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Sublinear time width-bounded separators and their application to the protein side-chain packing problem

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Abstract Given $d > 2$ and a set of n grid points Q in $\Re^d$, we design a randomized algorithm that finds a w-wide separator, which is determined by a hyper-plane, in $O(n^{\frac{2}{d}} \log n)$ sublinear time such that Q has at most $(\frac{d}{d+1} + o(1))n$ points on either side of the hyper-plane, and at most $c_d w n^{\frac{d-1}{d}}$ points within $\frac{w}{2}$ distance to the hyper-plane, where c_d is a constant for fixed d. In particular, $c_3 = 1.209$. To our best knowledge, this is the first sublinear time algorithm for finding geometric separators. Our 3D separator is applied to derive an algorithm for the protein side-chain packing problem, which improves and simplifies the previous algorithm of Xu (Research in computational molecular biology, 9th annual international conference, pp. 408–422, 2005).

Keywords Sublinear time algorithm · Width-bounded separator · Random sampling

1 Introduction

The work in this paper aims for efficient identification of width-bounded separators for a given set of points in the d-dimensional Euclidean space and their applications to intractable practical problems. Intuitively, a width-bounded separator utilizes a simple structured hyper-plane to divide the set into two *"balanced"* subsets, while at

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the same time maintaining a *"low density"* of the set within a given distance to the hyper-plane. This new notion of separators was initially introduced by Fu (2006), and it was shown that these separators are very suitable in solving a number of distance-bounded geometric problems such as the protein folding problem in the HP model in (Fu and Wang 2004) and some other intractable problems in (Fu 2006; Chen et al. 2006). The main contributions of this paper are summarized as follows.

In Sect. 5, we present an $O(n^{\frac{2}{d}}\log n)$ sublinear time randomized algorithm for finding a width-bounded separator in the dimensional Euclidean space $\Re^d$ for $d > 2$. To our best knowledge, this is the first sublinear time algorithm for finding geometric separators. For many other geometric problems, a higher dimension brings higher computational complexity. However, it is interesting to notice that the exponent of our algorithm's computational complexity is reversely proportional to the dimension of the space.

In Sect. 6, we exhibit an application of our sublinear time separator to the protein side-chain packing problem. One of the most fundamental problems in the molecular biology is to predict a protein's 3D structure when given its 1D amino-acid sequence. Although much effort has been made for decades, this problem remains unsolved. An important component of the general protein structure prediction problem is the protein side-chain packing problem. It determines the side-chain positions onto the fixed backbone (Ponter and Richards 1987). This problem has been proved to be NP-complete (Akutsu 1997). Recently, a $r_{\text{ave}}^{O(n^{\frac{2}{3}}\log n)}$ time algorithm was shown by Xu (2005), where r_{ave} is the average number of side-chain rotamers in a protein. We apply width-bounded separators to the protein side-chain packing problem. The length of side-chain of each amino acid is small compared to the size of one protein. Two side-chains in a protein molecular do not interact with each other if their distance is slightly larger than the sum of their lengths according to models used in (e.g. Canutescu et al. 2003; Chazelle et al. 2004; Xu 2005). Using our width-bounded separators, we obtain an algorithm with computational time $r_{\max}^{O(n^{\frac{2}{3}})}$, where $r_{\max}$ is the maximal number of side-chain rotamers among a protein. Since the number of rotamers is usually small, we assume both r_{ave} and $r_{\max}$ are constants, hence our new algorithm has a better complexity bound.

2 The related work

There have been extensive efforts on finding separators due to their critical roles in many issues of algorithm design and analysis. Because of space limit we cannot give a comprehensive review of the related work but list some representative results in this area. Lipton and Tarjan (1979) proved that every n vertex planar graph has at most $\sqrt{8n}$ vertices whose removal separates the graph into two disconnected parts of size at most $\frac{2}{3}n$. Their $\frac{2}{3}$-separator has been improved by a series of papers (Djidjev 1982; Gazit 1986; Alon and Thomas 1990; Djidjev and Venkatesan 1997) with the best record $1.97\sqrt{n}$ by Djidjev and Venkatesan (1997). Spielman and Teng (1996) showed a $\frac{3}{4}$-separator with size $1.82\sqrt{n}$ for planar graphs. Separators for more general graphs were derived in (Gilbert et al. 1984; Alon et al. 1990; Plotkin et al. 1990). A planar graph can be induced by a set of non-overlapping discs on the plane such that every vertex corresponds to a disc center and each edge corresponds to a tangent relationship between two discs. The separator developed by Miller et al. (1991) is a generalization of planar graph separators to the d-dimensional Euclidean space. Some $O(\sqrt{k \cdot n})$ size separators for k-thick systems and the related algorithms were derived in (Miller and Thurston 1990; Miller and Vavasis 1991; Miller et al. 1991; Smith and Wormald 1998).

The study of width-bounded separators were initiated by Fu (2006) and has yielded successful applications in (Fu and Wang 2004; Chen et al. 2006). Our width-bounded geometric separator has some interesting advantages over previous geometric separators such as the popular geometric separator by Miller et al. (1991). First, the width-bounded separator has a simple linear structure as the separator is determined by a hyper-plane and a width parameter w, but Miller et al.'s separator is a sphere, which can be also found in linear time (Eppstein et al. 1995). The linear structure is very crucial for us in deriving sublinear time algorithm in this paper. Second. the width-bounded separator has a smaller constant in its size upper bound factor than other separators. The constant factor was not clearly given in Miller et al.'s separator. Furthermore, their separator only has a balance condition bounded by $\frac{d+1}{d+2}n$ due to their transformation to a higher dimension, while the balance condition of the width-bounded separator is bounded by $\frac{d}{d+1}n$. Third, the width-bounded separator can be used to deal with an arbitrary set of points via using a set of grid points and weights to characterize the distribution of points from the input set.

3 Notations, definitions, and width-bounded separators

For any finite set A, $|A|$ denotes the number of elements in A. Let $\Re$ be the set of all real numbers. For two points p_1, p_2 in the d-dimensional Euclidean space $\Re^d$, $\mathrm{dist}(p_1, p_2)$ is the Euclidean distance between p_1 and p_2. For a set $A \subseteq \Re^d$, $\mathrm{dist}(p_1, A) = \min_{q \in A} \mathrm{dist}(p_1, q)$. The *diameter* of any $P \subseteq \Re^d$ is $\max_{p_1, p_2 \in P} \mathrm{dist}(p_1, p_2)$. For $a > 0$ and a set A of points in $\Re^d$, if the distance between every two points in A is at least a, then A is called *a-separated*. For $\epsilon > 0$ and a set Q of points in $\Re^d$, an *ϵ-sketch* of Q is another set P of points in $\Re^d$ such that each point in Q has a distance $\le \epsilon$ to some point in P. We say P is a sketch of Q if P is an ϵ-sketch of Q for some constant $\epsilon > 0$ (that does not necessarily depend on the size of Q). A sketch set is usually a 1-separated set such as a grid point set. A weight function $w : P \to [0, \infty)$ is often used to measure the density of Q near each point in P. Let $f : \Re^d \to \Re$ be a smooth function. Its *surface* is the set $L(f) = \{v \in \Re^d | f(v) = 0\}$. A *hyper-plane* in $\Re^d$ through a fixed point $p_0 \in \Re^d$ is defined by the equation $(p - p_0) \cdot v = 0$, where v is a normal vector of the plane and "$\cdot$" is the usual vector inner product. A hyper-plane in $\Re^d$ is determined by $L(f)$ for some linear function $f : \Re^d \to \Re$.

Definition 1 Given any $Q \subseteq \Re^d$ with a sketch $P \subseteq \Re^d$, a constant $a > 0$, and a weight function $w : P \to [0, \infty)$, an *a-wide-separator* is determined by the surface $L(f)$ for some linear function $f : \Re^d \to \Re$. The separator has two measurements for its quality of separation: (1) $\mathrm{balance}(L(f), Q) = \frac{\max(|Q_1|, |Q_2|)}{|Q|}$, where $Q_1 =$

$\{q \in Q | f(q) < 0\}$ and $Q_2 = \{q \in Q | f(q) > 0\}$; and (2) density$(L(f), P, \frac{a}{2}, w)$, where in general density$(A, P, x, w) = \sum_{p \in P, \mathrm{dist}(p,A) \le x} w(p)$ for any $A \subseteq \Re^d$ and $x > 0$. When f is fixed or no confusion arises, we use balance(L, Q) and density$(L, P, \frac{a}{2}, w)$ to stand for balance$(L(f), Q)$ and density$(L(f), P, \frac{a}{2}, w)$, respectively.

Definition 2 A (b, c)-*partition* of $\Re^d$ divides the space into a disjoint union of regions $P_1, P_2, \dots$, such that each P_i, called a *regular region*, has a volume of b and a diameter $\le c$. A (b, c)-*regular point set* A is a set of points in $\Re^d$ with a (b, c)-partition $P_1, P_2, \dots$, such that each P_i contains at most one point from A. For two regions A and B, if $A \subseteq B$ ($A \cap B \neq \emptyset$), we say B *contains* (*intersects* resp.) A.

For the case $b = 1$ and $c = \sqrt{2}$, the plane can be partitioned into 1×1 squares, where each 1×1-square is a region $\{(x, y) | i \le x < x + 1 \text{ and } j \le y < j + 1\}$ for some grid point (i, j) with two integers i and j. All grid points are $(1, \sqrt{2})$-regular points.

Let $B_d(r, o)$ be the d-dimensional ball of radius r at center o. Its volume is $V_d(r) = \frac{2^{(d+1)/2}\pi^{(d-1)/2}}{1\cdot 3 \cdots (d-2)\cdot d} r^d$ if d is odd, or $\frac{2^{d/2}\pi^{d/2}}{2\cdot 4 \cdots (d-2)\cdot d} r^d$ otherwise (see Trench 1978). Let $V_d(r) = v_d \cdot r^d$, where v_d is a constant for the fixed dimension d. In particular, $v_1 = 2$, $v_2 = \pi$ and $v_3 = \frac{4\pi}{3}$. We will use the following well-known fact that can be easily derived from Helly Theorem (see Pach and Agarwal 1995).

Lemma 3 *For an n-element set P in the d-dimensional space $\Re^d$, there is a point q with the property that any half-space that does not contain q, covers at most $\frac{d}{d+1}n$ elements of P. (Such a point q is called a centerpoint of P.)*

Definition 4 Let $a > 0$, p and o be two points in $\Re^d$. Define $Pr_d(a, p_0, p)$ to be the probability that the point p has $\le a$ perpendicular distance to a random hyper-plane L through the point p_0. Define function $f_{a,p,o}(L) = 1$ if p has a distance $\le a$ to the hyper-plane L through o, or 0 otherwise. The expectation of function $f_{a,p,o}(L)$ is $E(f_{a,p,o}(L)) = Pr_d(a, o, p)$. Assume $P = \{p_1, p_2, \dots, p_n\}$ is a set of n points in $\Re^d$ and each p_i has weight $w(p_i) \ge 0$. Define function $F_{a,P,o}(L) = \sum_{p \in P} w(p) f_{a,p,o}(L)$.

We give an upper bound for the expectation $E(F_{a,P,o}(L))$ for $F_{a,P,o}(L)$ in the lemma below.

Lemma 5 (Fu 2006) *Let $d \ge 2$. Let o be a point in $\Re^d$, $a, b, c > 0$ be constants and $\epsilon, \delta > 0$ be small constants. Assume that $P_1, P_2, \dots$, form a (b, c)-partition for $\Re^d$, and the weights $w_1 > \cdots > w_k > 0$ satisfy $k \cdot \max_{i=1}^k \{w_i\} = O(n^\epsilon)$. Let P be a set of n weighted (b, c)-regular points in a d-dimensional plane with $w(p) \in \{w_1, \dots, w_k\}$ for each $p \in P$. Let n_j be the number of points $p \in P$ with $w(p) = w_j$ for $j = 1, \dots, k$. We have $E(F_{a,P,o}(L)) \le (k_d \cdot (\frac{1}{b})^{\frac{1}{d}} + \delta) \cdot a \cdot \sum_{j=1}^k w_j \cdot n_j^{\frac{d-1}{d}} + O(n^{\frac{d-2}{d}+\epsilon})$, where $k_d = \frac{d \cdot h_d}{d-1} \cdot v_d^{\frac{1}{d}}$ with $h_d = \frac{2(d-1)v_{d-1}}{d \cdot v_d}$. In particular, $k_2 = \frac{4}{\sqrt{\pi}}$ and $k_3 = \frac{3}{2}(\frac{4\pi}{3})^{\frac{1}{3}}$.*

Definition 6 Let $a_1, \ldots, a_d > 0$ be positive constants. A $(a_1, \ldots, a_d)$*-grid regular partition* divides $\Re^d$ into a disjoint union of $a_1 \times \cdots \times a_d$ rectangular regions. A $(a_1, \ldots, a_d)$*-grid (regular) point* is a corner point of a rectangular region. Under certain translation and rotation, each $(a_1, \ldots, a_d)$-grid regular point is represented as $(a_1 t_1, \ldots, a_d t_d)$ for some integers $t_1, \ldots, t_d$. For a point $p = (x_1, \ldots, x_d) \in \Re^d$, if $x_1, \ldots, x_d$ are all integers, then p is simply called a *grid point* (it is a $(1, \ldots, 1)$*-grid regular point*). For each point q and a hyper-plane L in $\Re^d$, define $sd(q, L)$ to be the signed distance from q to L, which is $sd(q, L) = (q - q_0) \cdot v_L$, where q_0 is a point on L, and v_L is the normal vector of the plane L with the first nonzero coordinate to be positive.

Definition 7 For a hyper-plane L in $\Re^d$, if L is through a point q_0 and has the normal vector v, then it has linear equation $(u - q_0) \cdot v = 0$. If $q \in \Re^d$ and $d = sd(q, L)$, then the hyper-plane L' through q and parallel to L has equation $(u - (q_0 + dv)) \cdot v = 0$. We use $L(d)$ to represent such a hyper-plane L'.

For an interval $I \subseteq R$, $\|I\|$ is the length of I. For example, $\|[a, b)\| = b - a$. We often use $Pr(E)$ to represent the probability of an event E. For a real number x, $\lfloor x \rfloor$ is the largest integer $y \le x$, and $\lceil x \rceil$ are the least integer $z \ge x$. For an interval $[a, b] \subseteq R$, define $center([a, b])$ to be $\frac{a+b}{2}$.

Lemma 8 *Let P be a finite set of points in $\Re^d$ and q_0 be a fixed point in $\Re^d$. Then for a random hyper-plane L through q_0, $Pr(sd(p_1, L) = sd(p_2, L)$ for $p_1, p_2 \in P$ with $p_1 \ne p_2) = 0$.*

Proof A random hyper-plane L through a fixed point q_0 can be characterized by the equation $(q - q_0) \cdot v_L = 0$, where v_L is the normal vector of L. Each unit vector can be considered as a point of the surface of the unit ball $B_d(1, o)$, where $o = (0, \ldots, 0)$ is the origin point. The surface area size of $B_d(r, o)$ can be computed by the derivative $\frac{\partial V_d(r)}{\partial r} = d v_d r^{d-1}$. The surface area of $B_d(r, o)$ is of dimension $d - 1$.

For two fixed points p_1 and p_2, if $sd(p_1, L) = sd(p_2, L)$, then $(p_1 - q_0) \cdot v_L = (p_2 - q_0) \cdot v_L$. It implies that $(p_1 - p_2) \cdot v_L = 0$. Consider the sub-area on the surface of $B(1, o)$: $\{v | (p_1 - p_2) \cdot v = 0 \text{ and } v \cdot v = 1\}$, which is the intersection between a plane $(p_1 - p_2) \cdot v = 0$ and $B_d(1, o)$, and is of dimension $d - 2$. It is easy to see that it has area size 0 in the d-dimensional space. The lemma follows since the union of a finite number of areas of area size 0 still has 0 area size. □

4 An overview of our techniques

Given any set Q of points in $\Re^d$ with a sketch P, the idea of our techniques for finding an a-width-bound separator is to transform the problem from the d-dimensional space to the 1-dimensional space. By Lemma 3 and Lemma 5, we can see the existence of a hyper-plane that satisfies both the balance and the density conditions. Lemma 5 gives an upper bound on the expectation of $F_{a,P,o}(L)$. By Markov's inequality, $Pr(F_{a,P,o}(L) > (1 + \alpha)E(F_{a,P,o}(L))) \le \frac{1}{1+\alpha}$. Thus, with probability $\ge$

$1 - \frac{1}{1+\alpha} = \frac{\alpha}{1+\alpha}$, a random hyper-plane L has that $F_{a,P,o}(L) \le (1+\alpha)E(F_{a,P,o}(L))$. The chance is amplified if we repeat the random selection of the hyper-plane L multiple times.

Let $n_P = |P|$ and $n_Q = |Q|$. After a hyper-plane L is fixed, we try to find another hyper-plane L' that is parallel to L. We want L' to guarantee the desired balance and density conditions. To do so, we compute signed distances for all the points in Q and P to the hyper-plane L. Those signed distances are all different for the points in Q and, respectively, for the points in P (by Lemma 8). These signed distances are all in the 1-dimensional real axis, and finding L' can be done via finding a "right position" among these distances, hence this transforms the problem from the d-dimensional space into to the 1-dimensional space as follows: Find the interval $[D_{1,d+1}, D_{d,d+1}]$ such that both the left side $(-\infty, D_{1,d+1})$ and the right side $(D_{d,d+1}, +\infty)$ have roughly $\frac{n_Q}{d+1}$ signed distances from Q to L. So, every hyper-plane L' (parallel to L) with a signed distance in $[D_{1,d+1}, D_{d,d+1}]$ to L guarantees the balance condition. For an interval I, we compute its weight as the sum of the weights of the points of P with their signed distances in I. We then look for an interval $[x-a, x+a]$ that has $x \in [D_{1,d+1}, D_{d,d+1}]$ and the smallest weight. Finally, we let L' be a hyper-plane with a signed distance x to L. The balance boundaries $D_{1,d+1}$ and $D_{d,d+1}$ can be detected by sampling a small number of points from Q. Using the Chernoff bound, we have a high probability that there is a small fraction difference from the exact boundaries. Similarly, the desired interval can be also detected by sampling a small number of points from P.

5 The sublinear time randomized algorithm

We use the following well-known Chernoff bound (see Motwani and Raghavan 2000 for a proof) and simpled version in Lemma 10.

Theorem 9 (Motwani and Raghavan 2000) *Let $X_1, \ldots, X_n$ be n independent random* $0, 1$ *variables, where X_i takes* 1 *with probability p_i. Let $X = \sum_{i=1}^n X_i$, and $\mu = E[X]$. Then for any $\delta > 0$,* (1) *$Pr(X < (1-\delta)\mu) < e^{-\frac{1}{2}\mu\delta^2}$, and* (2) *$Pr(X > (1+\delta)\mu) < [\frac{e^\delta}{(1+\delta)^{(1+\delta)}}]^\mu$.*

Lemma 10 (Li et al. 2002) *Let $X_1, \ldots, X_n$ be n independent random* $0, 1$ *variables, where X_i takes* 1 *with probability p. Let $X = \sum_{i=1}^n X_i$. Then for any $\frac{1}{3} > \epsilon > 0$,* (1) *$Pr(X < pn - \epsilon n) < e^{-\frac{1}{2}n\epsilon^2}$, and* (2) *$Pr(X > pn + \epsilon n) < e^{-\frac{1}{3}n\epsilon^2}$.*

Proof For $X = \sum_{i=1}^n$, $\mu = E(X) = \sum_{i=1}^n E(X_i) = pn$. Let $\delta = \frac{\epsilon}{p}$. (1) follows from Theorem 9. By Taylor theorem, $\ln(1+\epsilon) \ge \epsilon - \frac{\epsilon^2}{2}$. We have that $(1+\frac{1}{\epsilon})\ln(1+\epsilon) \ge (1+\frac{1}{\epsilon})(\epsilon - \frac{\epsilon^2}{2}) = 1 + \frac{\epsilon}{2} - \frac{\epsilon^2}{2} > 1 + \frac{\epsilon}{3}$. Thus, $(1+\epsilon)^{\frac{1}{\epsilon}} > e^{1+\frac{\epsilon}{3}}$ that implies $\frac{e}{(1+\epsilon)^{(1+\frac{1}{\epsilon})}} < e^{-\frac{\epsilon}{3}}$. Since $pn + \epsilon n = (1+\delta)\mu$ and the function $(1+y)^{1+\frac{1}{y}}$ is increasing for $y > 0$, $Pr(X > pn + \epsilon n) = Pr(X > (1+\delta)\mu) < [\frac{e^{\frac{\epsilon}{p}}}{(1+\frac{\epsilon}{p})^{(1+\frac{\epsilon}{p})}}]^{pn} = [\frac{e}{(1+\frac{\epsilon}{p})^{(1+\frac{p}{\epsilon})}}]^{\epsilon n} \le [\frac{e}{(1+\epsilon)^{(1+\frac{1}{\epsilon})}}]^{\epsilon n} \le e^{-\frac{\epsilon^2 n}{3}}$. Thus (2) is proved. □

Theorem 11 *Let $d \geq 2$ be the fixed dimension number and v be a positive parameter. Let $a, b, c > 0$ be constants and $\delta, s_1, s_2 > 0$ be small constants. Let Q be another set of n_Q points in $\Re^d$, and P be a set of n_P (b, c)-regular points, which form a sketch for Q. Let $w_1 > w_2 > \cdots > w_k > 0$ be positive weights with $k \cdot w_1 = O(n_P^{s_1})$, $\frac{w_1}{w_k} = o(n_P^{\frac{1}{d}})$, $\frac{k}{w_k} = O(n_P^{s_2})$, and w be a mapping from P to $\{w_1, \ldots, w_k\}$. There exists an $O(v^2 \cdot (n_P^{\frac{2}{d}+2(s_1+s_2)} \cdot \log n_P + \log n_Q))$ time randomized algorithm to find a hyper plane M with probability $\geq 1 - \frac{1}{2^v}$ such that (1) each half space has $\leq (\frac{d}{d+1} + \delta)n_Q$ points from Q, and (2) $\sum_{p \in P \text{ and } \mathrm{dist}(p,M) \leq a} w(p) \leq (k_d \cdot b^{\frac{-1}{d}} + \delta) \cdot a \cdot \sum_{j=1}^{k} w_j n_j^{\frac{d-1}{d}} + O(n_P^{\frac{d-2}{d}+s_1})$ for all large n_P, where $n_j \geq 1$ is the number of points $p \in P$ with $w(p) = w_j$ $(j = 1, \ldots, k)$.*

Before proving Theorem 11, we give the following corollary, which is easier to understand than Theorem 11, but is not as general as Theorem 11. Corollary 12 will be applied to the protein side chain packing problem in Sect. 6.

Corollary 12 *Let $d \geq 2$ be the dimension number and the parameter $v > 0$. Let $a > 0$ be a constant and $\delta > 0$ be a small constant. There exists a randomized $O(v^2 n^{\frac{2}{d}} \log n)$ time such that given a set Q of n grid points in $\Re^d$, the algorithm finds a hyper-plane L with probability at least $1 - \frac{1}{2^v}$ such that each side of L has at most $(\frac{d}{d+1} + \delta)n$ points of Q, and the number of points of Q with distance $\leq a$ to L is $\leq (k_d + \delta)an^{\frac{d-1}{d}} + O(n^{\frac{d-2}{d}})$.*

Proof We convert the conditions of this corollary into the conditions of Theorem 11 so that we can use Theorem 11. The space $\Re^d$ is partitioned into $1 \times 1 \cdots \times 1$ unit cubes with grid points in the corners of all unit cubes. Clearly, the distance of two points in the same unit cube is at most $\sqrt{d}$. Let the two sets P and Q be the same. The weights of all points of P are equal to 1. This makes that $s_1 = s_2 = 0$, $b = 1$, $c = \sqrt{d}$, and $k = 1$. Then the corollary follows from Theorem 11. □

Proof of Theorem 11 We use two phases to find the separator hyper-plane. The first phase determines the orientation of the hyper-plane by selecting a random hyper-plane, and finds the region of the separator hyper-plane for a balanced partition. The second phase finds the position of the separator plane with a small sum of weights for the points of the set P close to it. Without loss of generality, we assume that $0 < \delta < 1$. Since $n_j \geq 1$ $(j = 1, \ldots, k)$ and $\sum_{j=1}^{k} n_j = n_P$, we have $k \leq n_P$. Select constant $c_0 > 0$ and let $\delta_1 = c_0\delta$ so that

$$(k_d \cdot b^{\frac{-1}{d}} + 3\delta_1)(1 + \delta_1)^2 \leq \left(k_d \cdot b^{\frac{-1}{d}} + \frac{\delta}{2}\right). \tag{1}$$

Let

$$a_1 = a(1 + \delta_1) \quad \text{and} \quad \alpha = \delta_1. \tag{2}$$

With the conditions of the theorem, let c_1 be a constant such that

$$k \cdot w_1 \le c_1 n_P^{s_1} \quad \text{and} \quad \frac{k}{w_k} \le c_1 n_P^{s_2}. \tag{3}$$

Let o be the center point from Lemma 3 (our algorithm does not need to find such a center point o, but will use its existence). By Lemma 5,

$$E(F_{a_1,P,o}) \le (k_d \cdot b^{\frac{-1}{d}} + \delta_1) \cdot a_1 \cdot \sum_{j=1}^{k} w_j n_j^{\frac{d-1}{d}} + O(n_P^{\frac{d-2}{d}+s_1}). \tag{4}$$

By the well known Markov inequality and (4),

$$Pr(F_{a_1,P,o}(L) \ge (1+\alpha)E(F_{a_1,P,o})) \le \frac{1}{1+\alpha}. \tag{5}$$

This tells us that for a random hyper-plane L, the probability is at least $1 - \frac{1}{1+\alpha}$ such that there exists a separator hyper-plane L' (it may be through o) that satisfies the conditions of the theorem and is parallel to L. The hyper-plane L' is determined by the signed distance from a point in L' to the hyper-plane L since L' and L are parallel. We assign the values to some parameters:

$$r = c_4 v, \text{ where } c_4 \text{ is a constant to be fixed later}, \tag{6}$$

$$\delta_2 = \frac{\delta_1 \cdot a}{c_1}, \tag{7}$$

$$\epsilon = \frac{\delta_2}{3c_1 n_P^{\frac{1}{d}+s_1+s_2}}, \tag{8}$$

$$\epsilon_0 = \frac{\delta}{7}, \tag{9}$$

$$\epsilon_1 = 5\epsilon_0, \tag{10}$$

$$m_1 = \frac{3(\ln 100 + r + \log n_Q)}{\epsilon_0^2}, \tag{11}$$

$$m_2 = \frac{3(\ln 100 + 2\log n_P + r)}{\epsilon^2}. \tag{12}$$

Algorithm: find separator in d-dimension
Input:
P (a set of weighted (b, c)-regular points in $\Re^d$),
Q (a set of points in $\Re^d$),
$n_P = |P|$ (the number of elements of set P), and
$n_Q = |Q|$ (the number of elements of set Q).
Phase 1:
begin
Select a fixed point $o^* \in \Re^d$ and a random hyper-plane L through o^*.

Randomly select a list m_1 points $Q' = \langle q_1, \ldots, q_{m_1} \rangle$ from Q.
For each $q_j \in Q'$, compute its signed distance to L $d_{q_i} = sd(q_i, L)$.
Find the $\lfloor (\frac{1}{d+1} - \epsilon_1) m_1 \rfloor$-th least point $D^*_{1,d+1} = d_{q_1^*}$ among $d_{q_1}, \ldots, d_{q_{m_1}}$.
Find the $\lceil (\frac{d}{d+1} + \epsilon_1) m_1 \rceil$-th least point $D^*_{d,d+1} = d_{q_2^*}$ among $d_{q_1}, \ldots, d_{q_{m_1}}$.
Randomly select a list of m_2 points $P' = \langle p_1, \ldots, p_{m_2} \rangle$ from P.
For each $p_i \in P'$, compute $d_{p_i} = sd(p_i, L)$.
end (Phase 1)
Phase 2:
begin
if $(|D^*_{1,d+1} - D^*_{d,d+1}| \geq 3an_P^{\frac{2}{d}})$ then (Case 1)
begin
Let $u = n_P^{\frac{2}{d}}$.
Partition $[D^*_{1,d+1}, D^*_{d,d+1}]$ into equal length intervals $[l_1, l_2), [l_2, l_3), \ldots, [l_{u-1}, l_u), [l_u, l_{u+1}]$.
Compute $W(P', L, [l_i, l_{i+1}])$ for $i = 1, \ldots, u$.
Select $[l_i, l_{i+1}]$ with the minimal sum of weights $W(P', L, [l_i, l_{i+1}])$.
end (Case 1)
if $(|D^*_{1,d+1} - D^*_{d,d+1}| \leq \delta_1 a)$ then (Case 2: Subcase 2.1)
begin
Select $J = [D^*_{1,d+1} - a, D^*_{1,d+1} + a]$.
end (Case 2: Subcase 2.1)
if $(\delta_1 a < |D^*_{1,d+1} - D^*_{d,d+1}| < 3an_P)$ then (Case 2: Subcase 2.2)
begin
Select the least integer $v \geq 2$ such that $\frac{|D^*_{d,d+1} - D^*_{1,d+1}| + 2a}{v} \leq \frac{\delta_1 a}{3}$.
Let $s = \frac{|D^*_{d,d+1} - D^*_{1,d+1}| + 2a}{v}$.
Partition $[D^*_{1,d+1} - a, D^*_{d,d+1} + a]$ into $[r_1, r_2) \cup [r_2, r_3) \cup \cdots \cup [r_{v-1}, r_v) \cup [r_v, r_{v+1}]$ of length s.
Compute $W(P', L, I_i)$ with $I_i = [r_i, r_{i+1})$ for $i = 1, \ldots, v-1$ and $I_v = [r_v, r_{v+1}]$.
Select an integer h with $2a < h \cdot s < 2a + 2s$.
Let $J_i^* = [r_i, r_{i+h}) = I_i \cup I_{i+1} \cup \cdots \cup I_{i+h-1}$ $(i = 1, 2, \ldots, v-h)$ and
$J^*_{v-h+1} = [r_{v-h+1}, r_{v+1}] = I_{v-h+1} \cup I_{v-h+2} \cup \cdots \cup I_{v+1}$.
Compute $W(P', L, J_i^*)$ via $W(P', L, J_i^*) = W(P', L, J^*_{i-1}) - W(P', L, I_{i-1}) + W(P', L, I_{i+h})$
$(i = 1, \ldots, v-h+1)$.
Select $J = J_i^*$ with the minimal sum of weights $W(P', L, J_i^*)$.
end (Case 2: Subcase 2.2)
Output $L(center(J))$ (see Definition 7) as the separator hyper-plane.
end (Phase 2)
End of the Algorithm

Phase 1 of the algorithm: The input of our algorithm is $P, Q, n_Q = |Q|$, and $n_P = |P|$. Each input point $p \in P$ has the format $\langle (x_1, \ldots, x_d), w(p) \rangle$, where $p = (x_1, \ldots, x_d)$ and $w(p)$ is the weight of p. The algorithm starts with the following steps: Select a fixed point $o^* \in \Re^d$ and a random plane L through o^* (random hyperplane can be selected via selecting a random normal vector). Randomly select m_1 points $q_1, \ldots, q_{m_1}$ from Q and let $Q' = \langle q_1, \ldots, q_{m_1} \rangle$ represent the list of these points just selected from Q (One point may appear multiple times. This is why we use list instead of set). For each $q_j \in Q'$, compute its signed distance $d_{q_i} = sd(q_i, L)$ to L. Find the $\lfloor(\frac{1}{d+1} - \epsilon_1)m_1\rfloor$-th least point $D^*_{1,d+1} = sd(q_1^*, L)$ for $d_{q_1}, \ldots, d_{q_{m_1}}$. Find the $\lceil(\frac{d}{d+1} + \epsilon_1)m_1\rceil$-th least point $D^*_{d,d+1} = sd(q_2^*, L)$ for $d_{q_1}, \ldots, d_{q_{m_1}}$. Randomly select m_2 points $p_1, \ldots, p_{m_2}$ from P and let $P' = \langle p_1, \ldots, p_{m_2} \rangle$ represent the list of these points just selected. For each $p_i \in P'$, compute $d_{p_i} = sd(p_i, L)$. It is well-known that finding the i-th element from a list takes linear steps (see Cormen et al. 2001). The computation above takes $(m_1 + m_2)$ steps. In the rest of the algorithm, we locate the position of the separator hyper-plane parallel to L by finding its signed distance to L. Its position will be at the center of an interval of size $2a$. In the rest of the proof, we treat both P and Q as lists of points from $\Re^d$. Each point appears only at most once on both P and Q. Let $t_d = k_d \cdot b^{\frac{-1}{d}} + \delta$. For $q \in \Re^d$ and $A \subseteq \Re^d$, define

$$Pr(A, L, \leftarrow q) = \frac{|\{q' | q' \in A \text{ and } sd(q', L) \le sd(q, L)\}|}{|A|}.$$

For a list of points $B = \langle x_1, \ldots, x_m \rangle$ from $\Re^d$ and a point $q \in \Re^d$, define $X_{B,L,q}(i) = 1$ if $sd(x_i, L) \le sd(q, L)$, or 0 otherwise. We also define

$$Y(B, L, q) = \sum_{i=1}^{m} X_{B,L,q}(i).$$

Lemma 13 *With probability* $\ge 1 - \frac{e^{-r}}{50}$, $Pr(Q, L, \leftarrow q_1^*) \in [\frac{1}{d+1} - \delta, \frac{1}{d+1} - \frac{\delta}{6}]$ *and* $Pr(Q, L, \leftarrow q_2^*) \in [\frac{d}{d+1} + \frac{\delta}{6}, \frac{d}{d+1} + \delta]$ *for all large* n_Q.

Proof By Lemma 8, with probability 0, we have that $sd(q_i, L) = sd(q_j, L)$ for some $q_i \ne q_j$ from Q or $sd(p_i, L) = sd(p_j, L)$ for some $p_i \ne p_j$ from P.

For a fixed $q \in Q$, by Lemma 10, we have probability $\le e^{-\frac{m_1\epsilon_0^2}{3}}$ such that $Y(Q', L, q) \notin [Pr(Q, L, \leftarrow q)m_1 - \epsilon_0 m_1, Pr(Q, L, \leftarrow q)m_1 + \epsilon_0 m_1]$. There are n_Q points in the set Q. This implies that the probability is at most $n_Q e^{-\frac{m_1\epsilon_0^2}{3}} < \frac{e^{-r}}{100}$ (see the assignment (11) for m_1) such that $Y(Q', L, q) \notin [Pr(Q, L, \leftarrow q)m_1 - \epsilon_0 m_1, Pr(Q, L, \leftarrow q)m_1 + \epsilon_0 m_1]$ for some $q \in Q$.

For each $q \in Q$, define $V_q(i)$ to be the random variable such that $V_q(i) = 1$ if $q = q_i$ or 0 otherwise. With probability $\frac{1}{n_Q}$, $V_q(i)$ is 1. When n_Q is large and m_1 elements are selected from Q, the probability is $\le e^{\frac{-1}{3}\epsilon_0^2 m_1}$ that at least $2\epsilon_0 m_1 > \frac{m_1}{n_Q} + \epsilon_0 m_1$ elements are equal to q (by Lemma 10). The probability is at most $n_Q e^{\frac{-1}{3}\epsilon_0^2 m_1} < \frac{e^{-r}}{100}$ that at least one element of Q is selected more than $2\epsilon_0 m_1$ times.

From the analysis above, the probability is $\ge 1 - (0 + \frac{e^{-r}}{100} + \frac{e^{-r}}{100}) = 1 - \frac{e^{-r}}{50}$ such that (a) $sd(q_i, L) \ne sd(q_j, L)$ for $q_i \ne q_j$ from Q, and $sd(p_i, L) \ne sd(p_j, L)$ for $p_i \ne p_j$ from P; (b) $Y(Q', L, q) \in [Pr(Q, L, \leftarrow q)m_1 - \epsilon_0 m_1, Pr(Q, L, \leftarrow q)m_1 +$

$\epsilon_0 m_1]$ for all $q \in Q$; and (c) no element of Q is selected more than $2\epsilon_0 m_1$ times into the list Q'.

Assume (a), (b) and (c) above are all true. Since $sd(q_1^*, L)$ is the $\lfloor(\frac{1}{d+1} - \epsilon_1)m_1\rfloor$-th least element among $d_{q_1}, d_{q_2}, \ldots, d_{q_{m_1}}$ and both (a) and (c) hold, the point q_1^* appears in the list Q' no more than $2\epsilon_0 m_1$ times and we also have

$$\left(\frac{1}{d+1} - \epsilon_1\right)m_1 + 2\epsilon_0 m_1 + 1 \geq Y(Q', L, q_1^*). \tag{13}$$

By (b), we conclude that

$$Y(Q', L, q_1^*) \geq Pr(Q, L, \leftarrow q_1^*)m_1 - \epsilon_0 m_1. \tag{14}$$

By (13) and (14), $(\frac{1}{d+1} - \epsilon_1)m_1 + 2\epsilon_0 m_1 + 1 \geq Pr(Q, L, \leftarrow q_1^*)m_1 - \epsilon_0 m_1$. Hence, $\frac{1}{d+1} - \epsilon_1 + 3\epsilon_0 + \frac{1}{m_1} \geq Pr(Q, L, \leftarrow q_1^*)$. Since $sd(q_1^*, L)$ is the $\lfloor(\frac{1}{d+1} - \epsilon_1)m_1\rfloor$-th least element among $d_{q_1}, d_{q_2}, \ldots, d_{q_{m_1}}$,

$$\left(\frac{1}{d+1} - \epsilon_1\right)m_1 - 1 \leq Y(Q', L, q_1^*). \tag{15}$$

By (b),

$$Y(Q', L, q_1^*) \leq Pr(Q, L, \leftarrow q_1^*)m_1 + \epsilon_0 m_1. \tag{16}$$

By (15) and (16), $Pr(Q, L, \leftarrow q_1^*) \geq \frac{1}{d+1} - \epsilon_1 - \epsilon_0 - \frac{1}{m_1}$. Thus, $Pr(Q, L, \leftarrow q_1^*) \in [\frac{1}{d+1} - \epsilon_1 - \epsilon_0 - \frac{1}{m_1}, \frac{1}{d+1} - \epsilon_1 + 3\epsilon_0 + \frac{1}{m_1}] \subseteq [\frac{1}{d+1} - \delta, \frac{1}{d+1} - \frac{\delta}{6}]$. Similarly, $Pr(Q, L, \leftarrow q_2^*) \in [\frac{d}{d+1} + \frac{\delta}{6}, \frac{d}{d+1} + \delta]$. □

Phase 2 of the algorithm: In this phase, we will find a position of the hyperplane L' (parallel to the hyperplane L) with the signed distance to L in the range $[D^*_{1,d+1}, D^*_{d,d+1}]$. Lemma 13 guarantees (with high probability) that each position in the interval $[D^*_{1,d+1}, D^*_{d,d+1}]$ gives a balance partition. We look for the position that has the small sum of weights for the points of P close to L'.

For a list $A = \langle x_1, \ldots, x_m\rangle$, $|A| = m$ is denoted to be the *length of* A and $x \in A$ means that x is one of the elements in A ($x = x_i$ for some $1 \leq i \leq m$). For a real number subset $J \subseteq \Re$ and a list A of finite points in $\Re^d$, define

$$Pr_*(A, L, J, w_j) = \frac{|\{p | p \in A \text{ and } w(p) = w_j \text{ and } sd(p, L) \in J\}|}{|A|}, \tag{17}$$

and

$$Z(A, L, J, w_j) = \sum_{p \in A} X^*_{L,p,J,w_j}, \tag{18}$$

where $X^*_{L,p,J,w_j} = 1$ if $sd(p, L) \in J$ and $w(p) = w_j$, or 0 otherwise. We also define

$$W(A, L, J) = \sum_{p \in A \text{ and } sd(p,L) \in J} w(p). \tag{19}$$

By the definitions (17–19), it is easy to see that

$$W(A, L, J) = \sum_{j=1}^{k} w_j Z(A, L, J, w_j) = \sum_{j=1}^{k} w_j Pr_*(A, L, J, w_j)|A|. \tag{20}$$

Since $\sum_{j=1}^{k} n_j = n_P$, we have that

$$n_j \geq \frac{n_P}{k} \tag{21}$$

for some $1 \leq j \leq k$. By (3) and the theorem condition $w_k \leq w_j$ for $j = 1, \ldots, k$, we have that

$$n_P^{s_2} \geq \frac{k}{c_1 w_k} \geq \frac{k^{\frac{d-1}{d}}}{c_1 w_j}. \tag{22}$$

By (21) and (22),

$$n_P^{\frac{d-1}{d} - s_2} = \frac{n_P^{\frac{d-1}{d}}}{n_P^{s_2}} \leq c_1 w_j \left(\frac{n_P}{k}\right)^{\frac{d-1}{d}} \leq c_1 w_j n_j^{\frac{d-1}{d}} \quad \text{for some } 1 \leq j \leq k. \tag{23}$$

By (7) and (23), for some $1 \leq j \leq k$,

$$\delta_2 \cdot n_P^{\frac{d-1}{d} - s_2} \leq \delta_1 \cdot a \cdot w_j n_j^{\frac{d-1}{d}}. \tag{24}$$

Lemma 14 *Let $f \leq n_P$ be an integer and $H_1, H_2, \ldots, H_f \subseteq R$ be f real intervals. With probability $\geq 1 - \frac{1}{100} e^{-r}$, we have that $W(P, L, H_i) \in [W(P', L, H_i)\frac{n_P}{m_2} - \delta_2 n_P^{\frac{d-1}{d} - s_2}, W(P', L, H_i)\frac{n_P}{m_2} + \delta_2 n_P^{\frac{d-1}{d} - s_2}])$ for $1 \leq i \leq f$.*

Proof For fixed interval H_i and weight w_j, by Lemma 10, the probability is $\leq e^{-\frac{m_2 \epsilon^2}{3}}$ such that $Z(P', L, H_i, w_j) \notin [Pr_*(P, L, H_i, w_j)m_2 - \epsilon m_2, Pr_*(P, L, H_i, w_j)m_2 + \epsilon m_2]$. Thus, the probability is $\leq k \cdot f e^{-\frac{m_2 \epsilon^2}{3}} \leq n_P^2 e^{-\frac{m_2 \epsilon^2}{3}} < \frac{1}{100} e^{-r}$ such that $Z(P', L, H_i, w_j) \notin [Pr_*(P, L, H_i, w_j)m_2 - \epsilon m_2, Pr_*(P, L, H_i, w_j)m_2 + \epsilon m_2]$ for some $i \leq f$ and $j \leq k$. In other words, with probability $\geq 1 - \frac{1}{100} e^{-r}$, we have $Z(P', L, H_i, w_j) \in [Pr_*(P, L, H_i, w_j)m_2 - \epsilon m_2, Pr_*(P, L, H_i, w_j)m_2 + \epsilon m_2]$ for all $i \leq f$ and $j \leq k$. We assume that for all $i \leq f$ and $j \leq k$,

$$\begin{aligned} &Z(P', L, H_i, w_j) \\ &\quad \in [Pr_*(P, L, H_i, w_j)m_2 - \epsilon m_2, Pr_*(P, L, H_i, w_j)m_2 + \epsilon m_2]. \end{aligned} \tag{25}$$

By (8) and (3),

$$\epsilon k w_1 \leq \frac{\delta_2}{3 c_1 n_P^{\frac{1}{d} + s_1 + s_2}} \cdot c_1 n_P^{s_1} = \frac{\delta_2}{3 n_P^{\frac{1}{d} + s_2}} \leq \frac{\delta_2}{n_P^{\frac{1}{d} + s_2}}. \tag{26}$$

By (20), (26) and (25),

$$W(P', L, H_i) = \sum_{j=1}^{k} w_j Z(P', L, H_i, w_j) \tag{27}$$

$$\geq \sum_{j=1}^{k} w_j (Pr_*(P, L, H_i, w_j)m_2 - \epsilon m_2) \tag{28}$$

$$\geq \sum_{j=1}^{k} w_j Pr_*(P, L, H_i, w_j)m_2 - \epsilon k w_1 m_2 \tag{29}$$

$$\geq \sum_{j=1}^{k} w_j Pr_*(P, L, H_i, w_j)m_2 - \frac{\delta_2 m_2}{n_P^{(1/d)+s_2}}. \tag{30}$$

Similarly, we also have

$$W(P', L, H_i) \leq \sum_{j=1}^{k} w_j Pr_*(P, L, H_i, w_j)m_2 + \frac{\delta_2 m_2}{n_P^{(1/d)+s_2}}. \tag{31}$$

By (30) and (31),

$$W(P', L, H_i) \in \left[\sum_{j=1}^{k} w_j \cdot Pr_*(P, L, H_i, w_j)m_2 - \frac{\delta_2 m_2}{n_P^{(1/d)+s_2}}, \right.$$

$$\left. \sum_{j=1}^{k} w_j \cdot Pr_*(P, L, H_i, w_j)m_2 + \frac{\delta_2 m_2}{n_P^{(1/d)+s_2}} \right]. \tag{32}$$

Since $W(P, L, H_i) = \sum_{j=1}^{k} w_j Pr_*(P, L, H_i, w_j)n_P$ (by (20)) and $W(P', L, H_i)$ is in the interval $[\sum_{j=1}^{k} w_j Pr_*(P, L, H_i, w_j)m_2 - \frac{\delta_2 m_2}{n_P^{(1/d)+s_2}}, \sum_{j=1}^{k} w_j Pr_*(P, L, H_i, w_j)m_2 + \frac{\delta_2 m_2}{n_P^{(1/d)+s_2}}]$ (by (32)), we have $W(P, L, H_i) \leq W(P', L, H_i)\frac{n_P}{m_2} + \delta_2 n_P^{\frac{d-1}{d}-s_2}$ and $W(P, L, H_i) \geq W(P', L, H_i)\frac{n_P}{m_2} - \delta_2 n_P^{\frac{d-1}{d}-s_2}$. We have proved the lemma. □

Case 1: $|D^*_{1,d+1} - D^*_{d,d+1}| \geq 3an_P^{\frac{2}{d}}$. Partition $[D^*_{1,d+1}, D^*_{d,d+1}]$ into disjoint intervals $[l_1, l_2), [l_2, l_3), \ldots, [l_{u-1}, l_u), [l_u, l_{u+1}]$ such that each $l_{i+1} - l_i (i = 1, \cdots, u)$ is equal to $\frac{|D^*_{1,d+1} - D^*_{d,d+1}|}{g_1(n_P)} \geq 3a$, where

$$g_1(n_P) = u = n_P^{\frac{2}{d}}. \tag{33}$$

Let $J_i = [l_i, l_{i+1})$ if $i < u$, and $J_u = [l_u, l_{u+1}]$. Compute $W(P', L, J_i)$ for $i = 1, \cdots, u$, which takes $O(m_2 + g_1(n_P)) = O(m_2)$ steps. The algorithm selects $J = J_{i_0}$ that has the least $W(P', L, J_{i_0})$ and let $L' = L(center(J_{i_0}))$ (see Definition 7), which takes $O(g_1(n_P)) = O(m_2)$ steps. Assume that J_{i_1} is the interval with the least $W(P, L, J_{i_1})$.

Lemma 15 *Assume Case* 1 *condition is true. With probability* $\geq 1 - \frac{1}{50}e^{-r}$, $W(P, L, J_{i_0}) \leq (k_d \cdot b^{\frac{-1}{d}} + \delta) \cdot a \cdot \sum_{j=1}^{k} w_j \cdot n_j^{\frac{d-1}{d}}$ *for all large* n_P.

Proof For a fixed interval J_i, by Lemma 10, the probability is $\leq e^{-\frac{m_2\epsilon^2}{3}}$ that $Z(P', L, J_i, w_j) \notin [Pr_*(P, L, J_i, w_j)m_2 - \epsilon m_2, Pr_*(P, L, J_i, w_j)m_2 + \epsilon m_2]$. Thus, the probability is $\leq g_1(n_P)e^{-\frac{m_2\epsilon^2}{3}} < \frac{1}{100}e^{-r}$ that $Z(P', L, J_i, w_j) \notin [Pr_*(P, L, J_i, w_j)m_2 - \epsilon m_2, Pr_*(P, L, J_i, w_j)m_2 + \epsilon m_2]$ for some $i \leq g_1(n_P)$ and $j \leq k$.

Since

$$\sum_{j=1}^{k} n_j = n_P, \tag{34}$$

and $w_1 > w_2 > \cdots > w_k$, the sum of weights of all points in P is

$$W(P, L, (-\infty, +\infty)) \leq w_1 \cdot n_P. \tag{35}$$

Because $J_1, J_2, \ldots, J_u$ are disjoint intervals,

$$\sum_{i=1}^{g_1(n_P)} W(P, L, J_i) \leq W(P, L, (-\infty, +\infty)). \tag{36}$$

There is J_i for some $i \leq u$ such that

$$W(P, L, J_i) \leq \frac{w_1 n_P}{n_P^{\frac{2}{d}}} \tag{37}$$

$$= \sum_{j=1}^{k} w_1 \frac{n_j}{n_P^{\frac{2}{d}}} \tag{38}$$

$$\leq \sum_{j=1}^{k} \frac{w_1}{n_P^{\frac{1}{d}}} n_j^{\frac{d-1}{d}} \tag{39}$$

$$\leq (k_d \cdot b^{\frac{-1}{d}} + \delta_1) \cdot a \cdot \sum_{j=1}^{k} w_k \cdot n_j^{\frac{d-1}{d}} \tag{40}$$

$$\leq (k_d \cdot b^{\frac{-1}{d}} + \delta_1) \cdot a \cdot \sum_{j=1}^{k} w_j \cdot n_j^{\frac{d-1}{d}}. \tag{41}$$

The inequality (37) is from (35), (36), and (33). The transition from (37) to (38) is by (34). The transition from (38) to (39) is because $n_j \leq n_P$. The transition from (39) to (40) is because n_P is large, $(k_d \cdot b^{\frac{-1}{d}} + \delta_1) \cdot a$ is a constant and we have the condition $\frac{w_1}{w_k} = o(n_P^{\frac{1}{d}})$ from the theorem. Therefore (by (37–41)),

$$W(P,L,J_{i_1}) \le W(P,L,J_i) \le (k_d \cdot b^{\frac{-1}{d}} + \delta_1)\cdot a \cdot \sum_{j=1}^{k} w_j \cdot n_j^{\frac{d-1}{d}}. \tag{42}$$

By Lemma 14, with probability $\ge 1 - \frac{1}{100}e^{-r}$, we have

$$W(P,L,J_i) \in \left[W(P',L,J_i)\frac{n_P}{m_2} - \delta_2 n_P^{\frac{d-1}{d}-s_2}, W(P',L,J_i)\frac{n_P}{m_2} + \delta_2 n_P^{\frac{d-1}{d}-s_2} \right]$$

for all $i \le u$. (43)

Assume (43) holds. Thus, $W(P',L,J_{i_1})\frac{n_P}{m_2} - \delta_2 n_P^{\frac{d-1}{d}-s_2} \le W(P,L,J_{i_1})$, which implies the following:

$$W(P',L,J_{i_1}) \le W(P,L,J_{i_1})\frac{m_2}{n_P} + \frac{\delta_2 m_2}{n_P^{(1/d)+s_2}}. \tag{44}$$

Since the algorithm selects the interval J_{i_0} with the least $W(P',L,J_{i_0})$, we have that

$$W(P',L,J_{i_0}) \le W(P',L,J_{i_1}). \tag{45}$$

Thus, we conclude that

$$W(P,L,J_{i_0}) \le W(P',L,J_{i_0})\frac{n_P}{m_2} + \delta_2 n_P^{\frac{d-1}{d}-s_2} \tag{46}$$

$$\le W(P',L,J_{i_1})\frac{n_P}{m_2} + \delta_2 n_P^{\frac{d-1}{d}-s_2} \tag{47}$$

$$\le \left(W(P,L,J_{i_1})\frac{m_2}{n_P} + \frac{\delta_2 m_2}{n_P^{(1/d)+s_2}} \right)\frac{n_P}{m_2} + \delta_2 n_P^{\frac{d-1}{d}-s_2} \tag{48}$$

$$= W(P,L,J_{i_1}) + 2\delta_2 n_P^{\frac{d-1}{d}-s_2} \tag{49}$$

$$\le W(P,L,J_{i_1}) + 2\delta_1 \cdot a w_j n_j^{\frac{d-1}{d}} \text{ for some } j \le k. \tag{50}$$

The inequality (46) is due to (43). The transition from (46) to (47) is due to (45). The transition from (47) to (48) is due to (44). The transition from (49) to (50) is due to (24).

By (42) and (46–50),

$$W(P,L,J_{i_0}) \le (k_d \cdot b^{\frac{-1}{d}} + \delta_1)\cdot a \cdot \sum_{j=1}^{k} w_j \cdot n_j^{\frac{d-1}{d}} + 2\delta_1 \cdot a w_j n_j^{\frac{d-1}{d}} \tag{51}$$

$$\le (k_d \cdot b^{\frac{-1}{d}} + 3\delta_1)\cdot a \cdot \sum_{j=1}^{k} w_j \cdot n_j^{\frac{d-1}{d}} \tag{52}$$

$$\le (k_d \cdot b^{\frac{-1}{d}} + \delta)\cdot a \cdot \sum_{j=1}^{k} w_j \cdot n_j^{\frac{d-1}{d}}. \tag{53}$$

The transition from (52) to (53) is due to (1). □

Case 2: $|D^*_{1,d+1} - D^*_{d,d+1}| < 3an_P^{\frac{2}{d}}$. Let J^* be interval such that $center(J^*) \in [D^*_{1,d+1}, D^*_{d,d+1}]$ and $|J^*| = 2a_1 = 2a(1+\delta_1)$ and $W(P, L, J^*)$ is the least.

Subcase 2.1: $|D^*_{1,d+1} - D^*_{d,d+1}| \le \delta_1 a$. Let $J = [D^*_{1,d+1} - a, D^*_{1,d+1} + a]$ and let $L' = L(D^*_{1,d+1})$ (In other words, $L' = L(center(J))$) (see Definition 7). Clearly, $J \subseteq J^*$ and $W(P, L, J) \le W(P, L, J^*)$.

Subcase 2.2: $\delta_1 a < |D^*_{1,d+1} - D^*_{d,d+1}| < 3an_P$. Let $g_2(n_P)$ be the least integer $v \ge 2$ such that $\frac{|D^*_{d,d+1} - D^*_{1,d+1}| + 2a}{v} \le \frac{\delta_1 a}{3}$. Since $v \ge 2$ and $\frac{|D^*_{d,d+1} - D^*_{1,d+1}| + 2a}{v-1} > \frac{\delta_1 a}{3}$, we have $\frac{|D^*_{d,d+1} - D^*_{1,d+1}| + 2a}{v} = \frac{v-1}{v} \frac{|D^*_{d,d+1} - D^*_{1,d+1}| + 2a}{v-1} > \frac{v-1}{v}\frac{\delta_1 a}{3} \ge \frac{\delta_1 a}{6}$. Therefore,

$$
\begin{aligned}
v &\le \frac{|D^*_{d,d+1} - D^*_{1,d+1}| + 2a}{\frac{\delta_1 a}{6}} \\
&\le \frac{3an_P^{\frac{2}{d}} + 2a}{\frac{\delta_1 a}{6}} \\
&= \frac{6(3n_P^{\frac{2}{d}} + 2)}{\delta_1} = O(n_P^{\frac{2}{d}}).
\end{aligned}
$$

Let $s = \frac{|D^*_{d,d+1} - D^*_{1,d+1}| + 2a}{g_2(n_P)} \in [\frac{\delta_1 a}{6}, \frac{\delta_1 a}{3}]$. Partition $[D^*_{1,d+1} - a, D^*_{d,d+1} + a]$ into the union of $g_2(n_P)$ disjoint intervals of size s: $[r_1, r_2) \cup [r_2, r_3) \cup \cdots \cup [r_{v-1}, r_v) \cup [r_v, r_{v+1}]$, where $v = g_2(n_P)$ and $r_{i+1} = r_i + s$ for $i = 1, \ldots, v$. Let $I_i = [r_i, r_{i+1})$ for $i = 1, \ldots, v-1$ and $I_v = [r_v, r_{v+1}]$. Let $J_i^* = I_i \cup I_{i+1} \cup \cdots \cup I_{i+h-1}$ for $i = 1, \ldots, v-h+1$, where h is an integer with $2a < h \cdot s \le 2a + s$. The algorithm selects the interval $J = J^*_{i_2}$ that has the least $W(P', L, J^*_{i_2})$. Finally, the algorithm outputs $L' = L(center(J))$ (see Definition 7) for the separator hyper-plane. We analyze the algorithm for the case 2.

Lemma 16 *Assume that J is the interval output from the case* 2 (*either subcase* 2.1 *or subcase* 2.2). *With probability* $\ge 1 - \frac{1}{100}e^{-r}$, *we have that* $W(P, L, J) \le W(P, L, J^*) + 2\delta_1 \cdot aw_j n_j^{\frac{d-1}{d}}$ *for some* $j \le k$.

Proof The subcase 2.1 is trivial since the small size of the interval implies that $J \subseteq J^*$. We only discuss the subcase 2.2. Let $I_t, I_{t+1}, \ldots, I_{t+m}$ be the intervals such that $J^* \cap J_{t+i} \ne \emptyset$ $(i = 0, \ldots, m)$. Then $I_{t+1}, I_{t+2}, \ldots, I_{t+m-1}$ are all subsets of J^*. Let K^* be the interval from the union $I_{t+1} \cup I_{t+2} \cup \cdots \cup I_{t+m-1}$. Since $\|I_i\| = s \le \frac{\delta_1 a}{3}$, $\|J^*\| = 2(1+\delta_1)a \ge \|K^*\| \ge \|J^*\| - \|I_t\| - \|I_{t+m}\| \ge 2(1+\delta_1)a - \frac{2\delta_1 a}{3} \ge 2a + \frac{4\delta_1 a}{3}$ (Remember that we use $\|[a, b)\|$ to represent the length $b - a$ of the interval $[a, b)$). We have the interval J^*_{t+1} with $\|J^*_{t+1}\| \ge 2a$ and $J^*_{t+1} \subseteq K^* \subseteq J^*$. This implies that

$$
W(P, L, J^*_{t+1}) \le W(P, L, J^*). \tag{54}
$$

By Lemma 14, the probability is $\ge 1 - \frac{1}{100}e^{-r}$ that $W(P, L, J_i^*) \in [W(P', L, J_i^*) \times \frac{n_P}{m_2} - \delta_2 n_P^{\frac{d-1}{d} - s_2}, W(P', L, J_i^*)\frac{n_P}{m_2} + \delta_2 n_P^{\frac{d-1}{d} - s_2}]$ for all $i \le g(n_P) - h + 1$. Thus,

$W(P', L, J^*_{t+1})\frac{n_P}{m_2} - \delta_2 n^{\frac{d-1}{d}-s_2} \le W(P, L, J^*_{t+1}) \le W(P, L, J^*)$. We assume that

$$W(P, L, J^*_i) \in \left[W(P', L, J^*_i)\frac{n_P}{m_2} - \delta_2 n_P^{\frac{d-1}{d}-s_2}, W(P', L, J^*_i)\frac{n_P}{m_2} + \delta_2 n_P^{\frac{d-1}{d}-s_2}\right]$$
$$\text{for every } 1 \le i \le g(n_P) - h + 1. \tag{55}$$

Thus, $W(P', L, J^*_{t+1})\frac{n_P}{m_2} - \delta_2 n^{\frac{d-1}{d}-s_2} \le W(P, L, J^*_{t+1}) \le W(P, L, J^*)$. Hence,

$$W(P', L, J^*_{t+1}) \le W(P, L, J^*)\frac{m_2}{n_P} + \frac{\delta_2 m_2}{n^{(1/d)+s_2}}. \tag{56}$$

Since the algorithm selects the interval $J^*_{i_2}$ with the least $W(P', L, J^*_{i_2})$,

$$W(P', L, J^*_{i_2}) \le W(P', L, J^*_{t+1}). \tag{57}$$

We have that

$$W(P, L, J^*_{i_2}) \le W(P', L, J^*_{i_2})\frac{n_P}{m_2} + \delta_2 n_P^{\frac{d-1}{d}-s_2} \tag{58}$$
$$\le W(P', L, J^*_{t+1})\frac{n_P}{m_2} + \delta_2 n_P^{\frac{d-1}{d}-s_2} \tag{59}$$
$$\le \left(W(P, L, J^*_{t+1})\frac{m_2}{n_P} + \frac{\delta_2 m_2}{n_P^{(1/d)+s_2}}\right)\frac{n_P}{m_2} + \delta_2 n_P^{\frac{d-1}{d}-s_2} \tag{60}$$
$$= W(P, L, J^*_{t+1}) + 2\delta_2 n_P^{\frac{d-1}{d}-s_2} \tag{61}$$
$$\le W(P, L, J^*) + 2\delta_2 n_P^{\frac{d-1}{d}-s_2} \tag{62}$$
$$\le W(P, L, J^*) + 2\delta_1 \cdot a w_j n_j^{\frac{d-1}{d}} \text{ for some } j \le k \text{ (by (24))}. \tag{63}$$

The inequality (58) follows from (55). The transition from (58) to (59) is due to (57). The transition from (59) to (60) is due to (56). The transition from (61) to (62) is due to (54). □

For a list A of finite points in $\Re^d$ and a hyper-plane M_1, define $F_1(M_1, a, A) = \sum_{p_i \in A}$ and $\text{dist}(p_i, M_1) \le aw(p_i)$. If M_1 and M_2 are two parallel hyper-planes with signed distance $d_{M_1,M_2} = sd(p, M_1)$ for some point p in the M_2, then $F_1(M_2, a, A) = W(A, M_1, [d_{M_1,M_2}, -a, d_{M_1,M_2} + a])$. The hyper-plane $L(center(J^*_{i_2}))$ (see Definition 7) output by the algorithm has that $F_1(L(center(J)), a, P) \le F_1(L(center(J^*)), a_1, P) + 2\delta_1 \cdot a w_j n_j^{\frac{d-1}{d}}$ for some $j \le k$ by Lemma 16.

Lemma 17 *With probability at least $1 - e^{-r}$, one can output an hyperplane L' in $O(v^2 \cdot (n_P^{\frac{2}{d}+2(s_1+s_2)} \cdot \log n_P + \log n_Q))$ steps such that $F_1(L', a, P) \le (k_d \cdot b^{\frac{-1}{d}} + \delta) \cdot a \cdot \sum_{j=1}^k w_j n_j^{\frac{d-1}{d}} + O(n_P^{\frac{d-2}{d}+s_1})$.*

Proof After the hyper-plane L is selected in phase one, by Lemma 13, the probability is at least $1-e^{-r}$ that both $Pr(Q, L, \leftarrow q_1^*) \in [\frac{1}{d+1}-\delta, \frac{1}{d+1}-\frac{\delta}{6}]$ and $Pr(Q, L, \leftarrow q_2^*) \in [\frac{d}{d+1}+\frac{\delta}{6}, \frac{d}{d+1}+\delta]$. This means every L' (parallel to L) with the signed distance (to L) in the interval $[D_{1,d+1}^*, D_{d,d+1}^*]$, it has at most $(\frac{d}{d+1}+\delta)n_Q$ points of Q in each of the half spaces. In phase 2, we have probability at least $1-e^{-r}$ to output the separator L' (the signed distance to L is in $[D_{1,d+1}^*, D_{d,d+1}^*]$) such that $F_1(L', a, P) \le (k_d \cdot b^{\frac{-1}{d}} + \delta) \cdot a \cdot \sum_{j=1}^k w_j \cdot n_j^{\frac{d-1}{d}}$ (Case 1 of Phase 2, see Lemma 15) or $F_1(L', a, P) \le F_1(L(J^*), a_1, P) + 2\delta_2 w_j n_j^{\frac{d-1}{d}}$ (Case 2 of Phase 2, see Lemma 16), where J^* is the interval of length $2a_1$ with the least $F_1(L(J^*), a_1, P)$ and center between $D_{1,d+1}^*$ and $D_{d,d+1}^*$.

Assume that L is a fixed hyper-plane and L^* is a another hyper-plane that is parallel to L and $F_1(L^*, a_1, P)$ is the least. By Lemma 15 and Lemma 16, the probability is $\ge (1-e^{-r})^2$ such that we can get another L' (parallel to L) such that $F_1(L', a, P) \le F_1(L^*, a_1, P) + 2\delta_1 w_j n_j^{\frac{d-1}{d}}$ for some $j \le k$ or $F_1(L', a, P) \le (k_d \cdot b^{\frac{-1}{d}} + \delta) \cdot a \cdot \sum_{j=1}^k w_j \cdot n_j^{\frac{d-1}{d}}$. The number of points in Q in each side of L' is $\le (\frac{d}{d+1}+\delta)n_Q$.

With probability at most $\frac{1}{1+\alpha}$, $F_{a_1,P,o}(L) \ge (1+\alpha)E(F_{a_1,P,o})$ (by (5)). If the algorithm repeats z times, let $L_1, \ldots, L_z$ be the random hyper planes selected for L. With probability $\ge (1-(\frac{1}{1+\alpha})^z)$, one of those L_is has another hyper-plane L_i^* such that L_i^* is parallel to L_i and has $F_{a_1,P,o}(L_i^*) \le (1+\alpha)E(F_{a_1,P,o})$. Therefore, we have probability at least $(1-(\frac{1}{\alpha+1})^z)(1-e^{-r})^{2z}$ to find out such a hyper-plane L' with

$$F_1(L', a, P) \le (1+\alpha)E(F_{a_1,P,o}) + 2\delta_1 w_j n_j^{\frac{d-1}{d}} \quad \text{for some } j \le k \tag{64}$$

or

$$F_1(L', a, P) \le (k_d \cdot b^{\frac{-1}{d}} + \delta) \cdot a \cdot \sum_{j=1}^{k} w_j \cdot n_j^{\frac{d-1}{d}}. \tag{65}$$

By (64), (65), (1), (2), and (4), we have $F_1(L', a, P) \le (k_d \cdot b^{\frac{-1}{d}} + \delta) \cdot a \cdot \sum_{j=1}^k w_j n_j^{\frac{d-1}{d}} + O(n_P^{\frac{d-2}{d}+s_1})$.

Now we give a bound for the probability. Let $z = \frac{2r}{\ln(1+\alpha)} = O(v)$ (by (6)). Then $1-(\frac{1}{1+\alpha})^z > 1-e^{-r}$.

$$\left(1-\left(\frac{1}{1+\alpha}\right)^z\right)(1-e^{-r})^{2z} > (1-e^{-r})^{2z+1} > 1-(2z+1)e^{-r} > 1-\frac{1}{2^v},$$

where we let $r = c_4 v$ for some constant c_4 large enough.

The phase 1 of the algorithm takes $O(m_1+m_2)$ steps. The case 1 of phase 2 takes $O(m_2)$ steps. The case 2 of phase 2 takes $O(m_2)$ steps. Totally, it takes $O(z(m_1 +$

$m_2)) = O(v \cdot (n_P^{\frac{2}{d}+2(s_1+s_2)} \cdot (\log n_P + v) + v \log n_Q)) = O(v^2 \cdot (n_P^{\frac{2}{d}+2(s_1+s_2)} \cdot \log n_P + \log n_Q))$ steps. □

Applying Lemma 17, we finish the proof of the Theorem. □

6 An application to protein side-chain packing problem

We follow the description of Xu (2005) for the model of protein side chain packing. The side-chain prediction problem can be formulated as follows. We use a reside interaction graph $G = (V, E)$ to represent a protein resides and their interactions. Each vertex in V represents a residue of the protein. For each reside $i \in V$, $D(i)$ is the set of all possible rotamers of side chain i. There is an interaction edge $(i, j) \in E$ if and only if there are $l \in D(i)$ and $k \in D(j)$ such that there exist an atom in the rotamer l conflicts with another atom in the rotamer k. Two atoms conflict each other iff their distance is less than the sum of their radii. For each two rotamers $l \in D(i)$ and $k \in D(j)$ $(i \neq j)$, there is an associated score $P_{i,j}(l, k)$ if residue i interacts with residue j. For each rotamer $l \in D(i)$, there is a score $S_i(l)$, which characterizes the interaction energy between l and the backbone of the protein. The prediction problem is to give $A(i) \in D(i)$ to residues $i \in V$ so that the following energy value is minimized. $E(G) = \sum_{i\in V} S_i(A(i)) + \sum_{i\neq j,(i,j)\in E} P_{i,j}(A(i), A(j))$.

For more detailed description about the protein side chain packing, see (e.g. Ponter and Richards 1987; Canutescu et al. 2003; Xu 2005; Chazelle et al. 2004). Let d_u^* be distance such that there is no interaction between two resides if their distance is $\geq d_u^*$. Let d_l^* be the minimal distance between two amino acids. Both d_u^* and d_l^* are constants.

Theorem 18 *There exists a $r_{\max}^{O(n^{\frac{2}{3}})}$-time algorithm to find the optimal solution for the protein side chain packing problem, where $r_{\max}$ is the maximal number of rotamers of one amino acid. In other words, $r_{\max} = \max_i |D(i)|$.*

Proof Our algorithm is based on the divide and conquer method. Let $d_0 = d_l^* \frac{\sqrt{2}}{2}$ be the unit distance. Since $d_l^* = \sqrt{2} d_0$, we consider that the minimal distance between two amino acids is $d_l = \sqrt{2}$ and the minimal distance for the interaction between two side chains is $d_u = \frac{d_u^*}{d_0}$. For a grid point $p = (x, y, z)$ $(x, y, z$ are integers), define $cube(p) = \{(u, v, w) \in \Re^3 | x - \frac{1}{2} \leq u < x + \frac{1}{2}$ and $y - \frac{1}{2} \leq v < y + \frac{1}{2}$ and $z - \frac{1}{2} \leq w < z + \frac{1}{2}\}$. The 3D space $\Re^3$ is partitioned into many cubes: $\Re^3 = cube(p_0) \cup cube(p_1) \cup \cdots$. For different grid points $p \neq p'$, $cube(p) \cap cube(p') = \emptyset$. Each amino acid is represented by the position of its C_α. Therefore, no two amino acids can stay at the same $cube(p)$ for any grid point p. Let P be the set of all grid points p such that $cube(p)$ contains the C_α for an amino acid.

Let $w = d_u + 2\sqrt{2}$. By Corollary 12, there exists a w-wide separator L plane such that each side has at most $(\frac{3}{4} + \delta)n$ contain amino acid, and the number of grid points (with amino acids in its cube) is bounded by $1.209 w n^{\frac{2}{3}}$, where $\delta > 0$ is an arbitrary small constant. The w-wide separator partitions the problem into P_1, S and P_2, where S is the separator area. Clearly, a side chain whose amino acid C_α is in $cube(p)$ with $p \in P_1$ does not interact another side chain in P_2 because of the w-wide separator between P_1 and P_2.

The number of ways to arrange the side chains in the separator area S is bounded by $r_{\max}^{1.209wn^{\frac{2}{3}}}$. We only need $O(n)$ time for computing the separator. We assume that $r_{\max} \geq 2$ (otherwise, it is trivial). Let $T(n)$ is the computational time for the protein side chain packing problem with n resides. Solving each sub-problem P_i $(i = 1, 2)$ takes $T((\frac{3}{4} + \delta)n)$ steps. We have the recursive $T(n) \leq 2(r_{\max}^{1.209wn^{\frac{2}{3}}} + O(n))T((\frac{3}{4} + \delta)n)$. This gives that $T(n) = r_{\max}^{O(n^{\frac{2}{3}})}$. □

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