1}), 1 - w_{i+1}\}$ for $i \in [2, n-2]$. Finally, from the discussion that immediately follows (1), we set $w_1 = \max\{\frac{d_2}{2d_1}w_2, 1\}$. To summarize, we have

$$w_{n-1} = \max\{R_{n-1}^{-1}(0), 1\},$$

$$w_i = \max\{R_i^{-1}(\xi_i w_{i+1}), 1 - w_{i+1}\}, \text{ for } i \in [2, n-2],$$

$$w_1 = \max\{\frac{d_2}{2d_1} w_2, 1\}.$$

It follows that we can obtain the optimal weights using a single Op 2 on each R_i .

3.1 Explicit representation of piecewise linear functions

Since R_i is a piecewise linear function, a natural representation is a sequence of linear functions, together with the sequence of breakpoints. Since R_i is strictly increasing, all three operations can then be implemented to run in time $O(\log k)$ using binary search, where k is the number of function pieces.

We construct the functions R_i , for i = 2, ..., n - 1, one by one.

The function R_2 consists of exactly two pieces. We construct it directly from d_1, d_2 , and ξ_1 using (2).

To construct R_{i+1} , we make use of the explicit representation of R_i that we have already computed. We first compute $w_i^{\circ} = R_i^{-1}(0)$ using Op 2 on R_i . If $w_i^{\circ} \ge 1$, then by (4) each piece of R_i , starting at the x-coordinate w_i° , gives rise to a linear piece of R_{i+1} , so the number of pieces of R_{i+1} is at most that of R_i .

If $w_i^{\circ} < 1$, then we compute w_i^{\bowtie} using Op 3 on R_i . The new function R_{i+1} has a breakpoint at $1 - w_i^{\bowtie}$ by (6) and (7). Its pieces for $x \ge 1 - w_i^{\bowtie}$ are computed from the pieces of R_i starting

at the x-coordinate w_i^{\bowtie} . Its pieces for $0 \leq x < 1 - w_i^{\bowtie}$ are computed from the pieces of R_i between the x-coordinates 1 and w_i^{\bowtie} . (Increasing w_{i+1} now corresponds to a decreasing w_i .)

Since a piece of R_i that covers x-coordinates in the range $[w_i^{\bowtie}, 1]$ gives rise to two pieces of R_{i+1} , the number of pieces of R_{i+1} can be twice the number of pieces of R_i . If this case occurs in every step of the construction, then function R_i will have 2^{i-1} pieces, leading to exponential time and space complexity.

It is hard to manually construct inputs that exhibit exponential growth in the number of pieces of R_i . We have therefore used the Z3 theorem prover [11] to try and satisfy the constraints under which R_{n-1} has 2^{n-2} pieces. For n = 10, which is the largest instance we have been able to solve using Z3, we obtain the following nine distances:

$$d_1$$
 d_2 d_3 d_4 d_5 d_6 d_7 d_8 d_9 11569 49184 65536 98304 109056 145408 146432 147456 32768

We have implemented the algorithm and verified using exact arithmetic that for these distances, the function R_i indeed has 2^{i-1} pieces, for $2 \le i \le 9$.

Based on this experiment, we find it unlikely that the explicit representation of the functions R_i will lead to a polynomial-time algorithm.

3.2 A quadratic time implementation

To guarantee a polynomial running time, we turn to an implicit representation of R_i . This representation is based on the fact that there is a linear relationship between points on the graphs of the functions R_i and R_{i+1} . Concretely, let $y_i = R_i(x_i)$, and $y_{i+1} = R_{i+1}(x_{i+1})$. Recall the following relation from (4) for the case of $w_i^{\circ} \ge 1$:

$$R_{i+1}(w_{i+1}) = 4d_{i+1}^2 w_{i+1} - \xi_i R_i^{-1}(\xi_i w_{i+1}).$$

We can express this relation as a system of two equations:

$$y_{i+1} = 4d_{i+1}^2 x_{i+1} - \xi_i x_i,$$

$$y_i = \xi_i x_{i+1}.$$

This can be rewritten as

$$y_{i+1} = 4d_{i+1}^2 y_i / \xi_i - \xi_i x_i,$$

$$x_{i+1} = y_i / \xi_i,$$

or in matrix notation

$$\begin{pmatrix} x_{i+1} \\ y_{i+1} \\ 1 \end{pmatrix} = M_{i+1} \cdot \begin{pmatrix} x_i \\ y_i \\ 1 \end{pmatrix}, \tag{8}$$

where

$$M_{i+1} = \begin{pmatrix} 0 & 1/\xi_i & 0 \\ -\xi_i & 4d_{i+1}^2/\xi_i & 0 \\ 0 & 0 & 1 \end{pmatrix}.$$

On the other hand, if $w_i^{\circ} < 1$, then R_{i+1} has a breakpoint at $1 - w_i^{\bowtie}$. The value w_i^{\bowtie} can be obtained by applying Op 3 to R_i . We compute the coordinates of this breakpoint: $(1 - w_i^{\bowtie}, R_{i+1}(1 - w_i^{\bowtie}))$. Note that $R_{i+1}(1 - w_i^{\bowtie}) = 4d_{i+1}^2(1 - w_i^{\bowtie}) - \xi_i R_i^{-1}(\xi_i(1 - w_i^{\bowtie}))$ which

can be computed by applying Op 2 to R_i . For $x_{i+1} > 1 - w_i^{\bowtie}$, the relationship between (x_i, y_i) and (x_{i+1}, y_{i+1}) is given by (8). For $0 \leq x_{i+1} < 1 - w_i^{\bowtie}$, recall from (5) that

$$R_{i+1}(w_{i+1}) = -R_i(1 - w_{i+1}) + (2\xi_i + 4d_{i+1}^2)w_{i+1} - \xi_i.$$

We again rewrite this as

$$y_{i+1} = -y_i + (2\xi_i + 4d_{i+1}^2)x_{i+1} - \xi_i,$$

$$x_i = 1 - x_{i+1},$$

which gives

$$y_{i+1} = -y_i + (2\xi_i + 4d_{i+1}^2)(1 - x_i) - \xi_i,$$

$$x_{i+1} = 1 - x_i,$$

or in matrix notation:

$$\begin{pmatrix} x_{i+1} \\ y_{i+1} \\ 1 \end{pmatrix} = L_{i+1} \cdot \begin{pmatrix} x_i \\ y_i \\ 1 \end{pmatrix},$$

where

$$L_{i+1} = \begin{pmatrix} -1 & 0 & 1\\ -2\xi_i - 4d_{i+1}^2 & -1 & \xi_i + 4d_{i+1}^2\\ 0 & 0 & 1 \end{pmatrix}.$$

We will make use of this relationship to store the function R_{i+1} , for $i \ge 2$, by storing the breakpoint $(x_{i+1}^*, y_{i+1}^*) = (1 - w_i^{\bowtie}, R_{i+1}(1 - w_i^{\bowtie}))$ as well as the two matrices L_{i+1} and M_{i+1} . The function R_2 is simply stored explicitly.

We now discuss how the three operations Op 1, Op 2, and Op 3 are implemented on this representation of a function R_i . For an operation on R_i , we progressively build transformation matrices $T_i^i, T_{i-1}^i, T_{i-2}^i, \ldots, T_3^i, T_2^i$ such that $(x_i, y_i, 1) = T_j^i \times (x_j, y_j, 1)$ for every $2 \leq j \leq i$ in a neighborhood of the query. Once we obtain T_2^i , we use our explicit representation of R_2 to express y_i as a linear function of x_i in a neighborhood of the query, which then allows us to answer the query.

The first matrix T_i^i is the identity matrix. We obtain T_j^i from T_{j+1}^i , for $j \in [2, i-1]$, as follows: If R_{j+1} has no breakpoint, then $T_j^i = T_{j+1}^i \cdot M_{j+1}$. If R_{j+1} has a breakpoint (x_{j+1}^*, y_{j+1}^*) , then either $T_j^i = T_{j+1}^i \cdot M_{j+1}$ or $T_j^i = T_{j+1}^i \cdot L_{j+1}$, depending on which side of the breakpoint applies to the answer of the query. We can decide this by comparing $(x', y', 1)^t = T_{j+1}^i \cdot (x_{j+1}^*, y_{j+1}^*, 1)^t$ with the query. More precisely, for Op 1 we compare the input x with x', for Op 2 we compare the input y with y', and for Op 3 we compute $x' + y'/\xi$ and compare with 1.

Assuming the Real-RAM model common in computational geometry, where arithmetic on real numbers takes constant time, it follows that the implicit representation of R_i supports all three operations on R_i in time O(i).

Finally, we discuss how the representation of all functions R_i is obtained. We again build it iteratively, constructing $R_2, R_3, R_4, \ldots, R_{n-1}$, one-by-one in this order. The first function R_2 is stored explicitly. To construct the implicit representation of R_{i+1} , we only need to perform on our representation of R_i (that we already computed) one Op 2 to get $w_i^{\circ} = R_i^{-1}(0)$, one Op 3 to get w_i^{\bowtie} , and one Op 2 to get $R_i^{-1}(\xi_i(1-w_i^{\bowtie}))$, which allows us to determine the breakpoint $(1-w_i^{\bowtie}, R_{i+1}(1-w_i^{\bowtie}))$, if there is one (when $w_i^{\circ} < 1$). The two matrices L_{i+1} and R_{i+1} can be computed in O(1) time.

Since operations on R_i take time O(i), the total time to construct R_{n-1} is $O(n^2)$.

Theorem 3.1. Given n points on a line, we can compute an optimal set of weights for minimizing the quality measure Q in $O(n^2)$ time under the Real-RAM model.

4 Conclusion

We do not have a polynomial time bound on the running time using the explicit representation of the functions R_i , and our experiments with the Z3 solver suggest that the complexity of R_i may indeed increase exponentially with i. It would be interesting to determine whether one can construct such a worst-case example for any n.

It would also be nice to obtain an algorithm for higher dimensions that is not based on a quadratic programming solver.

In two dimensions, we have conducted some experiments that indicate that the Delaunay triangulation of the point set contains a well-fitting graph. If we choose the graph edges only from the Delaunay edges and compute the optimal edge weights, the resulting quality measure is very close to the best quality measure in the unrestricted case. It is conceivable that one can obtain a provably good approximation from the Delaunay triangulation.

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