

Separation in Graphs: A Survey and Some Recent Results

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Abstract

Let G and H be graphs, with $|G| \leq |H|$. Consider a one-to-one map $f:G \rightarrow H$, and define $|f| = \min\{\text{dist}_H(f(x),f(y)): xy \in E(G)\}$. Now let the separation of G in H be defined by $\text{sep}(G,H) = \max\{|f|: \text{all one-to-one maps } f:G \rightarrow H\}$. We survey some results of the past several years on this parameter, in particular using Alon and Milman's results on the connection between the second largest eigenvalue of a graph and isoperimetric inequalities to obtain bounds for $\text{sep}(G,Q(n))$, where $Q(n)$ is the n -dimensional hypercube and G is arbitrary. Also included are two new results, one involving the Kruskal-Katona theorem as it applies to separating complete bipartite graphs into hypercubes, the other being an algorithmic solution to separating complete graphs into trees.

1. Introduction and Previous Results.

Given graphs G and H with $|V(G)| \leq |V(H)|$, a separator of G in H is any one-to-one map $f:V(G) \rightarrow V(H)$. Define the minimum distance of separator f by $|f| = \min\{d_H(f(x),f(y)): xy \in E(G)\}$, where d_H denotes distance in H . Now define $\text{sep}(G,H)$, the separation of G in H , to be the maximum of $|f|$ over separators f . The idea behind $\text{sep}(G,H)$ is to map G into H while keeping pairs of adjacent points in G as far apart as possible in H (perhaps the edges of G indicating which pairs of vertices are incompatible). It may be useful to think of G as being the "guest" graph and H as being the "host" graph. The separation parameter is a natural dual to the much studied bandwidth parameter $B(G,H) = \min_f \max\{d_H(f(x),f(y)): xy \in E(G)\}$, obtained by interchanging the min and the max in the definition, where H is ordinarily taken to be a path on $V(G)$ many vertices.

The motivation for a study of $\text{sep}(G,H)$ has several aspects. Probably the most intensely studied problem expressible in the form "determine $\text{sep}(G,H)$ " is that of determining $\text{sep}(K_p,Q(n))$, in connection with the theory of binary error-correcting codes. Here K_p denotes the complete graph on p points, and $Q(n)$ denotes the n -dimensional cube, whose vertex set is $(\mathbb{Z}_2)^n$, with two binary n -tuples adjacent when they differ in exactly one coordinate. The distance between two n -tuples in $Q(n)$ is then the number of coordinates in which they differ, otherwise known as the Hamming distance. A major subject of coding theory is the construction of sets $C \subset V(Q(n))$ such that $d_Q(x,y) \geq m$ for all $x,y \in C$, known as " (n,m) codes". Much attention is given to finding the maximum size $A(n,m)$ among all (n,m) codes. An (n,m) code C of size p exists if and only if $\text{sep}(K_p,Q(n)) \geq m$, and $A(n,m) = \max\{p: \text{sep}(K_p,Q(n)) \geq m\}$. Because of this connection with coding theory, $\text{sep}(G,Q(n))$ is of particular interest. The study of $\text{sep}(K_p,H)$ for any graph H is then also a natural extension of the study of codes in the hypercube.

In this first section we review some previous work on separation parameters, and in the last two sections we present some new results.

We use the following notation and conventions. Only finite simple graphs will be considered. Let $[1, n]$ denote the set of integers from 1 to n inclusive. Let $G \sqsubseteq H$ denote that G is isomorphic to a subgraph of H . Let $\chi(G)$, $\Delta(G)$ and $\delta(G)$ denote the chromatic number, maximum degree and minimum degree of G , respectively. For definitions of graph theoretic terms not given here, see [H].

Separation of G in paths:

To our knowledge, the first study of graph separation parameters is in [LVW], where H is taken to be a path or cycle on the same number of points as G . Let $s(G) = \text{sep}(G, P_n)$, where $n = |V(G)|$. The main concern in that paper was the algorithmic complexity of $s(G)$ and related parameters obtained by replacing P_n by C_n , also considering orientations of P_n and C_n . In particular it is shown in [LVW] that the problem "given a graph G and an integer k , is $s(G) > k$?" is NP-complete, even for the case $k=1$ (by a simple reduction from the Hamilton path problem). Their main results demonstrate the reducibility of various multiprocessor job scheduling problems to variants of the quoted problem.

Since we may let $V(P_n)$ be the set $[1, n]$, where vertices are adjacent in P_n when they are consecutive integers, a separator $f: V(G) \rightarrow P_n$ will also be regarded as a labeling $f: V(G) \rightarrow [1, n]$. Thus for any labeling f we have $\text{lfl} = \min \{ |f(x) - f(y)| : xy \in E(G) \}$ and of course $s(G) = \max \{ \text{lfl} : f \text{ is a labeling of } G \}$. The parameter $s(G)$ known as the separation number of the graph G .

In this subsection we review some relations between the separation number and other natural graph parameters.

Theorem 1.1 [MP1]: For G of order n with $\delta(G) > 0$, $s(G) \leq \lfloor n/2 \rfloor$.

Proof: Let f be a labelling satisfying $\text{lfl} = s(G)$. Then $f(x) = \lceil n/2 \rceil$ for some x . Letting y be a neighbor of x , we have $s(G) \leq |f(x) - f(y)| \leq \lfloor n/2 \rfloor$. ■

Alternatively, the separation number can be conveniently viewed via subgraphhood. Let $H_{n,s}$ (a "host" graph) be the graph with $V(H_{n,s}) = [1, n]$, where $ij \in E(H_{n,s})$ if and only if $|i - j| \geq s$. For G of order n , it follows that $s(G) = \max \{ s : G \sqsubseteq H_{n,s} \}$. Consequently, it is useful to study these graphs $H_{n,s}$.

Lemma 1.2 [MP1]: Suppose $s \leq n/2$.

- (i) For each $i \in [1, s-1]$, $H_{n,s}$ has exactly two vertices (namely i and $n-i+1$) of degree $n+1-s-i$. The remaining $n+2-2s$ vertices each have degree $n+1-2s$.
- (ii) $|E(H_{n,s})| = \binom{n+1-s}{2}$.
- (iii) $\chi(H_{n,s}) = \lceil n/s \rceil$.

Proof: (i) easily follows from the definition of $H_{n,s}$. Taking one-half of the sum of the degrees of $V(H_{n,s})$, one easily verifies (ii).

For (iii) observe that any subset of $[1, n]$ of cardinality greater than s has its smallest and largest elements differing by at least s . Hence no such set is independent. Therefore $\times(H_{n,s}) \geq n/s$. The proper coloring given by $f(i) = \lceil i/s \rceil$ verifies that $\times(H_{n,s}) \leq \lceil n/s \rceil$. ■

For convenience, in statements of results throughout the rest of the paper, we consider only graphs G with $\delta(G) > 0$. Thus we may assume that $s(G) \leq n/2$, so that the facts about $H_{n,s}$ presented in lemma 1.2 are relevant.

Theorem 1.3 [MP1]: For G with n vertices and q edges, $\times = \times(G)$, $\delta = \delta(G)$, $\Delta = \Delta(G)$,

$$(i) \quad s(G) \leq n + \frac{1}{2} (1 - \sqrt{1+8q})$$

$$(ii) \quad s(G) < n/(\times - 1)$$

$$(iii) \quad s(G) \leq \frac{1}{2} (n - \delta + 1)$$

$$(iv) \quad s(G) \leq n - \Delta$$

Proof: Let $s = s(G)$. From (ii) of lemma 1.2, $q \leq |E(H_{n,s})| = \binom{n+1-s}{2}$, so $0 \leq s^2 - (2n+1)s + n^2 + n - 2q$. Solving this inequality as a quadratic in s , we obtain that either $s \leq \frac{1}{2} (2n+1 - \sqrt{1+8q})$ or $s \geq \frac{1}{2} (2n+1 + \sqrt{1+8q}) > n$. Clearly the latter is impossible, proving (i).

To prove (ii), observe that $\times(G) \leq \times(H_{n,s}) = \lceil n/s \rceil$, so $\times < n/s + 1$.

Finally, (iii) and (iv) follow from $\delta(G) \leq \delta(H_{n,s}) = n-2s+1$ and from $\Delta(G) \leq \Delta(H_{n,s}) = n-s$. ■

Thus far we have only presented *upper* bounds on the separation number. A strategy for giving constructive lower bounds for the separation number of bipartite graphs is embodied in the following theorem. For bipartite B with bipartition X, Y with $|X| = m$, $|Y| = n - m$, with $Y = \{y_1, y_2, \dots, y_{n-m}\}$ (the y_i 's in a fixed order), consider all labelings $f: V(B) \rightarrow [1, n]$ for which $f(y_i) = m+i$ for all $i \in [1, n-m]$. Let $s(B, \{y_i\})$ be the maximum value of $|f|$ among all such labelings f . For each $x \in X$, let $j(x) = \min\{i : x \text{ is adjacent to } y_i\}$. For each $t \in [1, n-m]$, let $Nb(t) = \{x \in X : j(x) = t\}$, let $New(t) = |Nb(t)|$, and let $B(i) = \sum_{t=1}^i New(t)$, the number of vertices adjacent to any or all elements of $\{y_1, y_2, \dots, y_i\}$.

Theorem 1.4 [MP1]: $s(B, \{y_i\}) = m - \max_i \{B(i) - i\}$

Proof: Let f be any labeling for which $f(y_i) = m+i$ for all $i \in [1, n-m]$. Among the $B(i)$ many vertices adjacent to $\{y_1, y_2, \dots, y_i\}$, there exists $x \in X$ with $f(x) \geq B(i)$. Now x has a neighbor y_j

for some $j \leq i$, so $|f(y_j) - f(x)| \leq m - \max_i \{B(i) - i\}$, hence $|f| \leq m - \max_i \{B(i) - i\}$. Therefore $s(B, \{y_i\}) \leq m - \max_i \{B(i) - i\}$.

Conversely, we construct a labelling f with $|f| \geq m - \max_i \{B(i) - i\}$. Let $X = \{x_1, x_2, \dots, x_m\}$. We give a linear order \angle on X as follows. Define $x_h \angle x_i$ if and only if either $j(x_h) < j(x_i)$ or $j(x_h) = j(x_i)$ and $h < i$. One easily verifies that \angle is linear. For x_i the k^{th} least element in the ordering, assign the label $f(x_i) = k$, and as usual let $f(y_i) = m + i$ for each i . For this labelling, if x and y_i are adjacent, it follows that $f(x) \leq B(i)$, so $|f(y_i) - f(x)| \geq (m + i) - B(i) \geq m - \max_i \{B(i) - i\}$. Therefore $|f| = \min \{ |f(y_i) - f(x)| : xy_i \in E(B) \} \geq m - \max_i \{B(i) - i\}$, proving the theorem. ■

We now find asymptotically good lower bounds for the separation number of m by n grids. For $m \geq n$, let $G_{m,n}$ be the usual Cartesian product graph $P_m \times P_n$ of order mn , where P_k is a path on the points $[1, k]$. Thus (i, j) and (i', j') are adjacent if and only if either $i = i'$ and $|j - j'| = 1$, or $j = j'$ and $|i - i'| = 1$. $G_{m,n}$ is bipartite, so we may take advantage of theorem 1.4.

Let $X = \{(i, j) \in V(G_{m,n}) : i + j \text{ is odd}\}$ and $Y = \{(i, j) \in V(G_{m,n}) : i + j \text{ is even}\}$. Let Y be ordered lexicographically, i.e. $(i, j) < (i', j')$ if and only if either $i < i'$, or $i = i'$ and $j < j'$. Let y_i denote the i^{th} least element of Y .

Theorem 1.5 [MP1]: $s(G_{m,n}, \{y_i\}) = \lfloor (mn - n)/2 \rfloor$. Consequently $s(G_{m,n}) \geq \lfloor (mn - n)/2 \rfloor$.

Proof: $\text{New}(i) = 2$ for $1 \leq i \leq n/2$, and $\text{New}(i) \leq 1$ for $i > n/2$. Therefore $s(G_{m,n}, \{y_i\}) = |X| - \max_i \{B(i) - i\} = \lfloor mn/2 \rfloor - (B(\lfloor n/2 \rfloor) - \lfloor n/2 \rfloor) = \lfloor mn/2 \rfloor - 2\lfloor n/2 \rfloor + \lfloor n/2 \rfloor = \lfloor (mn - n)/2 \rfloor$. ■

Notice that the lower bound $\lfloor (mn - n)/2 \rfloor$ is asymptotically optimal, in the sense that the ratio of it compared to the upper bound $\lfloor mn/2 \rfloor$ goes to 1 as $m \rightarrow \infty$.

Since $Q(n)$ is bipartite we can make use of Theorem 1.4, again using a certain lexicographic ordering of one side of the bipartition, to give an asymptotically optimal labeling f for $Q(n)$. The choice of labeling f will therefore be easy to describe here, and the difficult work (the reader is referred to [MP1]) is in evaluating $|f|$ so as to obtain a lower bound for $s(Q(n))$.

As usual, we represent the vertices of $Q(n)$ by n -digit words over the alphabet $\{0, 1\}$, where two vertices are joined by an edge if and only if they disagree in exactly one coordinate. We let $\text{wt}(v)$, the weight of a vertex $v \in Q(n)$, be the number of 1's in v . We denote repetition of digits and subwords by exponents, so that $1^2 0^2 (10)^3 = 1100101010$. Prefix and suffix have their natural meanings, so that the above word has 11 and 11001 among its prefixes, and has 010 as a suffix. Also we let $\mathbf{N}(v)$ be the set of points in $Q(n)$ adjacent to v .

We make use of the following lexicographic ordering $<$ of the points of $Q(n)$. Define $v < w$ if and only if either $\text{wt}(v) < \text{wt}(w)$, or $\text{wt}(v) = \text{wt}(w)$ and the first coordinate in which v and w disagree is a 1 in v and a 0 in w . Letting $v_n(i)$ denote the i^{th} lowest ordered element, we get the ordering $v_n(1) < v_n(2) < \dots < v_n(2^n)$. This ordering for $Q(4)$ is $0000 < 1000 < 0100 < 0010 < 0001 < 1100 < 1010 < 1001 < 0110 < 0101 < 0011 < 1110 < 1101 < 1011 < 0111 < 1111$.

The ordering we actually use the ordering e_n of the points of $Q(n)$ of even weight. Thus given two even weight words $x, y \in Q(n)$, y is the successor of x under e_n if and only if y is the first even weight word which comes after x under v_n . As n will be fixed in our discussion, we henceforth refer to $e_n(j)$ (the j th point under e_n) by $\underline{e}(j)$. For any $1 \leq t \leq 2^{n-1}$, we let $Nb(t) = N(e(t)) \setminus \bigcup_{i < t} N(e(i))$. We also write $Nb(v)$ to refer to $Nb(t)$, where $v = e(t)$.

The labeling f of $Q(n)$ may now be described. We let $f(e(i)) = 2^{n-1} + i$. The odd weight words are mapped in the manner specified by theorem 1.4. That is, f first maps the n neighbors of $0^n = e(1)$ to $[1, n]$ in any order. Inductively, having defined f on $\bigcup_{i \leq t} N(e(i))$, $t \geq 1$, we assign $Nb(t+1)$ to the integers $r+1$ through $r+|Nb(t+1)|$, where $r = |\bigcup_{i \leq t} N(e(i))|$. We will call such an f a lexicographic layout via the even weight words (recall that there are choices of how f is to act on the odd weight words, but these choices do not affect $|f|$).

As an example, a lexicographic layout f for $Q(4)$ written in the order $f^{-1}(1), f^{-1}(2), \dots, f^{-1}(16)$ is $\{1000, 0100, 0010, 0001, 1110, 1101, 1011, 0111, 0000, 1100, 1010, 1001, 0110, 0101, 0011, 1111\}$. For $v = e(t)$, let $New(t) = New(v) = |Nb(t)|$, and recall that $B(k) = \sum_{t=1}^k New(t)$.

Theorem 1.6: Assume $n \geq 3$. Let e be whichever of $\lfloor \frac{n-1}{2} \rfloor$ or $\lfloor \frac{n+1}{2} \rfloor$ is even, and let

$$F(e, n) = \binom{n}{e+1} + \binom{2e}{e} - \binom{n}{e} - \binom{2e}{e+1} - (n - e - 1) + \sum_{i=1}^{e-1} \left[\binom{2e-2j}{e-j} - \binom{2e-2j}{e-j+1} \right]. \text{ Then}$$

$$a) \quad s(Q(n)) \geq 2^{n-1} - \left[\binom{n-1}{e-1} + (n - e - 1) + F(e-1, n-1) \right] \text{ if } n \equiv 3 \pmod{4}, \text{ and}$$

$$b) \quad s(Q(n)) \geq 2^{n-1} - \left[\binom{n-1}{e-1} + (n - e - 1) + F(e, n) \right] \text{ otherwise.}$$

Furthermore, this lower bound is asymptotically optimal.

Sketch of proof: For any lexicographic layout f of $Q(n)$, we have by the proof of Theorem 1.4 that $|f| = s(B, \{y_i\})$ for $y_i = e(i)$. Hence $|f| = 2^{n-1} - \max_k \{B(k) - k\}$. So in using such an f to get a lower bound for $s(Q(n))$, we are reduced to finding the maximum of the function $B(k) - k$ over $1 \leq k \leq 2^{n-1}$.

Let us pick a lexicographic layout f arbitrarily. For an even weight vertex x with $x = e(r)$, let $\text{value}(x) = B(r) - r$. Define some special vertices $Y(b, n)$ of weight b in $Q(n)$ by $Y(b, n) = 1^{2b-n}(10)^{n-b}$ if $b \geq \lceil n/2 \rceil$ and $Y(b, n) = 0^{n-2b}(10)^b$ if $b < \lceil n/2 \rceil$. In particular we have $Y(b, 2b) = (10)^b$.

The overall plan of how to maximize $B(k) - k$ is the following.

- (1) Show that $Y(b, n)$ has a maximum value among weight b vertices.
- (2) The sequence $\{\text{value}(Y(b, n)) : b \text{ even}, 0 \leq b \leq n\}$ is unimodal.

Using these two facts we can then show that $B(k) - k$ reaches a maximum at that k for which $e(k) = Y(e, n)$, where e is whichever of $\lfloor (n-1)/2 \rfloor$ or $\lfloor (n+1)/2 \rfloor$ is even. After finding $\text{value}(Y(e, n))$ for this e the statement of the theorem follows. ■

Bounds on separation of G in hypercubes and torus graphs, via eigenvalues:

Let H^c denote the usual graph complement of a simple graph H . Let $H(k)$ denote the graph with vertex set $V(H)$, edge set $E(H(k)) = \{xy: 0 < d_H(x,y) \leq k\}$. We refer to $H(k)$ as the k'th power of H. Let $H^{(k)}$ be the graph with vertex set $V(H)$, edge set $E(H^{(k)}) = \{xy: d_H(x,y) = k\}$.

Let H be a regular graph on n points, and let $p \leq n$ be an integer. Consider the function $f(H,p) = \max\{|E(G)|: G \text{ is an induced subgraph of } H \text{ on } p \text{ points.}\}$. The problem of determining $f(H,p)$ for each integer p is well known as the edge isoperimetric problem for H .

The relevance of this problem to separation is that bounds for the function f yield edge bounds for separation. Specifically, suppose we knew $f(H(k)^c,p)$ and consider any graph G satisfying $|G| \leq |H|$. We would then know that if $f(G,p) > f(H(k)^c,p)$ then G cannot be embedded in $H(k)^c$, since a certain p -point induced subgraph of G is denser than the densest p -point induced subgraph of $H(k)^c$. Thus we may conclude that $f(G,p) > f(H(k)^c,p)$ implies $\text{sep}(G,H) \leq k$. In particular, if $|E(G)| > f(H(k)^c,|G|)$, then $\text{sep}(G,H) \leq k$.

The following result in [BuCS] provides bounds for $f(H,p)$ in terms of the eigenvalues of H . This result can also be derived using results of Alon and Milman [AM, remark 2.4]. Let G be any induced subgraph on p points of a d -regular graph H on n points. Then the average degree $d_1(G)$ of G satisfies

$$d_1(G) \leq \frac{p\lambda_1}{n} + d - \lambda_1,$$

where λ_1 is the difference between d and the second largest eigenvalue of H . (For graphs in general, i.e. ones which are not necessarily regular, λ_1 is defined in terms of the adjacency matrix $A(H)$ as the second smallest eigenvalue of the "Laplacian" matrix $Q = \text{diag}(\deg(v))_{v \in H} - A(H)$. For regular H , this definition of λ_1 reduces to the difference given above.). Now let $d = \lambda(1)(H) = \lambda(1) \geq \lambda(2)(H) = \lambda(2) \geq \dots \geq \lambda(n)(H) = \lambda(n)$ be the eigenvalues of H , so that $\lambda_1 = d - \lambda(2)$. It follows that

$$f(H,p) \leq \frac{1}{2} \left(p\lambda(2) \left(1 - \frac{p}{n}\right) + d \frac{p^2}{n} \right). \quad (A)$$

We see then that an upper bound for $f(H,p)$ would follow from an upper bound for $\lambda(2)$.

Suppose now that H is a d -regular graph on n vertices, and that also $H(k)$ (and therefore $H(k)^c$) is regular for each integer k , $1 \leq k \leq n$. Then the inequality above applies to $H(k)^c$. Recall now the well known relation between the eigenvalues of a d -regular graph S on n points and the eigenvalues of its complement S^c : if S has the eigenvalues $\lambda(1)=d, \lambda(2), \dots, \lambda(n)$, then S^c has the eigenvalues $n-d-1, -1-\lambda(2), \dots, -1-\lambda(n)$. Hence the second largest eigenvalue of S^c is $-1 - \lambda_{\min}(S)$, where $\lambda_{\min}(S)$ is the smallest eigenvalue of S . Since $\lambda_{\min} < 0$ for any graph having an edge, it follows that a lower bound for $\lambda_{\min}(S)$ yields an upper bound for $\lambda(2)(S^c)$ and hence an upper bound for $f(H(k)^c)$.

We will use these ideas in a form summarized by the following lemma.

Lemma 1.7 [MP2]: Let H be a graph on n points, and suppose $H(k)$ is regular for some k . Let $H(k)^c$ be d -regular, and assume $\lambda_{\min}(H(k)) \geq b(k)$ for some function b . Let G be a graph on p points and q edges, $p \leq n$.

(a) If $q > \frac{1}{2} (p[-1-b(k)] (1 - \frac{p}{n}) + d \frac{p^2}{n})$, then $\text{sep}(G,H) \leq k$.

(b) If $p > n \left(1 - \frac{n-d-1}{n-d-1-b(k)} \right)$, then $\text{sep}(K_p,H) \leq k$.

Proof: First we have $\lambda(2)(H(k)^c) = -1 - \lambda_{\min}(H(k)) \leq -1 - b(k)$. Now inequality (A) implies that a necessary condition for G to be embeddable in $H(k)^c$ is that

$$q \leq \frac{1}{2} (p[-1-b(k)] (1 - \frac{p}{n}) + d \frac{p^2}{n}). \quad (*)$$

Part (a) follows since the hypothesis violates the condition. Thus G is not embeddable in $H(k)^c$ so $\text{sep}(G,H) \leq k$.

For part (b) we just apply (*) to the complete graph $G = K_p$. Substituting $q = \binom{p}{2}$ and solving the resulting inequality for p , we obtain a necessary condition for embeddability of K_p in $H(k)^c$ which is violated by the hypothesis on p . Hence $\text{sep}(K_p,H) \leq k$. ■

We will be concerned with graphs H which, in addition to having regular k 'th powers for all k , have the additional property that $A(H(k))$ is a polynomial in $A(H)$ for each k . For such graphs the eigenvalues of $H(k)$ are easily obtained as polynomials in the eigenvalues of H . We briefly describe a method for finding the eigenvalues of powers of direct products of such graphs. Then by lower bounding or determining exactly λ_{\min} in these powers when H is a hypercube or torus graph, we obtain edge bounds for separation in these graphs using lemma 1.7, and hence applications to separation of arbitrary G in hypercubes and torus graphs.

We now recall some basic definitions from matrix theory. Suppose A, B are $m \times n$ and $p \times q$ matrices respectively. Then the Kronecker product of A and B , denoted by $A \otimes B$, is the $mp \times nq$ matrix obtained by replacing each entry a_{rs} of A by the $p \times q$ matrix $a_{rs}B$. Now suppose A and B are adjacency matrices of graphs S and T , and let $x, x' \in V(S)$ and $y, y' \in V(T)$. The (y, y') entry of the submatrix $a_{xx'}B$ of $A \otimes B$ will be referred to as the $((x, y), (x', y'))$ entry of $A \otimes B$. Under a suitable ordering of the points in the graph $S \times T$, this entry is the one which corresponds in the adjacency matrix of $S \times T$ to the pair of points $\{(x, y), (x', y')\}$.

Lemma 1.8 [MP2]: Let G and H be two graphs. Then for any k , $1 \leq k \leq n$, we have the following adjacency matrix relationship:

$$A((G \times H)(k)) = \sum_{s+t=k} A(G^{(s)}) \otimes A(H^{(t)}).$$

Using Lemma 1.8 we can prove following theorem giving the eigenvalues of the k 'th power $(G \times H)(k)$ of the graph product $G \times H$, under the assumption that $A(G^{(i)})$ and $A(H^{(i)})$ are expressible as polynomials in the matrices $A(G)$ and $A(H)$ respectively for all $i \geq 1$. With this assumption let $p_i(x)$ and $q_i(x)$ be polynomials such that $p_i(A(G)) = A(G^{(i)})$ and $q_i(A(H)) =$

$A(H^{(i)})$. For eigenvalues λ and μ of G and H respectively, denote by $\lambda^{(s)}$ and $\mu^{(t)}$ the numbers $p_s(\lambda)$ and $q_t(\mu)$.

Theorem 1.9 [MP2]: Let G and H be graphs for which $A(G^{(i)})$ and $A(H^{(i)})$ are expressible as polynomials in $A(G)$ and $A(H)$ respectively for all $i \geq 1$. Then the set of eigenvalues of $(G \times H)(k)$ is given by

$$\left\{ \sum_{1 \leq s+t \leq k} \lambda^{(s)} \mu^{(t)} : \lambda, \mu \text{ eigenvalues of } G \text{ and } H \text{ respectively, listed with multiplicity} \right\}.$$

Using this result and a fair amount of analysis we can determine $\lambda_{\min}(Q(n)(k))$ precisely for k odd, and for k even in certain ranges, obtaining bounds for the remaining cases.

Theorem 1.10 [MP2]:

(I) If k is odd, then $\lambda_{\min}(Q(n)(k)) = -1 - \binom{n-1}{k}$.

(II) Suppose k is even. Then

(a) If $k \geq \frac{n}{2}$, then $\lambda_{\min}(Q(n)(k)) = \binom{n-2}{k} - \binom{n-2}{k-1} - 1$.

(b) If $k = \frac{n-1}{2}$, then $\lambda_{\min}(Q(n)(k)) = 2\binom{n-3}{k} + 2\binom{n-3}{k-2} - \binom{n-1}{k} - 1$.

(c) If $k < \frac{n-1}{2}$, then $\lambda_{\min}(Q(n)(k)) \geq \binom{n-2}{k-1} - \binom{n-2}{k} - 1$.

We can now combine these results and Lemma 1.7 to get edge bounds for separation in $Q(n)$.

Corollary 1.11 [MP2]: Let $N = |Q(n)| = 2^n$. Let G be a graph on p points and q edges.

Suppose k is odd.

If $q > \frac{1}{2} \left(p \binom{n-1}{k} \left(1 - \frac{p}{N}\right) + \frac{p^2}{N} \sum_{t=k+1}^n \binom{n}{t} \right)$, then $\text{sep}(G, Q(n)) \leq k$.

If $p > N \left(1 - \frac{N - \sum_{t=k+1}^n \binom{n}{t} - 1}{N - \sum_{t=k+1}^n \binom{n}{t} + \binom{n-1}{k}} \right)$, then $\text{sep}(K_p, Q(n)) \leq k$.

Suppose k is even, with $k \geq \frac{n}{2}$.

If $q > \frac{1}{2} \left(p \left(\binom{n-2}{k-1} - \binom{n-2}{k} \right) \left(1 - \frac{p}{N}\right) + \frac{p^2}{N} \sum_{t=k+1}^n \binom{n}{t} \right)$, then $\text{sep}(G, Q(n)) \leq k$.

Suppose k is even, with $k < \frac{n-1}{2}$.

If $q > \frac{1}{2} \left(p \left(\binom{n-2}{k} - \binom{n-2}{k-1} \right) \left(1 - \frac{p}{N}\right) + \frac{p^2}{N} \sum_{t=k+1}^n \binom{n}{t} \right)$, then $\text{sep}(G, Q(n)) \leq k$.

Suppose k is even, with $k = \frac{n-1}{2}$.

$$\text{If } q > \frac{1}{2} \left(p \left(\binom{n-1}{k} - 2 \binom{n-3}{k} - 2 \binom{n-3}{k-2} \right) \left(1 - \frac{p}{N} \right) + \frac{p^2}{N} \sum_{t=k+1}^n \binom{n}{t} \right), \text{ then } \text{sep}(G, Q(n)) \leq k.$$

A similar approach, consisting of theorem 1.9 and an extended analysis, bounds λ_{\min} in powers of the torus graph $C_n \times C_n$ and hence yields separation bounds via lemma 1.7. For brevity, we state here just the bounds on separation.

Corollary 1.12 [MP2]: Let G be a graph on p points and q edges, $p \leq n^2$, $k < n/2$.

(a) Suppose k is even.

$$\text{If } q > \frac{1}{2} \left(p \left(\frac{k+1}{\sin(\pi/(k+1))} + k^2 \right) \left(1 - \frac{p}{n^2} \right) + (n^2 - 2k^2 - 2k - 1) \frac{p^2}{n^2} \right) \text{ then } \text{sep}(G, C_n \times C_n) \leq k.$$

(b) Suppose k is odd.

$$\text{If } q > \frac{1}{2} \left(p \left(\frac{k}{\sin(\pi/k)} + (k+1)^2 \right) \left(1 - \frac{p}{n^2} \right) + (n^2 - 2k^2 - 2k - 1) \frac{p^2}{n^2} \right) \text{ then } \text{sep}(G, C_n \times C_n) \leq k.$$

2. Separation of $K(r,s)$ in Hypercubes.

In this section we present the first of our new results, an analysis of $\text{sep}(K(r,s), Q(n))$, where $K(r,s)$ is the complete r by s bipartite graph for positive integers r and s with $2^n \geq r+s$. This result follows directly from some classic theorems in extremal set theory, and our purpose here is to explain the interesting connection with these theorems.

The following definitions will be needed. Let $W(k,n)$ be the set of points of $Q(n)$ of weight k . For a point $x \in W(k,n)$, let $\Delta^{k-1}(x)$ be the set of neighbors of x of weight $k-1$. For $S \subseteq W(k,n)$, let $\Delta^{k-1}(S) = \bigcup_{x \in S} \Delta^{k-1}(x)$, and for $0 \leq d \leq k-1$ let $\Delta^d(S) = \Delta^d(\Delta^{d+1}(S))$. Thus $\Delta^d(S)$ consists of all points $y \in W(d,n)$ with $d_Q(x,y) = k-d$, i.e. all points y obtained from $x \in S$ by changing $k-d$ of the 1's in x to 0's. Given subsets X and Y of $V(Q(n))$, we use the notation $\text{dist}(X,Y)$ to refer to $\min\{d_Q(x,y) : x \in X, y \in Y\}$. For any integer k , let $\underline{b}(k) = \max \{p : \binom{n}{0} + \binom{n}{1} + \dots + \binom{n}{p} \leq k\}$ and let $\underline{e}(k) = k - \sum_{i=0}^{\underline{b}(k)} \binom{n}{i}$.

For integers n and k with $1 \leq k \leq n$, a k -binomial representation of n is an expression for n as a sum of binomial coefficients in the form

$$n = \binom{a_k}{k} + \binom{a_{k-1}}{k-1} + \dots + \binom{a_t}{t} \quad (\text{I})$$

where $a_k > a_{k-1} > \dots > a_t \geq t \geq 1$. Given n and k , it is well known that this expression is uniquely determined. Define the operator $L(k,-): \mathbb{Z} \rightarrow \mathbb{Z}$ which takes an integer n together with its k -binomial representation and produces the integer $L(k,n)$ together with its $(k-1)$ -binomial representation as follows:

$$L(k,n) = \binom{a_k}{k-1} + \binom{a_{k-1}}{k-2} + \dots + \binom{a_t}{t-1}. \quad (\text{II})$$

It is understood that if $t-1 = 0$, then $\binom{a_t}{0}$ is rewritten as $\binom{a_{t+1}}{0}$, and the last two terms are combined to give $\binom{a_{t+1}}{0} + \binom{a_{t+1}}{1} = \binom{1+a_{t+1}}{1}$. If $1+a_{t+1} = a_{t+2}$, then we add again to get $\binom{a_{t+2}}{1} + \binom{a_{t+2}}{2} = \binom{1+a_{t+2}}{2}$, continuing in this way until the representation for $L(k,n)$ satisfies the constraints of (I). To abbreviate notation, we let $L^{(2)}(k,n) = L(k-1, L(k,n))$, and inductively $L^{(r)}(k,n) = L(k-r+1, L^{(r-1)}(k,n))$, so that $L^{(r)}(k,n)$ is a $(k-r)$ -binomial representation of an integer.

For example, start with the 4-binomial representation of 23: $23 = \binom{6}{4} + \binom{4}{3} + \binom{3}{2} + \binom{1}{1}$. Our initial expression for $L_4(23)$ based on formula (II) is $\binom{6}{3} + \binom{4}{2} + \binom{3}{1} + \binom{1}{0}$. The term $\binom{1}{0}$ is not allowed under the constraints of (I), so we write $\binom{1}{0} = \binom{3}{0}$ and combine the last two terms to get $\binom{3}{0} + \binom{3}{1} = \binom{4}{1}$. This gives $\binom{6}{3} + \binom{4}{2} + \binom{4}{1}$ which again violates the constraints, so we combine the last two terms to finally get $L_4(23) = \binom{6}{3} + \binom{5}{2}$. We also have $L_4^{(2)}(23) = \binom{6}{2} + \binom{5}{1}$, and after applying (II) and combining terms $L_4^{(3)}(23) = \binom{7}{1}$.

Using the operator $L(k,-)$ and the previous definitions, we can now calculate $\text{sep}(K(r,s), Q(n))$.

Theorem 2: Let r and s be two positive integers. Then

- a) If $e(r) = e(s) = 0$, then $\text{sep}(K(r,s), Q(n)) = n - b(s) - b(r)$.
- b) If exactly one of $\{e(r), e(s)\}$ is 0 but the other is not, then $\text{sep}(K(r,s), Q(n)) = n - b(s) - b(r) - 1$.
- c) If $e(r) > 0$ and $e(s) > 0$, then
 - i) $\text{sep}(K(r,s), Q(n)) = n - b(s) - b(r) - 1$ if $e(r) \leq \binom{n}{b(r)+1} - L^{(n-b(s)-b(r)-2)}(n-b(s)-1, e(s))$.
 - ii) $\text{sep}(K(r,s), Q(n)) = n - b(s) - b(r) - 2$ otherwise.

Proof: Denote by A the independent r -set and B the independent s -set in the bipartition of $K(r,s)$. We note first that among all separators $f: K(r,s) \rightarrow Q(n)$, the maximum value of $|f|$ is achieved when A is mapped to a Hamming ball about some point v and B is mapped to a Hamming ball about the antipodal point w in $Q(n)$. (This follows from [Ha], with a simpler proof in [FF] that is described in [Bo]). So let f be a map with maximum value $|f|$ having this Hamming ball property, and we take the two points v and w to be 0^n and 1^n . Thus $f(A)$ consists of all points in $Q(n)$ of weight at most $b(r)$ together with $e(r)$ points of weight $b(r)+1$, while $f(B)$ consists of all points of weight at least $n - b(s)$ together with $e(s)$ points of weight $n - b(s) - 1$. Let $\underline{T}(A) = f(A) \cap W(b(r)+1, n)$ and $\underline{T}(B) = f(B) \cap W(n-b(s)-1, n)$.

We begin by noting that given integers k and k' satisfying $0 \leq k < k' \leq n$, and points $z \in W(k, n)$ and $z' \in W(k', n)$, we have

$$\begin{aligned} \text{dist}(z,z') &= k' - k && \text{if } z \in \Delta^k(z') \\ &\geq k' - k + 2 && \text{if } z \notin \Delta^k(z') \end{aligned} \quad (*)$$

It is understood here that $0^n \in \Delta^0(z')$ for all points z' .

Consider part a). There must exist a pair of points $y \in W(b(r),n)$ and $y' \in W(n-b(s),n)$ such that $y \in \Delta^{b(r)}(y')$. It follows that $\text{lfl} = \text{dist}(f(A),f(B)) = d_Q(y,y') = n-b(s)-b(r)$, as required. For part b), suppose without loss of generality that $e(r) > 0$ and $e(s) = 0$. For any point $y \in T(A)$ there is a point $y' \in W(n-b(s),n) \cap f(B)$ with $y \in \Delta^{b(r)+1}(y')$, from which it follows in the same way that $\text{lfl} = n-b(s)-b(r)-1$.

Now consider part c). If there is a pair of points $y \in T(A)$ and $y' \in T(B)$ with $y \in \Delta^{b(r)+1}(y')$, then $\text{dist}(T(A),T(B)) = \text{dist}(y,y') = n-b(s)-b(r)-2$. If no such pair exists, then $\text{dist}(T(A),T(B)) \geq n-b(s)-b(s)$ (by (*)), while $\text{dist}(T(A),f(B)) = \text{dist}(T(B),f(A)) = n-b(s)-b(r)-1$. It follows that $\text{lfl} = \text{dist}(f(A),f(B)) = n-b(s)-b(r)-2$ or $n-b(s)-b(r)-1$, depending on whether such a pair y and y' exists or not respectively. But such a pair exists if and only if $T(A) \cap \Delta^{b(r)+1}(T(B)) \neq \emptyset$. Hence (since lfl is a maximum) f may be assumed to have the following properties.

- (i) $T(B)$ is a subset of $W(n-b(s)-1,n)$ for which $|\Delta^{b(r)+1}(T(B))|$ is a minimum over all subsets of $W(n-b(s)-1,n)$ of size $|T(B)|$ ($= e(s)$).
- (ii) If $|T(A)|$ (which equals $e(r)$) $\leq \binom{n}{b(r)+1} - |\Delta^{b(r)+1}(T(B))|$ then $T(A) \subset W(b(r)+1,n) - \Delta^{b(r)+1}(T(B))$, and in this case we have $\text{lfl} = n-b(s)-b(r)-1$. Otherwise, $T(A)$ can be any subset of of size $e(r)$ in $W(b(r)+1,n)$, and in that case $\text{lfl} = n-b(s)-b(r)-2$.

The method of choosing $T(B)$ so that $|\Delta^{b(r)+1}(T(B))|$ is minimized is provided by the Kruskal-Katona theorem ([Kr],[Ka]). This theorem says that for integers p,k and d , where $1 \leq p \leq \binom{n}{k}$ and $d < k$, the minimum of $|\Delta^d(S)|$ over all subsets S of $W(k,n)$ of a given size p is achieved when S is taken to be the first p points in the "squashed" ordering of $W(k,n)$ (see [A]). For this optimal choice of S , it is a consequence of the Kruskal-Katona theorem (again see [A]) that $|\Delta^d(S)| = L^{(k-d)}(k,p)$. Now apply this discussion to the set $T(B)$ (of size $e(s)$) in place of S , $n-b(s)-1$ in place of k , and $b(r)+1$ in place of d . Part c) follows. ■

3. Separation of complete graphs in trees.

In this section we present a simple and efficient algorithm for finding $\text{sep}(K_p, T)$ for T any tree. First we present Algorithm A which, given positive integers p and t and a tree T , decides whether T has a set of p points in T that are t -separated (i.e. each pair in the set are at distance t or larger in T) and finds p such points when such a set exists. One can then run Algorithm A sequentially on the values $t = 1, 2, 3, \dots, \text{Diam}(T)$ to find the largest t for which T has p points that are t -separated, that largest t being $\text{sep}(K_p, T)$, thereby solving the separation problem.

Algorithm A:Input: Positive integers p, t and a tree T .Output: Determines whether T has a t -separated set of size p , and construct such a set when one exists.(Initialization) Let $T_1 = T$ and $R_1 = V(T)$.For $i = 1, 2, \dots, p$, do the following:

- (1) Select a vertex v in T_i , and let x_i be any vertex furthest from v in T_i . If $i = p$ then go to (4).
- (2) Let $R_{i+1} = R_i - \{\text{vertices of } T_i \text{ closer than } t \text{ away from } x_i\}$. If $R_{i+1} = \emptyset$ then go to (4).
- (3) Delete from T_i any leaf not in R_{i+1} , and continue removing leaves from the remaining tree if they are not in R_{i+1} , until all leaves of the remaining tree are in R_{i+1} . Let T_{i+1} be the remaining tree. Increase i by one and go to (1).
- (4) If $i = p$ then $\{x_1, x_2, \dots, x_p\}$ is t -separated in T . Otherwise, no p vertices are t -separated in T .

The proof that Algorithm A does what it is claimed to do is deferred until theorem 3.3. This is because we can generalize the algorithm to apply to edge-weighted trees, and indeed to tree structures in the plane where we seek p points that are t -separated, allowing those points to be in the interior of the tree edges. We can even solve the decision problem in which we restrict that the p points be selected from a specified subset of the points in the tree. In fact, as evidenced by the role of R_i in the operation of Algorithm A, this sort of restriction is natural to the solution process even when no restrictions are given for the original tree T .

We now extend the notion of $\text{sep}(G, H)$ to the notion of $\text{sep}(G, X)$, where $X = (X, d)$ is a metric space with metric function d (here G is still a graph). Much as before, an injective function $f: V(G) \rightarrow X$ is called a separator of G in X , whose minimum distance is given by

$|f| = \min\{d(f(x), f(y)) : xy \in E(G)\}$. An s -separator of G in X is a separator f with $|f| \geq s$. For G and (X, d) with $|V(G)| \leq |X|$, the separation number $\text{sep}(G, X)$ of G in X is defined as

$\text{l.u.b.}\{s : \text{there is an } s\text{-separator of } G \text{ in } X\} = \text{l.u.b.}\{|f| : f \text{ is a separator of } G \text{ in } X\}$. When the range of d is finite, $\text{sep}(G, X) = \max\{|f| : f \text{ is a separator of } G \text{ in } X\}$.

The reader may be familiar with the following examples of problems involving separation in metric spaces. There's a simple pigeon-hole principle argument (see pg. 23 of [Br]) that among any 5 points in a closed 2×2 square, some two must be $\sqrt{2}$ units apart or closer (i.e. the hard part of proving that $\text{sep}(K_5, SQ) = \sqrt{2}$ for SQ a 2×2 square under Euclidean metric). The problem of spreading out p points as far apart as possible on the unit sphere S , i.e. no two closer than $\text{sep}(K_p, S)$, is a compelling unsolved problem.

In keeping with the concepts of the theory of error-correcting codes, we make the following definitions. For (X, d) a metric space, refer to an arbitrary finite set $C \subseteq X$ as a code C in X , and define the minimum distance of C to be $\text{MinDist}(C) = \min\{d(x, y) : x, y \in C, x \neq y\}$. When the range of d is finite, notice that $\text{sep}(K_p, X) = \max\{\text{MinDist}(C) : C \subseteq X, |C| = p\}$. A code $C \subseteq X$ is s -separated if $d(x, y) \geq s$ for every pair of points x, y in C . For $x \in X$ and r in $[0, \infty)$, define the open ball of radius r about x as $B(x, r) = \{y \in X : d(x, y) < r\}$, and the closed ball of radius r about x as

$B[x,r] = \{ y \in X : d(x,y) \leq r \}$. Given t in $(0,\infty)$, let $A(X,t) = \max \{ |C| : C \text{ is } t\text{-separated in } X \}$, when such a maximum exists. This maximum exists for all t in $(0,\infty)$ exactly when (X,d) is totally bounded. In coding theory, $A(n,t)$ usually denotes what we can here call $A(Q(n),t)$, namely the largest number of words in a t -separated code of binary n -tuples. For H any graph observe that $\text{sep}(K_p, H) = \max \{ t : A(V(H),t) \geq p \}$ using the usual distance metric for $V(H)$, and that $A(V(H),t) = \max \{ p : \text{sep}(K_p, H) \geq t \}$.

A t -separated code C in X is called t -optimal if $|C| = A(X,t)$. A point $x \in X$ is called t -remote if $B(x,t) \subseteq B(y,t)$ for every $y \in B(x,t)$. If for some reason we wish to consider only those separators f for which $f(V(G)) \subseteq R$ for a specified restrictive set $R \subset X$, then we can replace (X,d) by (R,d_R) where d_R is the restriction of d to pairs of points in R , and concern ourselves with separators of G in R and $\text{sep}(G,R)$. In such cases, we make the slight abuse of notation by letting (R,d) denote (R,d_R) , and similarly $(X-R,d)$ will denote $(X-R,d_{X-R})$.

Lemma 3.1: If x is t -remote in $X = (X,d)$, then for every t -optimal code C in $(X-B(x,t),d)$ the code $C \cup \{x\}$ is t -optimal in X .

Proof: Let x be t -remote in X , let C be t -optimal in $X-B(x,t)$, and let C' be any t -separated code in X . Clearly $C \cup \{x\}$ is t -separated in X , so it suffices to show that $|C \cup \{x\}| \geq |C'|$. Suppose for contradiction that $|C \cup \{x\}| < |C'|$. Since $C' - B(x,t)$ is t -separated in $X - B(x,t)$, we have that $|C' - B(x,t)| \leq |C|$, so there exist distinct $y, z \in C' \cap B(x,t)$. Since x is t -remote in X , $z \in B(x,t) \subseteq B(y,t)$, so $d(y,z) < t$, contradicting that C' is t -separated. Therefore $|C \cup \{x\}| \geq |C'|$, completing the proof. ■

A sequence of points x_1, x_2, \dots, x_A in a metric space (X,d) is called a t -sequence if the sequence of sets $X = X_1, X_2, \dots, X_A$ generated by the recurrence $X_{i+1} = X_i - B(x_i, t)$ is such that for each i , x_i is t -remote in (X_i, d) , and $X_A \subseteq B(x_A, t)$. Iteratively applying lemma 3.1, notice that such a set $C = \{x_1, x_2, \dots, x_A\}$ forms a t -optimal code in (X,d) , and that $A = A(X,t)$. Thus we have fallen into good fortune when we can specify and/or iteratively generate a t -sequence for X . Indeed we show a simple way to iteratively generate a t -sequence in any of a wide variety of tree structures. Our interest will be in the case where X is a planar representation of a tree T , with d being a natural distance metric between points in X , as follows. Let $T = (V, E, \omega)$ be an edge-weighted tree, in which the weight of each edge $e \in E$ is given by $\omega(e)$ for some specified weight function $\omega : E \rightarrow (0, \infty)$. The weight $\omega(T)$ of the tree is defined as the sum of the weights of its edges. There exists an embedding of T in \mathbb{R}^2 , i.e. a set v of $|V|$ many points and a set e of $|E|$ many simple curves in \mathbb{R}^2 , and bijections $f : V \rightarrow v$, $g : E \rightarrow e$ such that for each $vw \in E$, $g(vw)$ is a simple curve of length $\omega(vw)$ whose ends are $f(v)$ and $f(w)$, such that for every $vw \neq xy$ in E , $g(vw) \cap g(xy) = \{f(v), f(w)\} \cap \{f(x), f(y)\}$. An embedding of T in \mathbb{R}^n would serve equally well for any $n \neq 2$. Let $X = \bigcup_{uv \in E}$

$g(u,v)$. To any points A,B in X there corresponds a unique simple curve $P(A,B) \subseteq X$ with ends A and B , referred to as a closed segment of X . Letting $d(A,B)$ denote the length of $P(A,B)$, d serves as a metric for X such that distances between vertices in T are the same as the distances between their images under f in X . Refer to the resulting metric space (X,d) as a representation of T .

For the remainder of the paper, a subset R of a representation X of a tree T is called a restriction of X if it is a finite union of closed segments of X . Note that a single point in X is always a closed segment of X . Let $\text{Diam}(X) = \max\{d(A,B) : A,B \in X\}$, the diameter of X . By the correspondence between X and T , we see that $\text{Diam}(X)$ is also the usual diameter of the weighted tree T , and points A,B at distance $\text{Diam}(X)$ in X must correspond to leaves at that same distance $\text{Diam}(X)$ in T .

Lemma 3.2: Let (X,d) be a representation of a weighted tree T , with R a restriction of X . Let $D = \text{Diam}(X)$. Suppose that $d(A_0, A_D) = D$ for some $A_0 \in R$, $A_D \in X$, and let $t \in (0, \infty)$. Then A_0 is t -remote in (R,d) .

Proof: We show that $B(A_0, t) \subseteq B(y, t)$ for each $y \in B(A_0, t)$, these being open balls in (X,d) . This suffices, because the corresponding property in (R,d) will hold, being inherited from X . For each $z \in [0, D]$, let A_z denote the unique point on $P(A_0, A_D)$ for which $d(A_0, A_z) = z$.

Claim: If $z \in [0, t/2)$ then $B(A_0, t) \subseteq B(A_z, t-z)$, and if $z \in [t/2, t)$ then $B(A_0, t) \subseteq B[A_z, z]$.

Proof of claim: Consider any $y \in B(A_0, t)$, and let A_w be the nearest point of $P(A_0, A_D)$ to y . It suffices to show that $d(A_z, y) < t-z$ when $z < t/2$ and that $d(A_z, y) \leq z$ when $z \geq t/2$.

Case I: Suppose $w \geq z$. Then $d(A_z, y) = d(A_0, y) - d(A_0, A_z) < t - z$. When $z \geq t/2$, we have that $t - z \leq z$, so that $d(A_z, y) < t - z \leq z$.

Case II: Suppose $w < z$. Then $d(A_z, y) = d(A_D, y) - d(A_D, A_z) \leq D - (D - z) = z$. When $z < t/2$, we have that $z < t - z$, so that $d(A_z, y) \leq z < t - z$, proving the claim.

Returning to the lemma, we now show that $B(A_0, t) \subseteq B(y, t)$ for each $y \in B(A_0, t)$, proving the lemma. We employ the facts that $d(A_w, y) \leq w$ (else $d(A_D, y)$ would exceed D) and that $w < t - d(A_w, y)$, as follows. If $w \in [0, t/2)$, then $B(A_0, t) \subseteq B(A_w, t - w) \subseteq B(y, t - w + d(A_w, y)) \subseteq B(y, t)$, where these containments (in order) follow from the claim, from the triangle inequality, and from $d(A_w, y) \leq w$, so we are done. If $w \in [t/2, t)$ then $B(A_0, t) \subseteq B[A_w, w] \subseteq B(A_w, t - d(A_w, y)) \subseteq B(y, t)$, where these containments (in order) follow from the claim, from $w < t - d(A_w, y)$, and from the triangle inequality, completing the proof. ■

For (X,d) a representation of an edge-weighted tree T , points of X corresponding to vertices of T are called vertices of X , and vertices of X corresponding to leaves of T are called leaves of X . Observe for any restriction R of X and point v in X that $R - B(v, t)$ is also a restriction of X . Further observe that if leaf L is such that $B(L, s)$ includes no vertices of X other than L , then

$(X-B(L,s),d)$ is a representation of some edge-weighted tree T' , for which $R-B(L,s)$ is a restriction (although we may have to designate a point of $X-B(L,s)$ as being a leaf now, even when it wasn't a vertex of the representation X). Now we present our algorithm for determining whether X has a t -separated set of p points in a given restriction R . Note that if any leaf L of X is in R , we can equivalently determine whether $X-B(L,s)$ has a t -separated set of p points in R , where s is the largest real number for which $B(L,s)$ contains no points of R and no vertices of X other than L . Therefore we lose no generality by treating only the case in which all leaves of X are in R .

Algorithm B:

Input: Positive integers p,t and a restriction R for X , where X is a representation $X = (X,d)$ of an edge-weighted tree T such that all leaves of X are in R .

Output: Determines whether a t -separated set of size p exists in (R,d) , and constructs such a set when one exists.

(Initialization) Let $X_1 = X$ and $R_1 = R$.

For $i = 1,2,\dots,p$, do the following:

- (1) Select a vertex v in X_i , and let x_i be any leaf furthest from v in X_i . If $i = p$ then go to (4).
- (2) Let $R_{i+1} = R_i - \{\text{points of } X_i \text{ closer than } t \text{ away from } x_i\}$. If $R_{i+1} = \emptyset$ then go to (4).
- (3) Find any leaf L of X_i that is not in R_{i+1} , and delete from X_i the set $B(L,s)$, where s is the largest real number for which $B(L,s)$ contains no points of R_{i+1} and no vertices of X_i other than L . Repeat until the remaining representation of a tree has all of its leaves in R_{i+1} . Let X_{i+1} be the remaining representation of a tree. Increase i by one and go to (1).
- (4) If $i = p$ then $\{x_1, x_2, \dots, x_p\}$ is t -separated in (R,d) . Otherwise, no p points of R are t -separated in X .

Theorem 3.3: Algorithm A and Algorithm B perform the tasks that they claim to do. Furthermore, Algorithm A applies equally well to edge-weighted trees.

Proof: Assume that Algorithm B does the task it claims to do. Given p,t and a tree T , assign each edge of T an edge-weight of 1, and perform Algorithm B on a representation X of this edge-weighted tree, using the restriction $R = \{\text{vertices of } X\}$. It is straightforward to verify that Algorithm B will perform steps on X corresponding exactly to the steps Algorithm A will perform on T , so Algorithm A does the task it claims to do. Indeed if T is an edge-weighted tree and we wish to determine whether it has p vertices that are t -separated, Lemma B will also succeed via the restriction $R = \{\text{vertices of } X\}$, and it is straightforward to verify that Algorithm A applies in its stated form to every edge-weighted tree T .

We now show that Algorithm B does the task it claims to do. Note that step (2) of the algorithm ensures that each R_i is a restriction of X_i . In X_i , let M be the midpoint of a longest path. It is a simple exercise to prove that a point q in X_i has a point at distance $D = \text{Diam}(X_i)$ away from

it in X_i if and only if q is a leaf of X_i such that $d(q, M) = D/2$. It is also easy to prove that if x_i is a leaf furthest from v in X_i then x_i has a point at distance D from it in X_i . Also, (1) and (3) ensure that each x_i is in R_i . Therefore by lemma 3.2, x_i is t -remote in (R_i, d) for each x_i that arises in performing Algorithm B.

Suppose that the algorithm terminates, having reached step (4). If $i = p$ when it terminates, then the set $\{x_1, x_2, \dots, x_p\}$ is t -separated in X , by the action of (2), so Algorithm B has done as claimed. If instead $i < p$ when it terminates, it is because $R_{i+1} = \emptyset$, in which case x_1, x_2, \dots, x_i is a t -sequence in (R, d) , so $\{x_1, x_2, \dots, x_i\}$ is t -optimal in (R, d) (by the discussion following lemma 3.1), so no p points of R are t -separated in X , and Algorithm B has done as claimed.

It remains only to prove that Algorithm B terminates in a finite number of steps! In the process of proving this, we also provide upper bounds for the number of times that certain parts of the algorithm can be iterated. In each execution of (3), either the weight of the associated tree drops by at least t with no increase in the number of edges, or else the number of edges drops by at least one with no increase in the weight of the associated tree. Therefore (3) is executed at most $\frac{\omega(T)}{t} + |E(T)|$ many times, so the algorithm proceeds only finitely many times through the cycle of items (1),(2) and (3). To resolve the concern that a single execution of (3) might involve infinitely many steps, observe that each execution of (3) can involve at most $|V|$ choices for the leaf L , since for each such L any new vertices created in deleting $B(L, s)$ must be in R_{i+1} . ■

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