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Expansion of layouts of complete binary trees into grids☆

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Abstract

Let T_h be the complete binary tree of height h. Let M be the infinite grid graph with vertex set Z^2, where two vertices (x_1, y_1) and (x_2, y_2) of M are adjacent if and only if $|x_1-x_2|+|y_1-y_2|=1$. Suppose that T is a tree which is a subdivision of T_h and is also isomorphic to a subgraph of M. Motivated by issues in optimal VLSI design, we show that the point expansion ratio $n(T)/n(T_h) = n(T)/(2^{h+1}-1)$ is bounded below by 1.122 for h sufficiently large. That is, we give bounds on how many vertices of degree 2 must be inserted along the edges of T_h in order that the resulting tree can be laid out in the grid. Concerning the constructive end of VLSI design, suppose that T is a tree which is a subdivision of T_h and is also isomorphic to a subgraph of the $n \times n$ grid graph. Define the expansion ratio of such a layout to be $n^2/n(T_h) = n^2/(2^{h+1}-1)$. We show constructively that the minimum possible expansion ratio over all layouts of T_h is bounded above by 1.4656 for sufficiently large h. That is, we give efficient layouts of complete binary trees into square grids, making improvements upon the previous work of others. We also give bounds for the point expansion and expansion problems for layouts of T_h into extended grids, i.e. grids with added diagonals.

1. Introduction

Embeddings appear in the literature [12,14] for the purpose of describing one of the following: (1) an efficient simulation of one parallel computer architecture by another,

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(2) an efficient method for using a parallel computer architecture to execute some standard computational processes, or (3) to give area-efficient patterns for printing circuits on VLSI chips or wafers. In an embedding, one has a *guest* graph $G=(V, E)$ that represents the parallel architecture to be simulated, the computation graph to be mapped to processors, or the circuit to be laid out. In addition, one has a *host* graph $H=(V', E')$ that represents the parallel computer architecture on which the computation is to be performed or the positions for gates and routing paths on a VLSI chip or wafer.

Here we consider embedding complete binary trees into grid and extended grid graphs. Both the grid graph $M[m,n]$ and extended grid graph $\mathrm{EM}[m,n]$ have the same set of m rows and n columns of vertices, namely the set of lattice points $\{(x,y) \mid 1 \leqslant x \leqslant m \text{ and } 1 \leqslant y \leqslant n\}$. $M[m,n]$ has an edge between (p,q) and (s,t) iff $|p-s|+|q-t|=1$, and $\mathrm{EM}[m,n]$ has an edge between (p,q) and (s,t) if and only if $\max\{|p-s|,|q-t|\}=1$. Alternatively, nodes of $M[m,n]$ are adjacent when their Euclidean distance is 1, and nodes of $\mathrm{EM}[m,n]$ are adjacent when their Euclidean distance is 1 or $\sqrt{2}$. Let T_h denote the complete binary tree of height h with $2^{h+1}-1$ vertices. We use standard notation from graph theory, in particular letting $n(G)$ denote the number of vertices in a graph G, $\Delta(G)$ the maximum degree among vertices of G, and $d_G(u,v)$ the distance in G between vertices u and v.

We consider one-to-one, congestion one embeddings f of complete binary trees into two-dimensional grids and extended two-dimensional grids. That is, such an f is an injection assigning to each vertex v in a tree T a single vertex $f(v)$ in a grid or extended grid M, also assigning to each edge uv of T a path $f(uv)$ in M between $f(u)$ and $f(v)$ such that the internal nodes of $f(uv)$ include neither $f(z)$, for any vertex z in T, nor any point in the path $f(st)$ for any edge $st \neq uv$ in T. In other words, the image of f is a subgraph of M which is homeomorphic to T. Such an embedding is commonly called a *layout*, and we shall use the two terms embedding and layout interchangeably. For a layout f of T_h (having a tree T homeomorphic to T_h) into $M[m,n]$ or $\mathrm{EM}[m,n]$ we consider the *expansion* ratio r of f, i.e. the number of points in $M[m,n]$ divided by the number of points in T_h, namely $r=mn/(2^{h+1}-1)$. For the most part we are interested in low expansion layouts of T_h into square grids (i.e. where $m=n$). We also consider the *point expansion* ratio r' of f, i.e. the number of points in T divided by the number of vertices in T_h, namely $r'=n(T)/(2^{h+1}-1)$. For example, the layout of T_8 into $M[24,39]$ shown in Fig. 7 has expansion $r=24\times 39/511 \approx 1.832$ and point expansion $r'=610/511 \approx 1.194$. The dashed line in the figure indicates a path (later called an "escape" or "channel") from the root of T_8 that could be used to iterate the construction by joining two such layouts of T_8 to obtain a layout of T_9. Since this path is not properly part of the layout of T_8, its vertices are not counted in the numerator of the point expansion.

More generally, let f be an embedding from a guest graph G to a host graph H. The *dilation* of an edge uv under f is the length of the path $f(uv)$. The *dilation* of the embedding f is the maximum dilation of any edge of G under f. The *load* of a vertex x in H under f, denoted by $\mathrm{load}(x)$, is the number of vertices mapped to x by f. The *congestion* of a vertex x in H under f, denoted by $\mathrm{congestion}(x)$, is the number of paths of the form $f(uv)$, for an edge uv in G containing x as an internal vertex. The *total congestion* of a vertex x is $\mathrm{load}(x)+\mathrm{congestion}(x)$. In this language, note

that the embeddings we consider have total congestion 1. By contrast, the embeddings given in [7,18] of complete binary trees into a nearly optimum grid generally have total congestion exceeding 1.

Many results on embeddings related to parallel computation deal with the problem of embedding different types of graphs into grids and hypercubes, since those structures are used in several large scale parallel computers (see [14]). It should be noted, however, that the MasPar computer (see [2,11]) allows each interior node to communicate directly with its eight nearest grid neighbors. Thus, embeddings into extended grids are also important (see [10]). We point out that, while extended grids have pairs of diagonal edges which "cross" (which may be viewed as a design flaw for some applications), none of our layouts use both edges from any pair of crossing diagonal edges.

In the areas of graph drawing and visualization (see [5]), the embeddings we study, called planar orthogonal grid drawings, are judged by further considerations for aesthetics. Since our objectives in this paper normally include laying out a complete binary tree into a *square* grid, our layouts are nice in that they have the ideal aspect ratio of length to width, namely 1. Our objective of minimizing the expansion ratio is the same problem as minimizing "area efficiency", whereas our objective of minimizing the point expansion ratio is the same problem as minimizing "total edge length". However, here we pay no mind to issues of whether the layouts have a natural "downward" structure to them (customarily useful for visualizing a binary tree), or whether our layouts possess symmetries, or whether we pay a cost per "bend" since our edges need not be laid out as straight line segments. See [4] for example concerning planar straight-line orthogonal grid drawings of binary trees, in which no such "bends" are allowed. Consequently, our layout results are more suitable from a VLSI point of view than from a visualization point of view.

The problem of embedding binary trees into grids has been studied extensively, although the objectives involved often vary from paper to paper. Embeddings of the complete binary tree T_{2n-1} into its optimum square grid $M[2^n, 2^n]$ with load one were considered in several papers. An embedding with nearly optimum dilation, namely $2 + (2^{n-1} - 1)/(n-1)$, is given in [9]. The vertex congestion of this embedding is $\Omega((2^{n-1} - 1)/(n-1))$. Embeddings with vertex congestion 2 are given in [19] with dilation $\frac{4}{3}2^{n-1} + O(1)$ and in [8] with dilation 2^{n-1}. Embeddings of trees into grids with small dilation are also the subject of several papers [1,8,16].

A famous example of the type of embedding we consider is the familiar H-tree layout [3] (see Fig. 1a). It embeds even height complete binary trees into square grids, specifically, T_{2n} into $M[2^{n+1} - 1, 2^{n+1} - 1]$, when one starts with an initial layout of T_0 into $M[1,1]$.

The H-tree construction: Assume we have an embedding of T_h into $M[n,n]$ such that there is a path of grid points, between the image of the root $M[n,n]$ and the border of $M[n,n]$, consisting of vertices that are not images of vertices in T_h (except for the image of the root). In VLSI applications such a free path is called a *channel*. Construct an embedding of T_{h+2} into $M[2n+1, 2n+1]$ as follows:

(1) Divide $M[2n+1, 2n+1]$ into four subgrids $M[n,n]$ separated by a middle row and middle column. Put an embedding of T_h into each of the four subgrids in

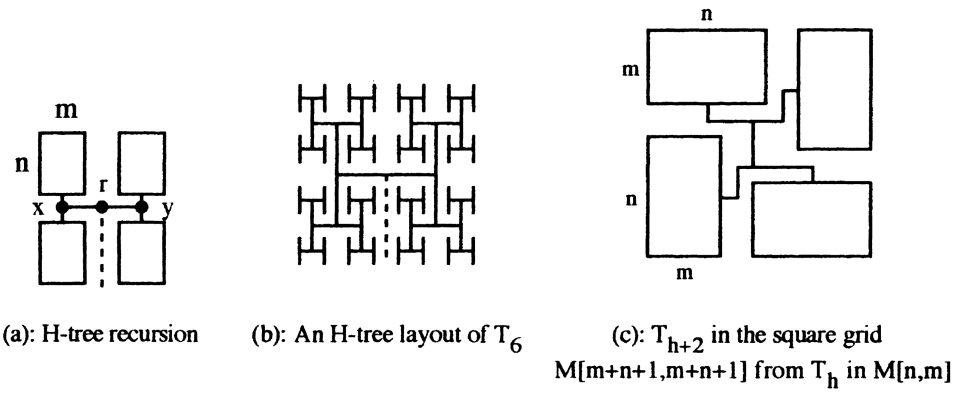


Fig. 1. H-tree and modified H-tree constructions. (a) H-tree recursion; (b) H-tree layout of T_6; and (c) T_{h+2} in the square grid $M[m+n+1, m+n+1]$ from T_h in $M[n,m]$.

such a way that the channels go from the images of the root to the middle row of $M[2n+1, 2n+1]$ (see Fig. 1a).

(2) The root r of T_{h+2} is mapped to the point at the intersection of the middle row and the middle column and its two children x and y are mapped to the intersection of the middle row and the columns containing the free channels associated with the T_h embeddings. Since the T_h subtrees joined at x are laid out the same inductively, x is in the same column as the channel columns it joins, and likewise for y.

(3) The images of the edges in T_{h+2} incident to r, x or y are laid out along the channels in the subgrids and segments of the middle row (they form an H-pattern). This construction allows a channel in the new middle column, so that the process can be iterated. See Fig. 1b for the H-tree layout of T_6 resulting from such iteration, where the new channel is the dashed line extending downward.

Notice that the H-tree construction uses only about 50% of the added middle row and column, and the unused space accumulates iteratively. Corresponding to this simple observation, it turns out that the expansion of the H-tree layout of T_{2n} approaches 2 as n grows. One way to reduce the total unused space in an iterative use of the H-tree construction is to start with initial embeddings of a complete binary tree which are constructed ad hoc to have less unused space than that given by an application of the usual H-tree construction. For this purpose rectangular grids can be more space efficient. The H-tree construction can be recursively applied to rectangles and an embedding into a square can be obtained as the last step of the construction using a modified H-tree construction, as shown in Fig. 1c.

Ducourthial and Mèrigot [6] used this strategy with initial embeddings of T_3 into $M[5,4]$ and T_6 into $M[15,13]$. This resulted in the following theorem, where by the *size* of an $n \times n$ grid we simply mean n, the number of points on a side.

Theorem 1 (Ducourthial [6]). *There exists a layout of the complete binary tree T_{2p+1} into a square grid of size $2^{p+1}+2^{p-1}+2^{p-2}-1$ for $p \geqslant 2$, and of T_{2p} into a square grid of size $2^p+2^{p-1}+2^{p-2}+2^{p-3}-1$ for $p \geqslant 3$. These embeddings have expansions approaching* 1.891 *for T_{2p+1} and* 1.758 *for T_{2p}.*

Opatrny and Sotteau [15] recently described an improvement, with initial embeddings of T_4 into $M[7,6]$ and $M[8,5]$ and T_7 into $M[20,18]$ and $M[19,19]$, then iteratively combining 16 copies of embeddings of T_{h-4} into $M[n,m]$ and $M[n-1,m+1]$ to obtain an embedding of T_h into $M[4n,4m+4]$ and $M[4n-1,4m+5]$, terminating with an embedding into a square grid by the step shown in Fig. 1c. This resulted in:

Theorem 2 (Opatrny and Sotteau [15]). *There exists a layout of the complete binary tree T_{2p+1} into a square grid of size $2^{p+1}+2^{p-2}+2^{p-3}+\lceil(1/3)(2^{p-2}-(-1)^{p \bmod 2})\rceil$ for $p \geqslant 4$, and of T_{2p} into a square grid of size $2^p+2^{p-1}+2^{p-2}+\lceil(1/3)(2^{p-2}-(-1)^{p \bmod 2})\rceil$ for $p \geqslant 3$. These embeddings have expansions approaching* 1.51 *for T_{2p+1} and* 1.606 *for T_{2p}.*

We improve upon these results, by techniques described in Section 2, showing:

Theorem 3. *For each integer $k \geqslant 0$,*
there exists a layout of T_{6k+15} into a square grid of size $\frac{1}{7}(2^{3k+5}(67)-2)$,
there exists a layout of T_{6k+17} into a square grid of size $\frac{1}{7}(2^{3k+6}(67)+3)$,
there exists a layout of T_{6k+19} into a square grid of size $\frac{1}{7}(2^{3k+7}(67)+13)$,
there exists a layout of T_{6k+16} into a square grid of size $\frac{1}{7}(2^{3k+2}(767)-2)$,
there exists a layout of T_{6k+18} into a square grid of size $\frac{1}{7}(2^{3k+3}(767)+3)$,
there exists a layout of T_{6k+20} into a square grid of size $\frac{1}{7}(2^{3k+4}(767)+13)$.

These layouts of T_p have expansions approaching $(67/56)^2 \approx 1.4315$ for p odd and $(767)^2/(2^{13}49) \approx 1.4656$ for p even.

For extended meshes, Opatrny and Sotteau [15] gave similar constructions and demonstrated an upper bound on expansion of 1.208 (resp., 1.247) for complete binary trees of even (resp., odd) heights. We improve the upper bounds on expansion to 1.115. Our construction is described in Section 3.

The point expansion $n(T)/n(T_{2n})$ of the H-tree layout turns out to approach 1.5 as n grows. In Sections 4–6 we obtain the lower bound $r' \geqslant 1.122$ for large values of h for the point expansion of layouts of T_h into grids and the lower bound $r' \geqslant 1.03$ for the point expansion of layouts of T_h into extended grids. Of course, $r \geqslant r'$ for any layout, so that these bounds also serve as lower bounds for the expansion r of such layouts.

Summarizing then, our results for expansion are that $1.122 \leqslant r \leqslant 1.4656$ (for large h) where r is the least expansion among layouts of T_h into grids, and $1.03 \leqslant r \leqslant 1.115$ (for large h) where r is the least expansion among layouts of T_h into extended grids. While the upper bounds are the latest improvements in a series of upper bounds by others (Tables 1 and 2), the lower bounds are the first to appear.

Table 1
Historical progress on the sizes of square grids into which complete binary trees of height h have been embedded

Height of tree	H-tree	Duc. & Mèr.	Opat. & Sott.	Ours
6	15	14	14	14
8	31	29	29	27
10	63	59	57	55
12	127	119	115	111
14	255	239	229	223
16	511	479	459	420

Table 2
Historical progress on the asymptotic ratio for expansion for embedding complete binary trees into square grids

Height of tree	H-tree	Duc. & Mèr.	Opat. & Sott.	Ours
Even	2	1.758	1.606	1.4656
Odd	Not applicable	1.892	1.510	1.4315

2. Embedding complete binary trees into grids

The following is an outline of our procedure for constructing layouts of complete binary trees into grids. We start with embeddings of T_7 and T_8 (see Figs. 2 and 3) into various rectangular grids. Using the schemes of Figs. 4 and 5, we pump these up to obtain our actual basis case embeddings of T_{13} and T_{14}. To these embeddings we iteratively apply the schemes of Fig. 6, obtaining layouts of complete binary trees of arbitrarily large height into rectangular grids. Finally, from these layouts we use the scheme of Fig. 1c to get layouts into square grids.

Before describing our recursive process for constructing layouts of larger complete binary trees from layouts of smaller ones, we describe the basis step for the process. The basis step consists of layouts of T_{13} into $M[158, 147]$ and into $M[157, 148]$, along with layouts of T_{14} into $M[230, 207]$ and into $M[229, 208]$. Essentially all of our layouts include an *escape* channel, i.e. a path from the image of the tree's root to the grid's periphery, as shown by example in Fig. 2a. We obtain each of the two layouts of T_{14} from 64 copies of layouts of T_8, as illustrated by Figs. 2a–c and 4a, and b.

Note: Be warned that while Fig. 4 (and figures to come that are like it) fairly explicitly illustrates how these 64 copies are to be connected, some minor details are nevertheless left to the reader. Consider for example the blocks labeled B and A at the left of the bottom row of blocks in Fig. 4a. The A block represents a copy of Fig. 2a flipped so that its escape opens to the left, and the B block represents a copy of Fig. 2b flipped so that its "L-shaped" escape opens to the right and then up. The figure suggests that the escapes of these two copies join exactly at the bend in the "L" of block B's escape, but this is not quite so! In actuality, the horizontal part of the escape

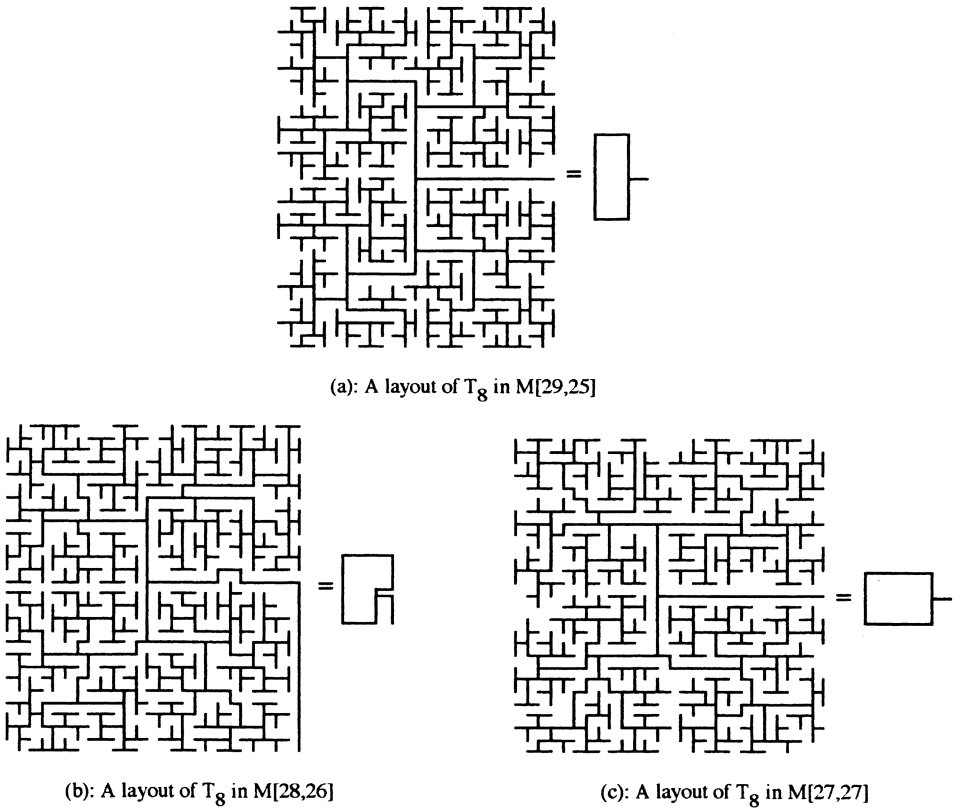


Fig. 2. Some layouts of T_8 into grids, and how they fit into Fig. 4. (a) Layout of T_8 in $M[29,25]$; (b) layout of T_8 in $M[28,26]$; and (c) a layout of T_8 in $M[27,27]$.

in the B block is in the 14th row from the bottom of $M[230,207]$, whereas the escape in the A block is in the 15th row from the bottom, so it joins the B block's escape one row above the bend. However, these figures do consistently follow the policy that once two such blocks join, these figures faithfully show how those junctions are further connected by paths so as to join the smaller layouts of complete binary trees to form a layout of a larger one, along with an escape path from the root to the periphery. A short "jog" in such a connecting path illustrates a change to an adjacent row or column. Also consider for example the 6th block in the first row of blocks in Fig. 4a. This B block is shown with a small portion taken out of it relative to the portrayal of other B blocks. This means that a single ordinarily unused vertex in that block (in this case the vertex in the last row, second column of the B block) is being used for the paths connecting the roots of the blocks in forming a layout of a larger complete binary tree.

Similarly, we obtain each of the two layouts of T_{13} from 64 copies of layouts of T_7, as illustrated by Figs. 3 and 5. It may be possible to find layouts of T_{13}

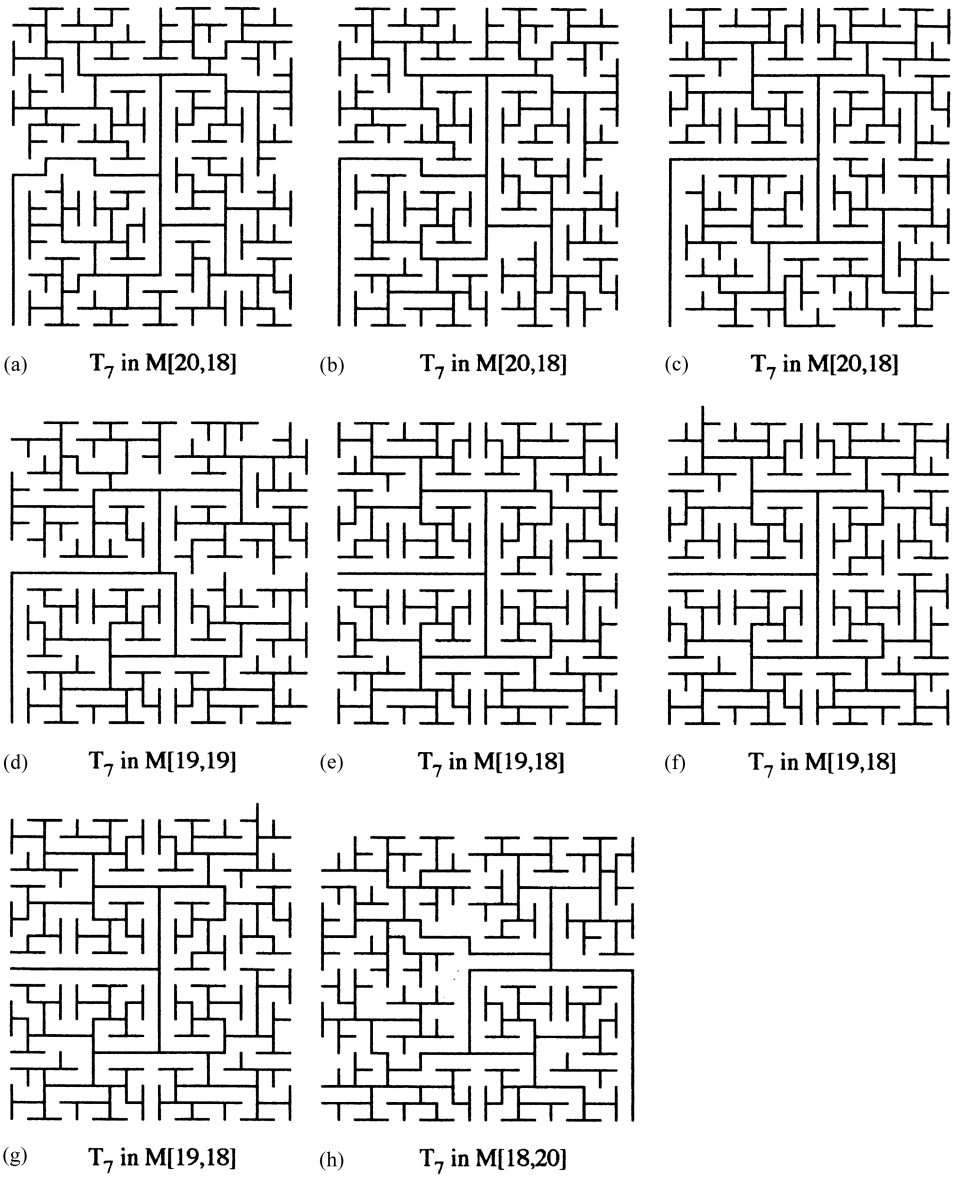


Fig. 3. Some layouts of T_7 into grids. (a) T_7 in $M[20,18]$; (b) T_7 in $M[20,18]$; (c) T_7 in $M[20,18]$; (d) T_7 in $M[19,19]$; (e) T_7 in $M[19,18]$; (f) T_7 in $M[19,18]$; (g) T_7 in $M[19,18]$; and (h) T_7 in $M[18,20]$.

and/or T_{14} (along with escapes) into smaller grids, but the reader probably needs no convincing that it took great effort for us to obtain layouts as compact as we have given. Note that the upper left and lower right vertices of Fig. 5a are unused, as are the lower left and lower right vertices in Fig. 5b, as well as all four

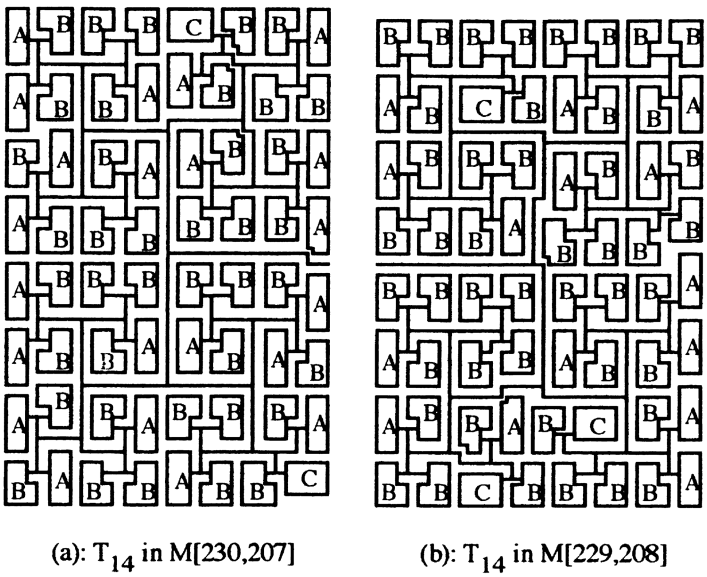


Fig. 4. Layouts of T_{14} from the pieces shown in Fig. 2a–c. (a) T_{14} in $M[230,207]$ and (b) T_{14} in $M[229,208]$.

corner vertices in Figs. 4a and b. We will use these available corners in the recursive construction.

Having specified the enormous pieces which constitute the basis step, now we consider the general induction process.

Construction 1 (see Fig. 6)

Input: For some integers a, b, a layout of T_h into $M[a,b]$ with an escape from the image of the root to the rectangle's side of length a (represented in Fig. 6 by the narrow rectangle), and a layout of T_h into $M[a-1, b+1]$ with an escape from the image of the root to the rectangle's side of length $a-1$ (represented in Fig. 6 by the wide rectangle). For purposes of this section, on each side of length a or $a-1$, a corner vertex must be unused.

Output: A layout of T_{h+6} into $M[8a, 8b+9]$ with an escape from the image of the root to the side of length $8a$ in the rectangle, as shown in Fig. 6a, and a layout of T_{h+6} into $M[8a-1, 8b+10]$ with an escape from the image of the root to the side of length $8a-1$ in the rectangle, as shown in Fig. 6b. For purposes of this section, on each side of length $8a$ or $8a-1$, a corner vertex will be unused (because we can flip the input copies so as to arrange for this feature). Note that Fig. 6 includes some "diagonal" edges. This is so that we can use the same figure in a later section on extended grids in which diagonal entries are allowed. For this section, regard those diagonal edges as representing a pair of edges, one horizontal and one vertical, which serve the same purpose as the diagonal edge shown but in fact meet at and use one of the otherwise unused corner vertices available by the nature of the input layouts.

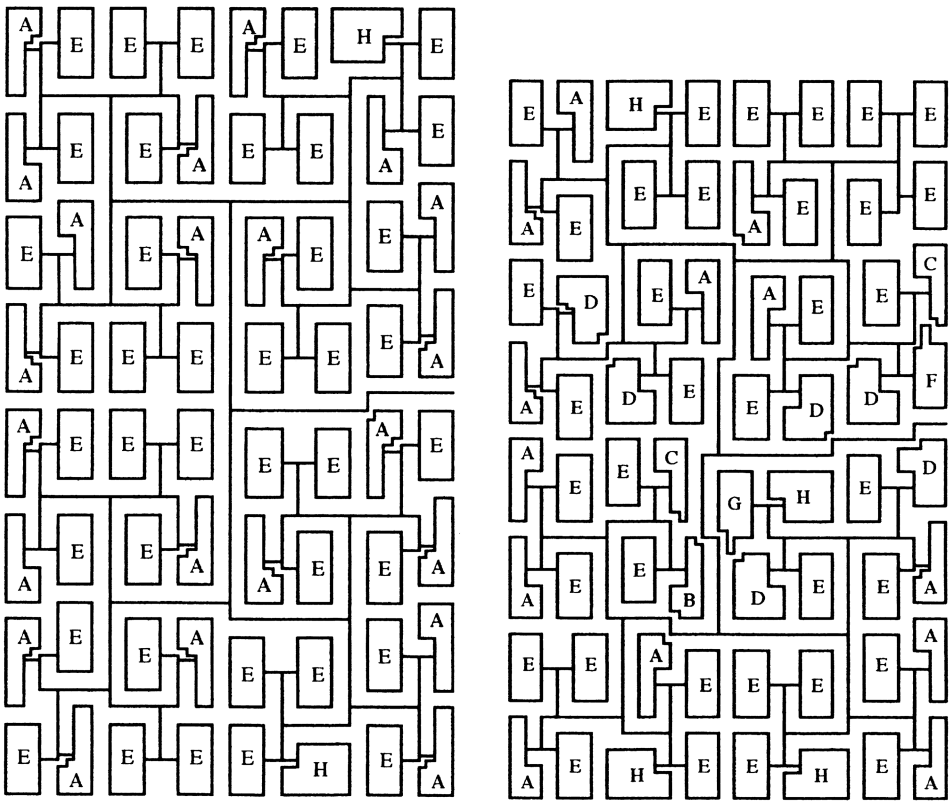


Fig. 5. Layouts of T_{13} from the pieces shown in Fig. 3. (a) T_{13} in $M[158,147]$ and (b) T_{13} in $M[157,148]$.

Notice that the output of Construction 1 can again be used as input to Construction 1. Thus, the construction can be iterated to produce layouts of T_{h+12} into $M[64a, 64b+81]$ and $M[64a-1, 64b+82]$, and then layouts of T_{h+18} into $M[2^9a, 2^9b+657]$ and $M[2^9a-1, 2^9b+658]$. In general, after k iterations, the recurrence produces a layout of T_{h+6k} into $M[a_k-1, b_k+1]$, where the a_k's and b_k's satisfy the recurrences $a_0=a$, $a_{k+1}=8a_k$, and $b_0=b$, $b_{k+1}=8b_k+9$. Clearly $a_k=2^{3k}a$, and a simple induction or solving of the linear recurrence for b_k yields that $b_k=2^{3k}b+\frac{9}{7}(2^{3k}-1)$, yielding the following:

Lemma 1. *Given layouts of T_h into $M[a,b]$ and $M[a-1,b+1]$ with escapes satisfying the assumptions of Construction* 1, *for each $k \geqslant 0$ there exists a layout of T_{h+6k} into $M[2^{3k}a,\ 2^{3k}b+\frac{9}{7}(2^{3k}-1)]$, having an escape from the image of the root to a side of size $2^{3k}a$ in the rectangle.*

Lemma 1 gives us a means for obtaining layouts for complete binary trees of arbitrarily large heights from layouts of smaller complete binary trees, but the results

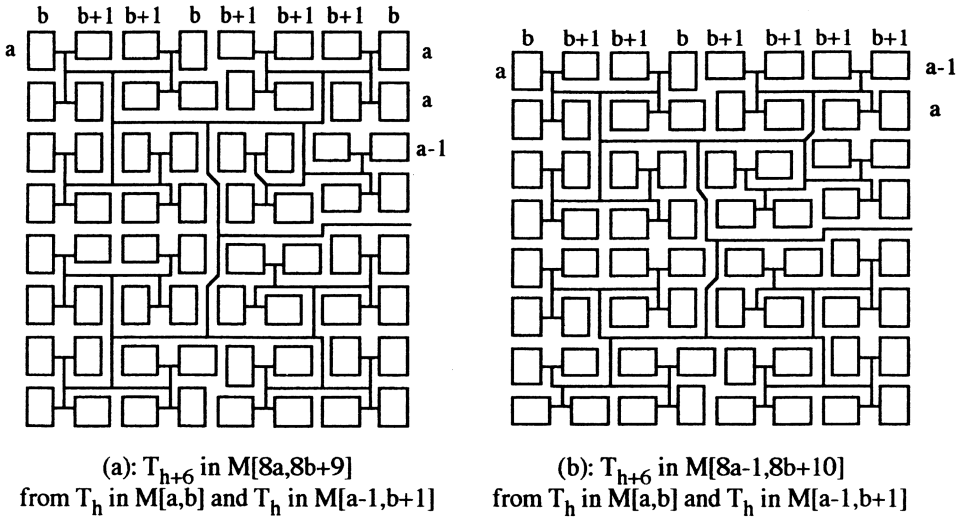


Fig. 6. Construction. (a) T_{h+6} in $M[8a, 8b+9]$ from T_h in $M[a,b]$ and T_h in $M[a-1, b+1]$ and (b) T_{h+6} in $M[8a-1, 8b+10]$ from T_h in $M[a,b]$ and T_h in $M[a-1, b+1]$.

are layouts into rectangular grids, not square ones. We use the following (used also in [6,15]) for "squaring up" large layouts, since grids in applications are often square, and so that the results can be easily compared to the results of others, using square grids as a standard. Since this step is not to be iterated, we need not include an escape in the output.

Construction 2 (see Fig. 1c)

Input: For some integers m, n, a layout of T_h into $M[m,n]$ with an escape from the image of the root to the rectangle's side of length n.

Output: A layout of T_{h+2} into the square grid of size $m+n+1$ (with no escape necessarily available).

Proof of Theorem 3 (from Section 1). Start with our layouts of T_{13} into $M[158, 147]$ and $M[157, 148]$, then apply Construction 1 iteratively k times, and then apply Construction 2 to obtain the desired layout of T_{6k+15}, where the size of the square into which it is embedded is easily verified. Similarly, from those same two starter layouts, instead apply Construction 1 iteratively k times, then apply the H-tree Construction once, and then apply Construction 2 to obtain the desired layout of T_{6k+17}. To obtain the desired layout of T_{6k+19} from those same starter layouts, apply Construction 1 iteratively k times, then apply the H-tree Construction twice, and then apply Construction 2. For layouts of complete binary trees of even heights, start with our layouts of T_{14} into $M[230, 207]$ and $M[229, 208]$. Applying Construction 1 iteratively k times and then Construction 2 yields the T_{6k+16} result, whereas applying Construction 1 iteratively k times and then the H-tree construction once and then Construction 2 yields the T_{6k+18} result, while applying Construction 1 iteratively k times and then the H-tree

construction twice and then Construction 2 yields the T_{6k+20} result. As for the asymptotics for the expansions of these layouts, $\lim_{k\to\infty}(\frac{1}{7}(2^{3k+5}(67)-2))^2 \div (2^{6k+15+1}-1) = \lim_{k\to\infty}(\frac{1}{7}(2^{3k+5})(67))^2 \div 2^{6k+16} = (67/56)^2$, which rounds up to 1.4315, and $\lim_{k\to\infty}(\frac{1}{7}(2^{3k+2}(767)-2))^2 \div (2^{6k+16+1}-1) = \lim_{k\to\infty}(\frac{1}{7}(2^{3k+2})(767))^2 \div 2^{6k+17} = (767)^2/(2^{13}49)$, which rounds up to 1.4656, and essentially the same computations hold for the other four cases in the theorem. We have rounded up so that we know for all large odd p that a layout of T_p into a square grid exists having expansion at most 1.4315 and for all large even p that a layout of T_p into a square grid exists having expansion at most 1.4656. Note that we know of very slightly improved layouts over those presented in Theorem 3, but the asymptotics involved give no improvement, and the exposition of how to obtain those layouts is a bit more complicated. □

3. Embedding complete binary trees into extended grids

We now turn to embedding complete binary trees into extended grids. In [15], Opatrny and Sotteau used a recursive construction which alternated between two schemes. Starting with embeddings of T_h into extended meshes $\mathrm{EM}[n,m]$ and $\mathrm{EM}[n-1,m+1]$, they use the first scheme (their modified Construction 2) to construct layouts of T_{h+4} into $\mathrm{EM}[4n-1,4m+4]$ and $\mathrm{EM}[4n,4m+4]$. Then they use the second scheme (their Construction 3) on T_{h+4} to get layouts of T_{h+8} into $\mathrm{EM}[16n-1,16m+18]$ and $\mathrm{EM}[16n,16m+19]$. Starting with embeddings of T_5 into $\mathrm{EM}[11,6]$ and $\mathrm{EM}[10,7]$, and embeddings of T_6 into $\mathrm{EM}[13,11]$ and $\mathrm{EM}[12,12]$, and alternating between these two schemes, they finally embed into a square extended grid to get the following.

Theorem 4 (Opatrny and Sotteau [15]). *There exist layouts of T_{2p} (for $p \geqslant 4$, $p \equiv 0 \pmod 4$) and T_{2p+1} (for $p \geqslant 3$, $p \equiv 3 \pmod 4$) into square extended grids of sizes $2^p + 2^{p-1} + 2^{p-4} + \frac{2}{15}(2^{p-4}-1)$ and $2^{p+1} + 2^{p-2} + \frac{2}{15}(2^{p-3}-1)$, respectively. These layouts have expansions approaching 1.234 for T_{2p} and 1.284 for T_{2p+1}.*

The modification of Construction 2 in [15] consists of adding an extra column to the scheme of their Construction 2, only part of which is used at each stage of the iteration. This waste then compounds itself upon successive iterations. In this section, we are able to improve upon their results by using better iteration schemes and by starting off with more efficient initial layouts.

Theorem 5. *For each integer $k \geqslant 0$,*

there exists a layout of T_{6k+15} into an extended square grid of size $\frac{1}{7}(2^{3k+2}(473)-2)$,
there exists a layout of T_{6k+17} into an extended square grid of size $\frac{1}{7}(2^{3k+3}(473)+3)$,
there exists a layout of T_{6k+19} into an extended square grid of size $\frac{1}{7}(2^{3k+4}(473)+13)$,
there exists a layout of T_{6k+16} into an extended square grid of size $\frac{1}{7}(2^{3k+2}(669)-2)$,
there exists a layout of T_{6k+18} into an extended square grid of size $\frac{1}{7}(2^{3k+3}(669)+3)$,
there exists a layout of T_{6k+20} into an extended square grid of size $\frac{1}{7}(2^{3k+4}(669)+13)$,

These layouts of T_p have expansions approaching $(473)^2/(2^{12}49) \approx 1.115$ *for* p *odd and* $(669)^2/(2^{13}49) \approx 1.115$ *for* p *even.*

Proof. Consider Construction 1, shown in Figs. 6a and b. This time, that figure is used to illustrate tree layouts into *extended* grids (not grids), where in this section we can treat the diagonal edges of those figures as literally representing diagonal edges. The figure shows how, given layouts of T_h into EM$[n,m]$ and EM$[n-1,m+1]$, we can produce layouts of T_{h+6} into EM$[8n,8m+9]$ and EM$[8n-1,8m+10]$, where we can treat the diagonal edges of those figures as literally representing diagonal edges in the extended mesh. By partially ad hoc methods we obtain layouts of T_{13} in each of EM$[144,125]$ and EM$[143,126]$ (using layouts of T_7 in EM$[18,15]$ and EM$[17,16]$), and layouts of T_{14} in each of EM$[192,189]$ and EM$[191,190]$ (using layouts of T_8 in EM$[24,23]$ and EM$[23,24]$). We use these two layouts of T_{13} and two layouts of T_{14} as the basis step for our iterative procedure. Details on these layouts of T_{13} and T_{14} into EM, and of T_7 and T_8 on which they are based are omitted here for brevity, but are given in the Electronic Appendix.[1]

Observe that Lemma 1 still holds if we replace each M by EM in its statement, where concerning Construction 1 (as in its statement) we no longer require in this section that there are any unused corner vertices. This holds because the diagonal edges in Fig. 6 are interpreted literally. So, for layouts of complete binary trees of odd heights, start with our layouts of T_{13} into EM$[144,125]$ and [143,126], then apply Construction 1 iteratively k times, and then apply Construction 2 to obtain the desired layout of T_{6k+15}, where the size of the square into which it is embedded is easily verified. Similarly, from those same two starter layouts, instead apply Construction 1 iteratively k times, then apply the H-tree Construction once, and then apply Construction 2 to obtain the desired layout of T_{6k+17}. To obtain the desired layout of T_{6k+19} from those same starter layouts, apply Construction 1 iteratively k times, then apply the H-tree Construction twice, and then apply Construction 2. For layouts of complete binary trees of even heights, start with our layouts of T_{14} into EM$[192,189]$ and EM$[191,190]$. Applying Construction 1 iteratively k times and then Construction 2 yields the T_{6k+16} result, whereas applying Construction 1 iteratively k times and then the H-tree construction once and then Construction 2 yields the T_{6k+18} result, while applying Construction 1 iteratively k times and then the H-tree construction twice and then Construction 2 yields the T_{6k+20} result. As for the asymptotics for the expansions of these layouts, for the T_{6k+15} result we have

$$\lim_{k\to\infty} \left(\tfrac{1}{7}(2^{3k+2}(473)-2)\right)^2 \div (2^{6k+15+1}-1)$$
$$= \lim_{k\to\infty} \left(\tfrac{1}{7}(2^{3k+2})(473)\right)^2 \div 2^{6k+16} = (473)^2/(2^{12}49),$$

which rounds up to 1.115, and for the T_{6k+16} result $\lim_{k\to\infty} (\frac{1}{7}(2^{3k+2}(669)-2))^2 \div (2^{6k+16+1}-1) = \lim_{k\to\infty} (\frac{1}{7}(2^{3k+2})(669))^2 \div 2^{6k+17} = (669)^2/(2^{13}49)$, which rounds up to 1.115. Each of the "p odd" cases is essentially the same as the T_{6k+15} case, and the

[1] See the online version of this paper at doi: 10.1016/S0166-218X(02)00550-4.

"p even" cases the same as the T_{6k+16} case. We have rounded up so that we know for all large p that a layout of T_p into a square grid exists having expansion at most 1.115.

4. Terminology and an overview concerning our lower bounds

As discussed before, for our purposes a layout of T_h is simply a subgraph T of $M[m,n]$ (or of $\mathrm{EM}[m,n]$) which is homeomorphic to T_h. Recall having defined the *point expansion* ratio r' for such a layout as being the number of points in T divided by the number of points in T_h, namely $r' = |V(T)|/(2^{h+1}-1)$. The remainder of the paper is devoted to finding reasonable lower bounds for r', separately for grids and for extended grids. Since m and n are irrelevant to the computation of r', we cease in specifying particular parameters for m and n, and essentially allow that m and n be infinite, as follows. For a given h we let $E(h)$ denote the minimum r' for which there exist values of m and n for which there exists a layout of T_h in $M[m,n]$ having expansion ratio r'. Likewise, for a given h we let $E'(h)$ denote the minimum r' for which there exist values of m and n for which there exists a layout of T_h in $\mathrm{EM}[m,n]$ having expansion ratio r'. These minima are easily seen to be well-defined, since for example the H-tree construction shows that T_{2h} has a layout in a suitably large grid. Our objective is to give reasonable lower bounds for each of $E(h)$ and $E'(h)$.

With the dimensions m and n in grid notations $M[m,n]$ and $\mathrm{EM}[m,n]$ no longer relevant, for the rest of the paper we avoid further reference to particular dimensions m and n by changing notation as follows. Let M be the graph of the 2-*dimensional infinite grid graph*. That is, M has as vertices the set Z^2 of ordered integer pairs, where two vertices (x_1,y_1) and (x_2,y_2) of M form an edge in M iff $|x_1-x_2|+|y_1-y_2|=1$. Likewise, we define the *infinite extended grid* EM as having the same vertex set as M, where by definition a pair of vertices (x_1,y_1) and (x_2,y_2) in EM are adjacent if and only if $\max(|x_1-x_2|,|y_1-y_2|)=1$. Thus M is 4-regular and EM is an 8-regular graph containing M as a subgraph, where EM is the result of adding "diagonals" to M. We write $T \sim T_h$ to indicate that T is a tree which is a subgraph of M and T is isomorphic to a subdivision of T_h (i.e. T is homeomorphic to T_h and results from T_h by inserting points of degree 2 along edges of T_h), and in this case we call such a T a *layout of T_h in M*. In other words, $T \sim T_h$ means that T is a translate in the plane of some layout of T_h in some grid $M[m,n]$. Likewise, we write $T \sim \times T_h$ to indicate that T is a tree which is a subgraph of EM and T is isomorphic to a subdivision of T_h, and in this case we call such a T a *layout of T_h in EM*. (Here, the symbol "$\times$" is simply a reminder that diagonals are allowed.) In this notation, we have that $E(h)=\min\{n(T)/n(T_h): T \sim T_h\}$ and $E'(h)=\min\{n(T)/n(T_h): T \sim \times T_h\}$.

Our main lower bound results are that $E(h) \geqslant 1.122$ and $E'(h) \geqslant 1.03$ for h sufficiently large. The constructions from Theorems 3 and 5 imply that $E(h) \leqslant 1.4656$ and that $E'(h) \leqslant 1.115$ for h sufficiently large. While considerable gaps remain between our upper and lower bounds, our lower bounds are the first improvements upon the trivial lower bounds $E(h) \geqslant E'(h) \geqslant 1$.

For an illustration, observe that the "northeastern" portion of Fig. 14b shows a layout of T_6 rooted at u, having point expansion 1, thus showing that $E'(6)=1$. For this layout

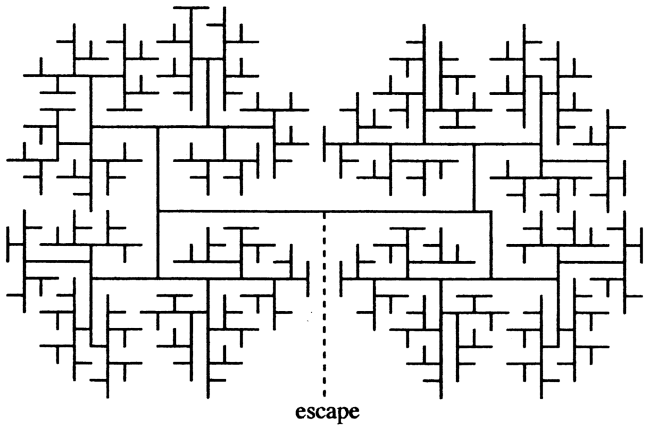
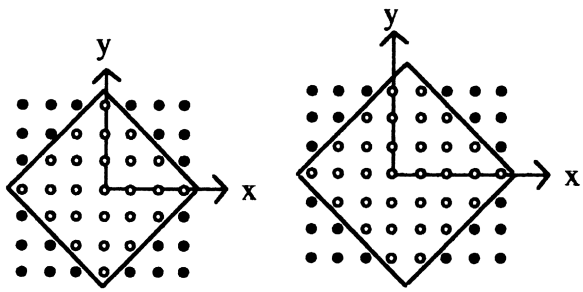


Fig. 7. Layout of T_8 in M having 99 waste vertices, so point expansion 610/511.

to be useful in constructing layouts of T_h for $h \geqslant 7$ there must be points of EM that are as yet unused by the layout, so that these points can be used for connecting the root u and the root of another layout of T_6 to a point v which can serve as the root of the resulting layout. Additional unused points of EM (shown by the dashed path in Fig. 14b) must exist to serve as an "escape" so that the resulting layout of T_7 can ultimately be part of a layout of a larger T_h.

If $T \sim \times T_h$ or $T \sim T_h$ we let $R = R(T)$ denote the root of T according to the homeomorphism, and let $W = W(T)$ denote the set of vertices of degree 2 in T, other than R. A vertex of W is called a *waste vertex*, or a *W-vertex* (Fig. 7). Clearly the point expansion of a layout of T_h is $r' = 1 + |W|/(2^{h+1} - 1)$. We pointed out earlier that the H-tree construction uses only about 50% of the added middle row and column, and that the unused space accumulates iteratively. But now that we measure the efficiency of a layout according to its point expansion, observe that these unused points in the middle row and column are not waste vertices, since they are unused. As previously mentioned, the H-tree construction yields a layout of T_{2n} into the $(2^{n+1} - 1) \times (2^{n+1} - 1)$ grid and has expansion $(2^{n+1} - 1)^2/(2^{2n+1} - 1)$ which approaches 2 as n grows. By contrast, simple induction shows that the point expansion $n(T)/n(T_{2n})$ of the H-tree layout is $(3(2^{2n}) - 3(2^n) + 2)/(2^{2n+1} - 1)$, which approaches 1.5 as n grows. In other words, in an H-tree layout $T \sim T_{2n}$, roughly half of the grid points in the host $(2^{n+1} - 1) \times (2^{n+1} - 1)$ grid are not vertices of the underlying T_{2n}, and among those roughly half are waste vertices in W and roughly half are not in T at all. So when measured by point expansion instead of expansion the H-tree construction is seen as wasteful, motivating in part our study of point expansion. Naturally, the lower bounds we obtain in this paper for the minimum point expansion serve also as lower bounds for the minimum expansion.

We now present an overview of our lower bound technique for layouts in M. Joining two layouts of T_h to form a layout of T_{h+1} requires that two separate "escape" paths (such as the dashed paths in Figs. 1b and 14b) lead from the roots of the T_h's to



(a) (b)

Fig. 8. Diamond $D_3(S)$, where $S = \{(0,.0)\}$ in (a) and $S = \{(0,.0),(1,0)\}$ in (b).

the root of the T_{h+1}. Thus for inductive purposes we will lower bound the number of W-vertices in a layout of T_h together with the W-vertices in the "escape" path from its root to the root of the T_{h+1}.

To start on such a bound, observe that any layout T of T_h must occupy at least $2^{h+1}-1$ lattice points. But we can prove that among any $2^{h+1}-1$ lattice points there must be a pair of points x' and y' fairly far apart in the host grid, separated by a distance D which we can quantify. Then T must contain leaf vertices x and y for which the x,y-path in T visits x' and y' and has length D or more. Let u and v be the leaf vertices of T_h mapped to x and y, so that u and v are at distance at most $2h$ in T_h. Then the x,y-path in T will have at least $D+1$ points along it, among which at most $2h+1$ are images of the points of the u,v-path in T_h. Thus, the x,y-path has at least $D-2h$ points which are W-vertices, driving up the point expansion of the embedding.

Determining D from h is based on some "taxicab" geometry. A set of grid points, each at grid distance d or less from the others, can have at most $(d^2/2)+d+1$ points. In fact, such a set necessarily resides in a "diamond" that is "centered" in a $(d+1)\times(d+1)$ square grid, as indicated by the open dots in Fig. 8. Thus, we could take D to be the least positive integer for d which $(d^2/2)+d+1=2^{h+1}-1$. (Later we use a different, better choice of D.)

It might be hoped that $D-2h$ is so large as to force so many W-vertices to exist in one such path as to give a reasonable lower bound based on the W-vertices in just that one path, but we can do better by working recursively with subtrees of T_h. We examine the forest F resulting from T by deleting the edges of such an x,y-path P, as in Fig. 13. Then F will contain the disjoint union of layouts of complete binary trees of various heights, where each such complete binary tree will have its own escape. As in Fig. 13, if the path P is the image of a path of length $2h$ in T_k, then F will contain layouts of two complete binary trees (with escapes) of heights 1 through $h-2$, and (if $h<k$) of one complete binary tree for each of the heights h through $k-1$.

We are led to the following inductive strategy. Having determined numbers $B(1)$, $B(2),\ldots,B(k-1)$ for which we have verified that every layout of T_i with its escape $(i=1,2,\ldots,k-1)$ in the grid has at least $B(i)$ many W-vertices, and having determined a number D for which it is known that every layout of T_k with its escape in the grid

has a path of length D, use that information to determine a number $B(k)$ such that every layout of T_k in the grid has at least $B(k)$ many W-vertices. To determine $B(k)$, consider a longest path P in a layout T of T_k, and consider the possible values for $2h$, the length of the path in T_k for which P is its image. It follows that T has at least $2B(1)+2B(2)+\cdots+2B(h-2)+B(h)+B(h+1)+\cdots+B(k-1)$ many W-vertices just within the components of the forest $F=T-E(P)$, plus an additional $D-2h$ or more W-vertices internal to P. With a bit of optimization analysis, it works out in our induction process that this grand total is generally minimized when $h=k$, i.e. if P happens to pass through the root of T. This explains why, in our Theorem 6, the expression $2s_{k-2}=2(B(1)+B(2)+\cdots+B(k-2))$ appears added to what is essentially $D-2k$: we can be sure that at least $2s_{k-2}+D-2k$ many W-vertices are present in such a layout.

5. Bounding a layout using taxicab geometry

The following lemma puts an upper bound on $n(T)$ for any subtree T of M or EM having a given diameter d. We later use this fact to inductively drive up the diameter of any layout T of T_h once we know that $n(T)$ is large enough.

Lemma 2.

(a) *Suppose that a binary tree T of diameter $d \geqslant 4$ is a subgraph of EM. Then* $n(T) \leqslant d^2+2d-3$.
(b) *Suppose that a binary tree T of diameter $d \geqslant 4$ is a subgraph of M. Then* $n(T) \leqslant (d^2/2)+d-1$.

Proof. For (a), consider a binary tree T of diameter $d \geqslant 4$ (so $\Delta(T) \leqslant 3$), T a subgraph of EM. Among the x-coordinates of the points of T, no two can differ by more than d, and likewise for the y-coordinates. Thus without loss of generality $V(T) \subseteq \{0,1,\ldots,d\} \times \{0,1,\ldots,d\}$, so $n(T) \leqslant d^2+2d+1$. We bother to reduce this bound by 4 to $n(T) \leqslant d^2+2d-3$, since iterative applications of this bound will later affect the constant in our main result.

Suppose for contradiction that there are fewer than four points of $\mathrm{SQ}=\{0,1,\ldots,d\} \times \{0,1,\ldots,d\}$ unoccupied by T. Recall that a *center* vertex of a tree of diameter d is a vertex along a path of length d in T at distance $\lfloor d/2 \rfloor$ from an end of that path. Every vertex of T is within distance $d/2$ of a center vertex of T, and T has exactly one center vertex if d is even, exactly two if d is odd. Tree T has a center vertex (x,y), where without loss of generality $x,y \geqslant d/2$, and T has a second center vertex (x',y') [which would be adjacent to (x,y)] if and only if d is odd.

Case 1: d is even. If $x>d/2$ then no points of $\{0\} \times \{0,1,\ldots,d\}$ are occupied by T, a contradiction, so $x=d/2$. By symmetric argument, $y=d/2$. Consider the set $S=\{0,1,d-1,d\} \times \{0,1,d-1,d\}$, a set of 16 points, of which at least 13 must be occupied by T, as in Fig. 9a in which the center and nearby parts of the tree are illustrated. Then, since (x,y) has 3 or fewer neighbors in T, at least one of those

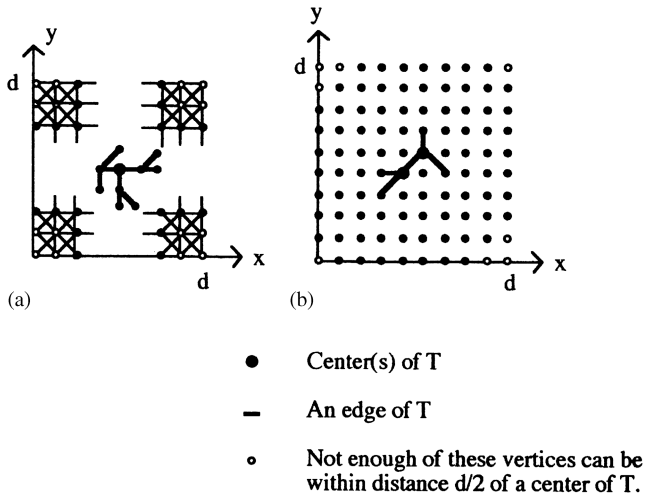


Fig. 9. In the proof of Lemma 2a, illustrations of why at least 4 points of SQ must be unoccupied by T.

neighbors is within distance $(d/2)-1$ of 5 of the points of S. But no point of SQ is within distance $(d/2)-1$ of 5 points of S, a contradiction.

Case 2: d is odd. Then each point of T is within distance $(d-1)/2$ of one of (x,y) and (x',y'). If $x'>d/2$ then since also $x \geqslant d/2$, no points of $\{0\}\times\{0,1,\ldots,d\}$ are occupied by T, a contradiction. By a symmetric argument, $y'>d/2$ leads to a contradiction. Since (x,y) and (x',y') are adjacent, we have that $(x,y)=((d+1)/2,(d+1)/2)$ and $(x',y')=((d-1)/2,(d-1)/2)$. See Fig. 9b for an illustration of the following. Neither $(d,0)$ nor $(0,d)$ is within distance $(d-1)/2$ from (x,y) or (x',y'). Also, since each end of the edge connecting (x,y) and (x',y') is incident to at most two other edges of T, at least one of $(0,0)$, $(0,d-1)$ and $(d-1,0)$ is not in T, and at least one of (d,d), $(d,1)$ and $(1,d)$ is not in T (because to reach each of these vertices from a center in T within $(d-1)/2$ steps requires a different choice for the first edge taken). All told, there are 4 points of S not in T, a contradiction.

Therefore (whether d is even or odd) there are at least 4 points of SQ unoccupied by T, so $n(T)\leqslant d^2+2d-3$, proving (a).

Now we move to the proof of (b), wherein we consider a binary tree T of diameter $d\geqslant 4$ (so $\Delta(T)\leqslant 3$), T a subgraph of M. We first show that T must lie in a "diamond" shaped region of M consisting of a sphere in taxicab geometry. More precisely, let S be a set of lattice points in M. Then the *diamond* $D_r(S)$ of radius r about S is the set of all lattice points at taxicab distance at most r from some point of S, i.e. $D_r(S)=\{(x,y)\in M\colon |x-s|+|y-t|\leqslant r \text{ for some } (s,t)\in S\}$ (see Fig. 8 illustrating diamonds with $S=\{(0,0)\}$ and $\{(0,0),(1,0)\}$). Observe that if S is a single point, then $|D_r(S)|=2r^2+2r+1$. Let v and w be two endpoints of T at distance d in T, and let P be the path of length d joining v and w. Let S be the set of (at most 2) center points of T, on P at distance $\lfloor d/2\rfloor$ in T from at least one of v or w. The set S consists of one point if d is even, two adjacent points if d is odd. After suitably

translating we may suppose that $S=\{(0,0)\}$ or $\{(0,0),(1,0)\}$ when d is even or odd, respectively. Then since every point of T must be at taxicab distance at most $\lfloor d/2\rfloor$ from some center point of T, it follows that $V(T)\subseteq D_{\lfloor d/2\rfloor}(S)$.

Case 1: $d=2r$ is even. Set $D=D_r(\{(0,0)\})$ It is easy to verify that $|D|=(d^2/2)+d+1$, so it suffices to show that D has some 2 points unoccupied by T. Not all 4 neighbors of $(0,0)$ in D can be neighbors of $(0,0)$ in T, so assume without loss of generality that $(0,-1)$ is not a neighbor of (0,0) in T. Then $(0,-d/2)$ and $(0,1-d/2)$ are in D but not T, as desired.

Case 2: d is odd. Set $D=D_{\lfloor d/2\rfloor}(\{(0,0),(1,0)\})$. It is easy to verify that $|D|=(d+1)^2/2$, so again it suffices to show that D has some 2 points unoccupied by T, using the knowledge that every point of T is within distance $(d-1)/2$ of one of the adjacent centers $(0,0)$ and $(1,0)$ of T. Since each end of the edge joining $(0,0)$ and $(1,0)$ is incident to at most two other edges of T, at least one of $(1,(d-1)/2)$, $(1,-(d-1)/2)$ and $((d+1)/2,0)$ is not in T, and at least one of $(-(d-1)/2,0)$, $(0,(d-1)/2)$ and $(0,-(d-1)/2)$ is not in T (because to reach each of these vertices from a center of T within $(d-1)/2$ steps requires a different choice for the first edge taken). Thus we have shown that D has some 2 points not in T, as desired. □

6. A recursive lower bound technique

Suppose $T\sim\times T_h$ or $T\sim T_h$. That is, the complete binary tree of height h is embedded in tree T, which is a subgraph of M or EM depending on the case. Let $\mathrm{CB}(T)$ denote the complete binary tree of height h with vertex set $V(T)-W(T)$ (i.e. non-waste vertices of T), with an edge joining distinct vertices x,y of $\mathrm{CB}(T)$ if and only if there exists an x,y-path in T each of whose internal vertices is in W. Note that while $\mathrm{CB}(T)$ and T_h are isomorphic, the vertices of $\mathrm{CB}(T)$ are formally part of the layout T; they are the non-waste vertices. For each vertex x of T we associate a subtree $T(x)$, rooted at x, as follows. For R the root of T we let $T(R)=T$, and for any other vertex x of T we let $T(x)$ denote the subtree of T induced by the vertices of T not in the same component as R in $T-x$. The *descendants* of vertex x of T are the vertices of $T(x)-x$. The *parent* of a vertex x of $\mathrm{CB}(T)-R$ is the unique neighbor $p(x)$ of x in $\mathrm{CB}(T)$ for which x is a descendant of $p(x)$. For x a vertex of $\mathrm{CB}(T)$ let the *eccentricity* $e(x)$ of x be defined by $e(x)=\max\{d_T(x,y): y\in V(T(x))\}$, and let the *level* $L(x)$ of x be defined by $L(x)=\max\{d_{\mathrm{CB}(T)}(x,y): y\in V(T(x))\cap V(\mathrm{CB}(T))\}$. For a vertex x of $\mathrm{CB}(T)-R$ let $\bar{T}(x)$ denote the subtree of T induced by the union of $V(T(x))$ and the path from x to $p(x)$. Also let $e'(x)$ denote $e(x)+d_T(x,p(x))$. See Fig. 10 for illustrations of definitions for $p(x)$, $T(x)$ and $\bar{T}(x)$. See Fig. 14a for a layout of T_5 in M, where for example $e(x)=4$ (since w is furthest from x among points in $T(x)$) while $e'(x)=6$ (6 being the length of the shaded path), where for instance $L(x)=L(y)=3$ and $L(w)=0$.

As mentioned previously, a crucial step in obtaining a lower bound for the number of W-vertices in $T\sim T_h$ is a lower bound for the number of W-vertices forced to exist in $\bar{T}(x)$ for x with $L(x)<h$. Formally then, let $w(x)$ denote the number of W-vertices residing in $\bar{T}(x)$, and let $w_k=\min\{w(x): x\in\mathrm{CB}(T),\ T\sim T_h,\ L(x)=k,\ h\geqslant k+2\}$.

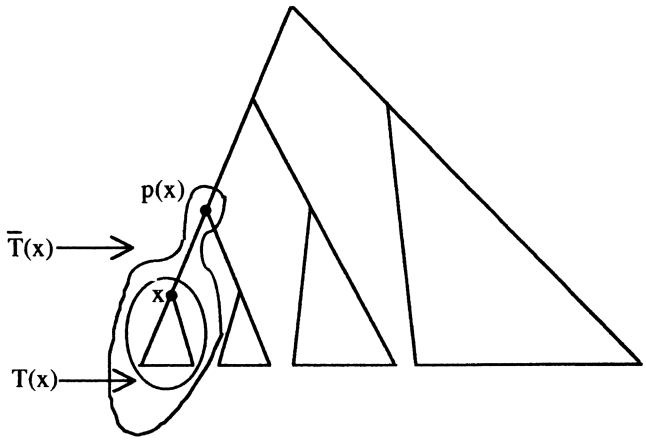


Fig. 10. Trees $T(x)$ and $\bar{T}(x)$.

The condition $h \geqslant k+2$ ensures that under suitable conditions a certain "large" subtree $T(x,E)$ of T containing x exists. This subtree will be defined next, and its existence drives up the value of $w(x)$.

Suppose $T \sim \times T_h$ or $T \sim T_h$, and consider a vertex x of $\mathrm{CB}(T)-R$ with $p(x) \neq R$ and a positive integer E. Let the path P in T joining x and $p(x)$ have exactly t W-vertices. Suppose further that in T there are two paths P' and P'' (possibly of length 0) starting at $p(x)$, each of length at least $E-t-1$, such that P, P' and P'' are edge-disjoint. Thus P' can be taken as a path containing an initial subpath from $p(x)$ toward $p(p(x))$, and continuing past $p(p(x))$ (if E is large enough) in one of two possible ways (i.e. toward either $p(p(p(x)))$ or toward the brother of $p(x)$). Similarly P'' is a path containing an initial subpath from $p(x)$ toward the brother of x and continuing past the brother of x (if E is large enough) toward one of the two descendants of the brother of x. Now define $T(x,E)$ to be the subtree of T induced by vertex set $V(T(x)) \cup \{y : y \in V(P \cup P' \cup P'')$ and $d_T(x,y) \leqslant E\}$ if the above paths P' and P'' exist. Note that $T(x,E)$, when it exists, has at most two vertices of $P \cup P' \cup P''$ which are at distance E from x in T, and that the structure of $T(x,E)$ is independent of the choice of paths P' and P''. Note also that the number of vertices in $T(x,E)-T(x)$ is $2E-t-1$ and is also at least E. See Fig. 11 for an illustration. As a technical note, observe that if $t+1>E$ then it would not have made sense for us to require that P' and P'' have length *exactly* $E-t-1$, and that $T(x,E)$ will not even contain all of P.

Our approach to the lower bound for the numbers w_k is as follows. Let $T'(x,E)$ denote the subtree of $T(x,E)$ induced by $\{v \in V(T(x,E)) : d_T(x,v) \leqslant E\}$. Every point in $T'(x,E)$ must be embedded inside a sphere of radius at most E in M; that is, $T'(x,E)$ fits (after being suitably translated) inside the diamond $D_E(\{(0,0)\} = \{(a,b) \in V(M) : |a|+|b| \leqslant E\}$. It turns out that only a proper subset S_E of $D_E(\{(0,0)\})$ can serve as the image of $T'(x,E)$, as shown in Lemma 3 below. Then using the resulting inequality $|S_E| \geqslant |T'(x,E)|$ and setting $E = e(x)$ we obtain a lower bound for $e'(x)$ in Lemma 5.

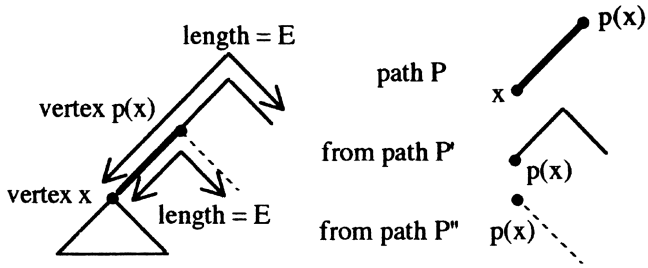


Fig. 11. Tree $T(x,E)$ and the parts of paths P, P' and P'' it typically contains.

The latter bound is a basic element in obtaining the recursive lower bounds for the numbers w_k expressed in Theorem 6.

Lemma 3. *Suppose that $T \sim T_h$ and that $T'(u,E)$ exists for vertex u of T and a value $E \geqslant 3$. Then $n(T'(u,E)) \leqslant 2E^2 + 2E - 2$.*

Proof. For brevity set $T'=T'(u,E)$. Let $D=D_E(\{(0,0)\})$. We can assume that $u=(0,0)$, so that $V(T') \subseteq D$, so that D contains $2E^2 + 2E + 1$ many lattice points.

We show that T' cannot reach all "extreme" points of D; in fact, that it must miss at least 3 such points, thereby proving the lemma. T' is a binary tree, so $\Delta(T') \leqslant 3$, so we can assume that $(0,-1)$ is not adjacent to $(0,0)$ in T'. Therefore points $(0,-E)$ and $(0,1-E)$ of D are not occupied by T, since to reach them in E or fewer steps from $u=(0,0)$ requires that the first step taken be to $(0,-1)$. If at least one of the points $(-E,0)$, $(-1,1-E)$, $(-1,E-1)$, $(0,E)$, $(1,E-1)$, $(E,0)$ and $(1,1-E)$ in D is unoccupied by T' then we are done, having three points of D unoccupied by T'. Therefore suppose that all seven of these points of D are in T'. Since each is E away in M from $(0,0)$ and since vertices of T' are all within distance E of $(0,0)$ in T' and since the edge from $(0,0)$ to $(0,-1)$ is not in T', it is not hard to verify (see Fig. 12) that the paths in T' from $(0,0)$ to each of $(-E,0)$ and $(E,0)$ and $(0,E)$ and $(-1,1-E)$ and $(1,1-E)$ are uniquely determined as in the figure, being

$(0,0) \to (-1,0) \to (-2,0) \to \cdots \to (-E,0)$
$(0,0) \to (1,0) \to (2,0) \to \cdots \to (E,0)$
$(0,0) \to (0,1) \to (0,2) \to \cdots \to (0,E)$
$(0,0) \to (-1,0) \to (-1,-1) \to (-1,-2) \to \cdots \to (-1,2-E) \to (-1,1-E)$
$(0,0) \to (1,0) \to (1,-1) \to (1,-2) \to \cdots \to (1,2-E) \to (1,1-E)$, respectively.

Since $(0,0)$ is distance E away from each of $(-1,E-1)$ and $(1,E-1)$ in D, the paths in T' from $(0,0)$ to each of $(-1,E-1)$ and $(1,E-1)$ must stay within the zone $-1 \leqslant x \leqslant 1$ of the plane. But $\Delta(T') \leqslant 3$, and we already have 3 edges out of each of $(-1,0)$ and $(1,0)$ in T', so $(-1,0)$ is not adjacent to $(-1,1)$ and $(1,0)$ is not adjacent to $(1,1)$ in T'. Therefore, the paths in T' from $(0,0)$ to each of the three points $(0,E)$, $(-1,E-1)$ and $(1,E-1)$ (each at distance E from $(0,0)$) must use the edge from $(0,0)$ to $(0,1)$. Since $P \cup P' \cup P''$ has at most two vertices at distance E from u, the edge from $(0,0)$ to $(0,1)$ must not be in $P \cup P' \cup P''$. Therefore,

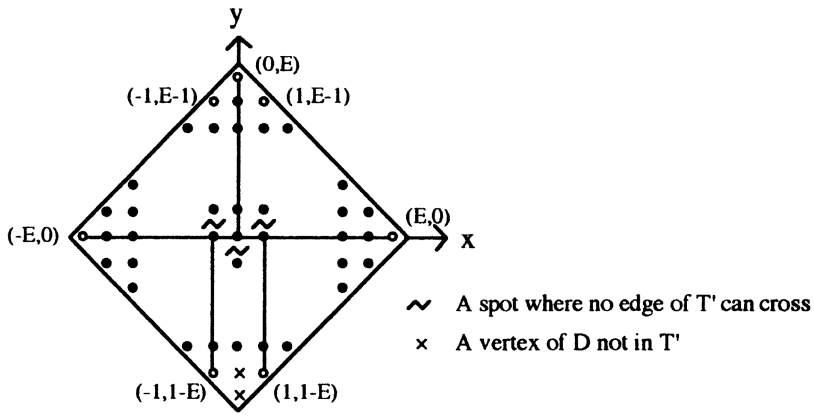


Fig. 12. In the proof of Lemma 3, the seven points among which we show at least one is not in T'.

without loss of generality the edges of $P \cup P' \cup P''$ are precisely the edges of the paths $(0,0) \to (1,0) \to (2,0) \to \cdots \to (E,0)$ and $(0,0) \to (1,0) \to (1,-1) \to (1,-2) \to \cdots \to (1,2-E) \to (1,1-E)$, with $p(u) = (1,0)$.

Suppose then that $(E-1,-1)$ lies in T'. Then from the above $(E-1,-1)$ must be in $T(u)$, so that the path from u to $(E-1,-1)$ must be vertex disjoint from $P \cup P' \cup P''$. But the vertices of $P \cup P' \cup P''$ block access from $(0,0)$ to $(E-1,-1)$ via paths of length E, a contradiction.

Thus the point $(E-1,-1)$ of D is unoccupied by T'. We conclude that $(0,-E)$, $(0,1-E)$ and $(E-1,-1)$ are 3 vertices of D unoccupied by T', so in this case too we have $n(T') \leqslant 2E^2 + 2E - 2$. $\square$

Occasionally, we require some analysis of expressions involving square roots, for which the following elementary lemma, whose proof we omit, is useful.

Lemma 4. *For all* $a, b \geqslant 0$,

(i) $a + \sqrt{b} \geqslant \sqrt{b + a^2}$
(ii) *If* $b \leqslant 2\sqrt{a+1}$, *then* $1 + \sqrt{a} - \sqrt{a+b} \geqslant 0$.

Recall that $w_k = \min\{w(x) : x \in \mathrm{CB}(T),\ T \sim T_h,\ L(x) = k,\ h \geqslant k+2\}$, and recall that $w(x)$ includes W-vertices in both $T(x)$ and in the path from x to $p(x)$.

Lemma 5. *Suppose that* $T \sim T_h$ *and that vertex* x *in* $\mathrm{CB}(T)$ *has level* $L(x) = k-1$ *with* $4 \leqslant k < h$.

Then $e'(x) \geqslant 1 + \sqrt{2^{k-1} + \frac{1}{2} w_{k-1}}$.

Proof. Consider such a T, x, and k, and choose x to be a vertex with least value $e'(x)$. Let $e = e(x)$. Then $T(x,e)$ exists by minimality of $e'(x)$ and since $k < n$. Also, since

$e = e(x)$, we have that $T'(x,e) = T(x,e)$. Let t denote the number of W-vertices on the path in T from x to $p(x)$.

Case 1: $t = 0$. Now $T(x)$ has at least w_{k-1} many W-vertices, so within $T(x,e)$ there are at least $2^k - 1 + w_{k-1} + 2e - 1$ points. From Lemma 3 we have $2^k - 1 + w_{k-1} + 2e - 1 \leqslant 2e^2 + 2e - 2$, so $e \geqslant \sqrt{2^{k-1} + \frac{1}{2}w_{k-1}}$. The result follows on observing that $e'(x) = 1 + e(x)$ since $t = 0$.

Case 2: $t \geqslant 1$. Here $T(x)$ has at least $w_{k-1} - t$ many W-vertices, so within $T(x,e)$ there are at least $2^k - 1 + w_{k-1} - t + e$ points. Again from Lemma 3 we have $2^k - 1 + w_{k-1} - t + e \leqslant 2e^2 + 2e - 2$, or $2e^2 + e - [2^k + w_{k-1} - t + 1] \geqslant 0$. Thus $e \geqslant \frac{1}{4}(-1 + \sqrt{1 + 8[2^k + w_{k-1} - t + 1]})$, so $e'(x) \geqslant 1 + t + \frac{1}{4}(-1 + \sqrt{1 + 8[2^k + w_{k-1} - t + 1]}) = 1 + (t - \frac{1}{4}) + \sqrt{2^{k-1} + \frac{1}{2}w_{k-1} - \frac{1}{2}t + \frac{9}{16}}$. By (i) of Lemma 4 we have $e'(x) \geqslant 1 + \sqrt{2^{k-1} + \frac{1}{2}w_{k-1} - \frac{1}{2}t + \frac{9}{16} + (t - \frac{1}{4})^2} = 1 + \sqrt{2^{k-1} + \frac{1}{2}w_{k-1} + t^2 - t + \frac{5}{8}} \geqslant 1 + \sqrt{2^{k-1} + \frac{1}{2}w_{k-1}}$, as desired. □

We plan to recursively produce non-negative lower bounds $B(i)$ for each w_i (i.e. where $w_i \geqslant B(i)$) satisfying $B(i+1) \geqslant 2B(i)$ for all i. We call such a sequence of bounds $B(i)$ a *lower bound sequence*. For such a lower bound sequence we let s_k denote $B(1) + B(2) + \cdots + B(k)$.

Theorem 6. *For any lower bound sequence $\{B(i)\}$, the sequence $\{w_i\}$ satisfies the recursive lower bound*

$$w_k \geqslant \max(2w_{k-1}, 2s_{k-2} - 2k + \sqrt{2^{k+2} + 4s_{k-2} + 4E - 4k - 2}),$$

for each integer $k \geqslant 4$, where $E = 1 + \lceil \sqrt{2^{k-1} + \frac{1}{2}B(k-1)} \rceil$.

Proof. Clearly, $w_k \geqslant 2w_{k-1}$ since for each x at level k with descendants y and z at level $k-1$ the tree $T(x) \subset \bar{T}(x)$ decomposes into $\bar{T}(y) \cup \bar{T}(z)$, where each of $\bar{T}(y)$ and $\bar{T}(z)$ contains at least w_{k-1} many W-vertices, and they intersect only at the non-waste vertex x. Therefore it suffices to prove that $w_k \geqslant 2s_{k-2} - 2k + \sqrt{2^{k+2} + 4s_{k-2} + 4E - 4k - 2}$.

So suppose $h \geqslant k+2$ with $k \geqslant 4$, and let $T \sim T_h$ with E as in the statement. Let vertex u of $\mathrm{CB}(T)$ have level $L(u) = k$, and let $d = \mathrm{diam}(T(u))$. Let P be a path of length d in $T(u)$, and let m denote the highest level among vertices of $P \cap \mathrm{CB}(T)$. If there exist any W-vertices of T adjacent to any leaves, those leaves may be deleted with the effect of decreasing the number of W-vertices, so it suffices to prove the result for the case in which no leaf of T is adjacent to a W-vertex of T. Therefore $m \geqslant 2$. Let $t = \min\{E-1$, number of W-vertices on the path in T from u to $p(u)\}$. For any vertex x of $\mathrm{CB}(T)$ with $L(x) = k-1$, by Lemma 5 we have that $e'(x) \geqslant 1 + \sqrt{2^{k-1} + \frac{1}{2}w_{k-1}} = E$. This lower bound holds in particular for $e'(y)$ and $e'(z)$, where y and z are the two descendants of u at level $k-1$.

Observe that $T(u,E)$ exists, by identifying the paths P' and P'' in the definition of $T(u,E)$ as follows. Let v be a cousin of u in $\mathrm{CB}(T)$; that is, v is a child of the brother

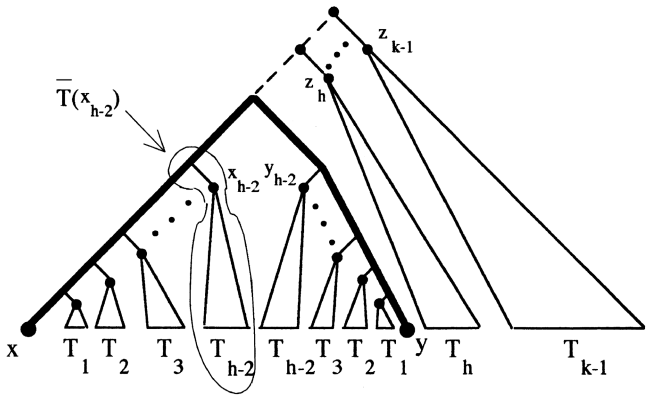


Fig. 13. Forest F formed by deleting the edges of the darkened path from a layout of T_k.

of $p(u)$, so $L(v)=k$. Then either child c of v in CB(T) satisfies $e'(c) \geqslant E$. Hence, we can take P' to be the path in T from $p(u)$ to v, together with whatever segment of the path in T of length $e'(c)$ from v through c that is needed to get a path of total length E starting from $p(u)$. Similarly let g be a nephew of u in CB(T); that is, g is a child of u's brother $b(u)$ in CB(T). Then $e'(g) \geqslant E$ also, and we take P'' as the path in T from $p(u)$ to $b(u)$, together with a segment (if necessary) of the path in T of length $e'(g)$ from $b(u)$ through g.

We also show that $T(u,E)$ has diameter $\mathrm{diam}(T(u,E))=d$. Clearly $\mathrm{diam}(T(u,E)) \geqslant \mathrm{diam}(T(u))=d$, so it suffices to show that any path Q in $T(u,E)$ not contained in $T(u)$ has length at most d. Note first that any path in $T(u)$ from u to an endpoint of $T(u)$ has length at least E, since $e'(x) \geqslant E$ for any point x at level $k-1$. It follows that $d \geqslant 2E$. If $Q \subseteq (P' \cup P'')$, then clearly $\mathrm{length}(Q) \leqslant 2E \leqslant d$. If $Q \nsubseteq (P' \cup P'')$, then we can suppose that $Q = Q_1 \cup Q_2$, where Q_1 is a path from u to an endpoint of $T(u)$, and Q_2 is a path from u to an endpoint of either P' or P''. Then $\mathrm{length}(Q_2) \leqslant E$. But now let Q' be any path from u to an endpoint of $T(u)$, so as above, $\mathrm{length}(Q') \geqslant E$. Choose such a Q' so that it has no vertices in common with Q_1 except u, and form the path $Q'' = Q_1 \cup Q'$. Then $\mathrm{length}(Q'') \geqslant \mathrm{length}(Q)$ since $\mathrm{length}(Q') \geqslant \mathrm{length}(Q_2)$, while $d \geqslant \mathrm{length}(Q'')$ since $Q'' \subseteq T(u)$. We get $\mathrm{length}(Q) \leqslant d$ as claimed.

There are at least $2E-t-1$ vertices in $T(u,E)-T(u)$. As for the vertices of $T(u)$, there are exactly $2^{k+1}-1$ many such vertices that are not W-vertices. There are $d-2m$ waste vertices in P. As for the number of W-vertices in $T(u)-E(P)$ (where $E(P)$ is the edge set of path P), note that $T(u)-E(P)$ decomposes naturally into disjoint subgraphs $\bar{T}(x_0), \bar{T}(x_1), \ldots, \bar{T}(x_{m-2}), \bar{T}(y_0), \bar{T}(y_1), \ldots, \bar{T}(y_{m-2}), \bar{T}(z_m), \bar{T}(z_{m+1}), \ldots, \bar{T}(z_{k-1})$, where each x_i, y_i, z_i is a vertex of CB(T) at level i, where each $p(x_i)$ and $p(y_i)$ is a vertex of P and each z_i is not a descendant of any vertex of P. The vertices of these subgraphs partition the non-isolated vertices of $T(u)-E(P)$, and we illustrate these subgraphs in Fig. 13. Therefore, the number of W-vertices in $T(u)-E(P)$, being lower bounded by the sum of the number of W-vertices in the various $\bar{T}(x_i), \bar{T}(y_i), \bar{T}(z_i)$, is at least $2s_{m-2}+s_{k-1}-s_{m-1} = s_{k-1}+s_{m-2}-B(m-1)$. Combined, the number of vertices in

$T(u,E)$ is at least $2E-t-1+2^{k+1}-1+d-2h+s_{k-1}+s_{m-2}-B(m-1)$. Since $T(u,E)$ has diameter d, Lemma 2 gives us

$$2E-t-1+2^{k+1}-1+d-2m+s_{k-1}+s_{m-2}-B(m-1)\leqslant \frac{d^2}{2}+d-1,$$

so that $d\geqslant\sqrt{2^{k+2}+2s_{k-1}+2s_{m-2}-2B(m-1)+4E-4h-2t-2}$. Therefore, since $T(u)$ has at least $d-2m+s_{k-1}+s_{m-2}-B(m-1)$ W-vertices and the path from u to $p(u)$ has at least t many W-vertices, we have

$$\begin{aligned} w(u)\geqslant{}&\sqrt{2^{k+2}+2s_{k-1}+2s_{m-2}-2B(m-1)+4E-4m-2t-2}\\ &-2m+s_{k-1}+s_{m-2}-B(m-1)+t. \end{aligned}$$

Let $f(m,t)$ denote $s_{k-1}+s_{m-2}-B(m-1)+t-2m$ $+\sqrt{2^{k+2}+2s_{k-1}+2s_{m-2}-2B(m-1)+4E-4m-2t-2}$, the right side of the above inequality. Observe that $f(k,0)=2s_{k-2}-2k+\sqrt{2^{k+2}+4s_{k-2}+4E-4k-2}$, so it suffices to prove that $f(m,t)\geqslant f(k,0)$ for all m and t, with $2\leqslant m\leqslant k$, $0\leqslant t\leqslant E-1$.

First we observe that $f(m,t)$ is monotone in t in the sense that $f(m,t+1)-f(m,t)=1+\sqrt{2^{k+2}+2s_{k-1}+2s_{m-2}-2B(m-1)+4E-4m-2t-4}$ $-\sqrt{2^{k+2}+2s_{k-1}+2s_{m-2}-2B(m-1)+4E-4m-2t-2}\geqslant 0$ by (ii) of Lemma 4 [using $b=2$], since $2\leqslant 2\sqrt{2^{k+2}+2s_{k-1}+2s_{m-2}-2B(m-1)+4E-4m-2t-4}+1$. That is, $f(m,t+1)-f(m,t)\geqslant 0$. Therefore, it suffices to prove that $f(m,0)\geqslant f(k,0)$ for all m with $2\leqslant m\leqslant k$. Fortunately, $f(m,0)$ is also monotone as a function of m, as follows:

$$\begin{aligned} f(m,0)-f(m+1,0)={}&s_{m-2}-B(m-1)-s_{m-1}+B(m)+2\\ &+\sqrt{2^{k+2}+2s_{k-1}+2s_{m-2}-2B(m-1)+4E-4m-2}\\ &-\sqrt{2^{k+2}+2s_{k-1}+2s_{m-1}-2B(m)+4E-4m-6}. \end{aligned}$$

But $s_{m-2}-B(m-1)-s_{m-1}+B(m)=B(m)-2B(m-1)\geqslant 0$. Likewise, the first radical exceeds the second radical, because the difference of their radicands is $2(s_{m-2}-B(m-1)-s_{m-1}+B(m))+4=2(B(m)-2B(m-1))+4\geqslant 4$. Therefore $f(m,0)\geqslant f(m+1,0)$ for all m, so $f(m,0)\geqslant f(k,0)$ for all m with $2\leqslant m\leqslant k$, as desired, completing the proof. □

Theorem 7. *The minimum point expansion $E(h)$ for any layout of T_h in M satisfies $E(h)\geqslant 1.12222$ for $h\geqslant 26$.*

Proof. Theorem 6 allows us to recursively produce a lower bound sequence $B(1)$, $B(2),\ldots$ First we obtain lower bounds for early values of w_i. We start with the lower bounds $w_1\geqslant 0$, $w_2\geqslant 0$, $w_3\geqslant 0$, $w_4\geqslant 1$ and $w_5\geqslant 5$, the last of which is done with computer assistance (see the last section). Then we begin our lower bound sequence by setting $B(1)=0$, $B(2)=0$, $B(3)=0$, $B(4)=1$ and $B(5)=5$, and thereafter (for $k=6,7,8,\ldots$) follow the recursive definition $B(k)=\max(2B(k-1),2s_{k-2}-2k+$

$\lceil\sqrt{2^{k+2}+4s_{k-2}+4E-4k-2}\rceil)$, where $E=1+\lceil\sqrt{2^{k-1}+\frac{1}{2}B(K-1)}\rceil$. Theorem 6 assures us that each $B(k)$ thus generated is a lower bound for w_k. For example, from $s_4=0+0+0+1=1$, when $k=6$ we obtain that $E=1+\lceil\sqrt{32+\frac{1}{2}5}\rceil=7$, and $B(6)=\max(2(5),2(1)-2(6)+\lceil\sqrt{256+4(1)+4(7)-4(6)-2}\rceil)=\max(10,7)=10$.

Continuing, $s_5=s_4+B(5)=1+5=6$, so when $k=7$ we obtain that $E=1+\lceil\sqrt{64+\frac{1}{2}10}\rceil=10$, and $B(7)=\max(2(10),2(6)-2(7)+\lceil\sqrt{512+4(6)+4(10)-4(7)-2}\rceil)=\max(20,22)=22$. Continuing in this manner, one obtains $B(8)=50$, $B(9)=106$, $B(10)=224$, $B(11)=462$, $B(12)=947$, $B(13)=1926$, $B(14)=3897$, $B(15)=7859$, $B(16)=15,810$, $B(17)=31,751$, $B(18)=63,687$, $B(19)=127,636$, $B(20)=255,643$, $B(21)=511,812$, $B(22)=1,024,367$, $B(23)=2,049,786$, $B(24)=4,101,060$, and eventually $B(48)\geqslant 6.886464\times 10^{13}$. Now for a layout T of T_k in M, there are $2^{k+1}-1$ non-waste vertices. In addition, the layout will have four vertices x_i, $1\leqslant i\leqslant 4$, of $\mathrm{CB}(T)$ at level $k-2$ (these being the grandchildren of the root of $\mathrm{CB}(T)$) for which $\bar{T}(x_i)$ and $\bar{T}(x_j)$ share no W-vertices for $i\neq j$, and hence T has at least $4B(k-2)$ many waste vertices. Now taking $k\geqslant 26$, we have $4B(k-2)\geqslant 8B(k-3)\geqslant\cdots\geqslant 2^{k-24}B(24)$. Therefore, the point expansion for T is

$$\frac{n(T)}{n(T_k)}=1+\frac{|W(T)|}{2^{k+1}-1}\geqslant 1+\frac{2^{k-24}B(24)}{2^{k+1}-1}\geqslant 1+\frac{4,101,060}{2^{25}}\geqslant 1.12222.$$

Likewise, for $k\geqslant 50$ the point expansion for T is at least $1+(6.886464\times 10^{13}/2^{49})\geqslant 1.122328$. □

Very minor improvements can be made by calculating more values of $B(k)$ for $k>48$ or by rounding off more carefully. Presumably, more significant improvements can be made by instead starting with improved starting values, say for $B(6)$, $B(7)$ or $B(8)$, (noting that in the last section we sketch roughly why 5 is the optimal value for $B(5)$) or by improving on the recurrence rule for $B(k)$.

The same technique for obtaining lower bounds for w_k for layouts T of T_k in M allows us to obtain lower bounds for the point expansion of any layout T of T_k in the extended grid EM. Not surprisingly, the lower bounds turn out to be considerably smaller, since it is much easier to avoid W-vertices when embedding T_k in the 8-regular extended grid EM than when embedding T_k in the 4-regular grid M. Let $\omega_k=\min\{w(x):T\sim\times T_h$ for $h\geqslant k+2$, $x\in V(\mathrm{CB}(T))$, $L(x)=k\}$, analogous to our notation w_k for layouts in M.

Lemma 6. *Suppose that $T\sim\times T_h$ and that vertex x in* $\mathrm{CB}(T)$ *has level $L(x)=k-1$ with $4\leqslant k<h$. Then $e'(x)\geqslant\frac{3}{4}+\sqrt{2^{k-2}+\frac{1}{4}\omega_{k-1}+\frac{5}{16}}$.*

Proof. Consider such a T, x and k, and choose x to be a vertex with least value $e'(x)$. Let $e=e(x)$. Then $T(x,e)$ is well defined, and has diameter $d=2e$. Let t denote the number of W-vertices on the path in T from x to $p(x)$.

Case 1: $t=0$. Then $T(x)$ has at least ω_{k-1} W-vertices, so within $T(x,e)$ there are at least $2^k-1+\omega_{k-1}+2e-1$ points. By Lemma 2, $2^k-1+\omega_{k-1}+2e-1\leqslant(2e)^2+2(2e)-3$,

i.e. $4e^2 + 2e - [2^k + \omega_{k-1} + 1] \geqslant 0$. Therefore $e \geqslant \frac{-1}{4} + \sqrt{2^{k-2} + \frac{1}{4}\omega_{k-1} + \frac{5}{16}}$. So, adding in the 1 or more edges in $T(x)$ between x and $p(x)$, we get $e'(x) \geqslant \frac{3}{4} + \sqrt{2^{k-2} + \frac{1}{4}\omega_{k-1} + \frac{5}{16}}$ as desired.

Case 2: $t \geqslant 1$. Then $T(x)$ has at least $\omega_{k-1} - t$ W-vertices, so within $T(x,e)$ there are at least $2^k - 1 + \omega_{k-1} - t + e$ points. By Lemma 2, $2^k - 1 + \omega_{k-1} - t + e \leqslant 4e^2 + 4e - 3$, or $4e^2 + 3e - [2^k + \omega_{k-1} - t + 2] \geqslant 0$. Thus $e \geqslant \frac{1}{8}(-3 + \sqrt{9 + 16(2^k + \omega_{k-1} - t + 2)})$, so $e'(x) \geqslant 1 + (t - \frac{3}{8}) + \sqrt{2^{k-2} + \frac{1}{4}\omega_{k-1} - \frac{1}{4}t + \frac{41}{64}}$. By (i) of Lemma 4 we have $e'(x) \geqslant 1 + \sqrt{2^{k-2} + \frac{1}{4}\omega_{k-1} - \frac{1}{4}t + \frac{41}{64} + (t - \frac{3}{8})^2} = 1 + \sqrt{2^{k-2} + \frac{1}{4}\omega_{k-1} + t^2 - t + \frac{25}{32}} \geqslant \frac{3}{4} + \sqrt{2^{k-2} + \frac{1}{4}\omega_{k-1} + \frac{5}{16}}$, as desired. □

As before, we recursively produce non-negative lower bounds $\beta(i)$ for each ω_i satisfying $\beta(i+1) \geqslant 2\beta(i)$ for all i (and of course $\omega_i \geqslant \beta(i)$). We call such a sequence of bounds $\beta(i)$ an *extended lower bound sequence*. For such a lower bound sequence we let σ_k denote $\beta(1) + \beta(2) + \cdots + \beta(k)$.

Theorem 8. *For any extended lower bound sequence $\{\beta(i)\}$, the sequence $\{\omega_i\}$ satisfies the recursive lower bound*

$$\omega_k \geqslant \max(2\omega_{k-1}, 2\sigma_{k-2} - 2k - \tfrac{1}{2} + \sqrt{2^{k+1} + 2\sigma_{k-2} + 2E - 2k + \tfrac{5}{4}}),$$

where $E = \lceil \frac{3}{4} + \sqrt{2^{k-2} + \frac{1}{4}\beta(k-1) + \frac{5}{16}} \rceil$.

Proof. Clearly $\omega_k \geqslant 2\omega_{k-1}$ since for each x at level k with descendants y and z at level $k-1$ the tree $T(x)$ decomposes into $\bar{T}(y)$ and $\bar{T}(z)$ [which overlap only at the non-waste vertex x], where each of $\bar{T}(y)$ and $\bar{T}(z)$ contain at least ω_{k-1} W-vertices. Therefore it suffices to prove that $\omega_k \geqslant 2\sigma_{k-2} - 2k - \frac{1}{2} + \sqrt{2^{k+1} + 2\sigma_{k-2} + 2E - 2k + \frac{5}{4}}$.

Suppose $h \geqslant k+2$ with $k \geqslant 4$, and let $T \sim \times T_h$ with E as in the statement. Let vertex u of $\mathrm{CB}(T)$ have level $L(u) = k$, and let $d = \mathrm{diam}(T(u))$. Let P be a path of length d in $T(u)$, and let m denote the highest level among vertices of $P \cap \mathrm{CB}(T)$. If there exist any W-vertices of T adjacent to any leaves, those leaves may be deleted with the effect of decreasing the number of W-vertices, so it suffices to prove the result for the case in which no leaf of T is adjacent to a W-vertex of T. Therefore $m \geqslant 2$. Let t denote $\min(E - 1$, number of W-vertices on the path in T from u to $p(u))$. For any vertex x of $\mathrm{CB}(T)$ with $L(x) = k - 1$, by Lemma 6 we have that $e'(x) \geqslant \frac{3}{4} + \sqrt{2^{k-2} + \frac{1}{4}\omega_{k-1} + \frac{5}{16}}$. This bound holds in particular for $e'(y)$ and $e'(z)$ for the two descendants y and z of u at level $k-1$. Therefore $T(u,E)$ exists, and has diameter d (since adding a limb at u to the tree T has not increased the length of the longest path through u, and no pairs of points in that limb are further than d apart).

There are at least $2E - t - 1$ vertices in $T(u,E) - T(u)$. As for the vertices of $T(u)$, there are exactly $2^{k+1} - 1$ many such vertices that are not W-vertices. There are $d - 2m$ waste vertices in P. As in the proof of Theorem 6, there are at least

$\sigma_{k-1}+\sigma_{m-2}-\beta(m-1)$ W-vertices in $T(u)-P$. Combined, the number of vertices in $T(u,E)$ is at least $2E-t-1+2^{k+1}-1+d-2m+\sigma_{k-1}+\sigma_{m-2}-\beta(m-1)$. By Lemma 2 we have that $2E-t-1+2^{k+1}-1+d-2m+\sigma_{k-1}+\sigma_{m-2}-\beta(m-1)\leqslant d^2+2d-3$, or $d^2+d-[2^{k+1}+\sigma_{k-1}+\sigma_{m-2}-\beta(m-1)+2E-2m-t+1]\geqslant 0$, from which $d\geqslant -\frac{1}{2}+\sqrt{2^{k+1}+\sigma_{k-1}+\sigma_{m-2}-\beta(m-1)+2E-2m-t+\frac{5}{4}}$. Therefore, since $T(u)$ has at least $d-2m+\sigma_{k-1}+\sigma_{m-2}-\beta(m-1)$ many W-vertices and the path from u to $p(u)$ has at least t many W-vertices, we get

$$\begin{aligned} w(u) \geqslant & -\tfrac{1}{2}+\sqrt{2^{k+1}+\sigma_{k-1}+\sigma_{m-2}-\beta(m-1)+2E-2m-t+\tfrac{5}{4}} \\ & -2m+\sigma_{k-1}+\sigma_{m-2}-\beta(m-1)+t. \end{aligned}$$

Let $f(m,t)$ denote $\sigma_{k-1}+\sigma_{m-2}-\beta(m-1)+t-2m-\frac{1}{2}$ $+\sqrt{2^{k+1}+\sigma_{k-1}+\sigma_{m-2}-\beta(m-1)+2E-2m-t+\frac{5}{4}}$, the right side of the above inequality. Observe that $f(k,0)=2\sigma_{k-2}-2k-\frac{1}{2}+\sqrt{2^{k+1}+2\sigma_{k-2}+2E-2k+\frac{5}{4}}$, so it suffices to prove that $f(m,t)\geqslant f(k,0)$ for all m and t, with $2\leqslant m\leqslant k$, $0\leqslant t\leqslant E-1$.

As before we observe that $f(m,t)$ is monotone in t, since $f(h,t+1)-f(h,t)=1+\sqrt{2^{k+1}+\sigma_{k-1}+\sigma_{m-2}-\beta(m-1)+2E-2m-t+\frac{1}{4}}$ $-\sqrt{2^{k+1}+\sigma_{k-1}+\sigma_{m-2}-\beta(m-1)+2E-2m-t+\frac{5}{4}}\geqslant 0$, by (ii) of Lemma 4 [using $b=1$]. Therefore $f(m,t+1)-f(m,t)\geqslant 0$. So, it suffices to prove that $f(m,0)\geqslant f(k,0)$ for all m with $2\leqslant m\leqslant k$. Also, $f(m,0)$ is also monotone as a function of m, since

$$\begin{aligned} f(m,0)-f(m+1,0) = & \sigma_{m-2}-\beta(m-1)-\sigma_{m-1}+\beta(m)+2 \\ & +\sqrt{2^{k+1}+\sigma_{k-1}+\sigma_{m-2}-\beta(m-1)+2E-2m+\tfrac{5}{4}} \\ & -\sqrt{2^{k+1}+\sigma_{k-1}+\sigma_{m-2}-\beta(m-1)+2E-2m-\frac{3}{4}}. \end{aligned}$$

But $\sigma_{m-2}-\beta(m-1)-\sigma_{m-1}+\beta(m)=\beta(m)-2\beta(m-1)\geqslant 0$. Likewise, the first radical exceeds the second radical, because the difference of their radicands is $\sigma_{m-2}-\beta(m-1)$ $-\sigma_{m-1}+\beta(m)+2=\beta(m)-2\beta(m-1)+2\geqslant 2$. Therefore $f(m,0)\geqslant f(m+1,0)$ for all m, so $f(m,0)\geqslant f(k,0)$ for all m with $2\leqslant m\leqslant k$, as desired, completing the proof. □

Theorem 9. *The minimum point expansion $E'(h)$ for any layout of T_h in* EM *satisfies $E'(h)\geqslant 1.03137$ for $k\geqslant 29$.*

Proof. Theorem 8 allows us to recursively produce an extended lower bound sequence $\beta(1),\beta(2),\ldots$ We start with the lower bounds $\omega_1=\omega_2=\omega_3=\omega_4=\omega_5=\omega_6=0$ and $\omega_7\geqslant 3$, all from the last section. Thus, our lower bound sequence begins with $\beta(1)=\beta(2)=\beta(3)=\beta(4)=\beta(5)=\beta(6)=0$ and $\beta(7)=3$, and thereafter (for $k=8,9,10,\ldots$)

it follows the recursive definition

$$\beta(k) = \max(2\beta(k-1), 2\sigma_{k-2} - 2k - \tfrac{1}{2} + \lceil \sqrt{2^{k+1} + 2\sigma_{k-2} + 2E - 2k + \tfrac{5}{4}} \rceil),$$

where $E = \lceil \frac{3}{4} + \sqrt{2^{k-2} + \frac{1}{4}\beta(k-1) + \frac{5}{16}} \rceil$.

Theorem 8 assures us that each $\beta(k)$ thus generated is a lower bound for ω_k. In this manner, we obtain $\beta(8) = 7$, $\beta(9) = 20$, $\beta(10) = 46$, $\beta(11) = 103$, $\beta(12) = 220$, $\beta(13) = 462$, $\beta(14) = 953$, $\beta(15) = 1952$, $\beta(16) = 3963$, $\beta(17) = 8018$, $\beta(18) = 16157$, $\beta(19) = 32496$, $\beta(20) = 65238$, $\beta(21) = 130838$, $\beta(22) = 262173$, $\beta(23) = 525065$, $\beta(24) = 1051133$, $\beta(25) = 2103697$, $\beta(26) = 4209407$, $\beta(27) = 8421673$, and eventually $\beta(50) \geqslant 7.070388 \times 10^{13}$. The layout T of T_k in EM has $2^{k+1} - 1$ non-waste vertices. In addition, the layout will have four vertices x_i, $1 \leqslant i \leqslant 4$, of CB($T$) at level $k-2$ (these being the grandchildren of the root of CB(T)) for which $\bar{T}(x_i)$ and $\bar{T}(x_j)$ share no W-vertices for $i \neq j$, and hence T has at least $4\beta(k-2)$ many waste vertices. Now taking $k \geqslant 29$, we have $4\beta(k-2) \geqslant 8\beta(k-3) \geqslant \cdots \geqslant 2^{k-27}\beta(27)$. Therefore the point expansion for T is

$$\frac{n(T)}{n(T_k)} = 1 + \frac{|W(T)|}{2^{k+1} - 1} \geqslant 1 + \frac{2^{k-27}B(27)}{2^{k+1} - 1} \geqslant 1 + \frac{8,421,673}{2^{28}} \geqslant 1.03137.$$

Likewise, for $k \geqslant 52$ the point expansion for T is at least $1 + (7.070388 \times 10^{13}/2^{51}) \geqslant 1.0313988$. □

7. Conclusions

In the first part of the paper we constructed improved layouts of complete binary trees into grids and extended grids. In the second part we gave lower bounds for the expansion of such layouts, the first non-trivial such lower bounds on record. Nevertheless, there is still a large "gap" between the lower and upper bounds produced. This is partly due to the fact that the upper bounds are for expansion, whereas the lower bounds are really for "point expansion". Point expansion is clearly a natural lower bound for ordinary expansion. Fig. 7 shows a layout of T_8 and its escape channel into a grid, with "only" 99 grid vertices that are "W-vertices" in the sense that they show up as degree 2 vertices inserted along the edges of T_8, i.e. points which drive up the point expansion. Using essentially the H-tree construction initialized with the layout of Fig. 7, one can obtain an asymptotic upper bound of 1.28 for point expansion, somewhat closing the "gap" between the upper and lower bounds. Clearly, improvements in both the upper and lower bounds can be made through added effort. We believe that making significant improvements in the lower bounds will either require significant computer assistance in showing that many waste vertices are required in laying out T_h for particular small values of h, or will require a fairly new idea.

Since $M[m,n]$ has no vertex of degree exceeding four, it is reasonable to attempt obtaining similar results concerning efficient layouts of complete ternary trees, but not for r-ary trees with $r > 4$. It is already known that O($n(T)$) area can be obtained for planar orthogonal grid drawings of trees T with maximum degree four [13,17].

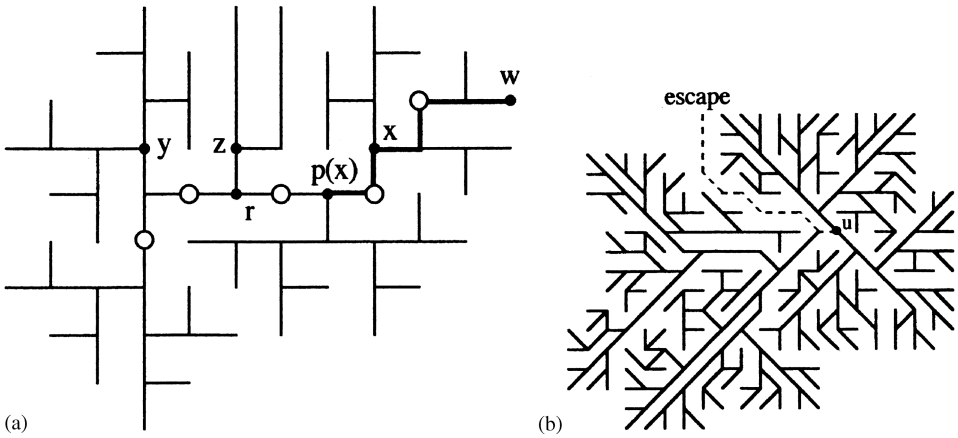


Fig. 14. Constructions showing in (a) that $w_5 \leqslant 5$, and in (b) that $\omega_6 = 0$.

8. Miscellaneous cases: values of w_k and ω_k for small k

Our purpose in this short section is to discuss briefly the values w_k for $k \leqslant 5$, and ω_k for $k \leqslant 7$. When we can show by example that our lower bounds for these values are exact, we often do so by example, but what we need to fuel the lower bound sequences of Theorems 7 and 9 are lower bounds. Some details not given here are included in the Electronic Appendix.[2]

It is easily seen that $w_i = 0$ for $i \leqslant 3$, as demonstrated in Fig. 14a, where for the point y illustrated, $\bar{T}(y)$ is laid out with no W-vertices (as part of a larger layout), and where $T(y) \sim T_3$. We leave as an exercise the verification that $w_4 = 1$: it is a simple matter to show by example a layout of T_4 in which there is just one waste vertex (including along the escape), and it is a sobering experience to try producing a short proof that at least one such waste vertex is required. The proof that $w_5 \leqslant 5$ follows from the layout of T_5 shown in Fig. 14a as containing just 5 degree 2 points (circled). That we can obtain the required layout T of T_7 containing such a T_5 can be seen by using the pair of paths extending upward from the point z in the figure, this z being the root of a layout V of T_6. One of the two paths leads to the root of another copy of V, while the other leads to the root of T. By extending these paths sufficiently, one obtains enough room to suitably join together 4 copies of this V to form such a T.

Proving that $w_5 \geqslant 5$ turned out to be an enormous struggle. Upon supposing for contradiction that a suitable T_5 layout exists with at most 4 waste vertices, our proof is a synthesis of using reasoning to narrow down the possibilities for the structure of such a hypothetical counterexample, followed by a computer search to eliminate the possibility of embedding in M any of the remaining narrowed down possibilities. An example of the "hand" reasoning showing that a layout of a particular T_5 with 3 waste

[2] See the online version of this paper at doi: 10.1016/S0166-218X(02)00550-4.

vertices is impossible, as well as the list of narrowed possibilities which were then shown unembeddable in M by computer, are given in the Electronic Appendix.

By contrast, there was no need for a computer assisted proof in the extended grid case.

Lemma 7. $\omega_i = 0$ *for* $1 \leqslant i \leqslant 6$, *and* $\omega_7 \geqslant 3$.

Proof. Fig. 14b shows a layout of T_7 in EM, in which the vertex u of level 6 has $w(u) = 0$, so $\omega_6 = 0$, and by subgraph inclusion also $\omega_i = 0$ for $1 \leqslant i \leqslant 5$.

Our proof that $\omega_7 \geqslant 3$ is three pages long, and is included in the Electronic Appendix.[3] □

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