Spanning Trees of n-Dimensional Cubes

Joseph Malkevitch

Dots and lines diagrams known as graphs are a powerful tool for problem solving across many academic disciplines. Graphs are also a rich source of relatively easy-to-state unsolved problems that are fun to think about. Two fascinating kinds of graphs with many applications (error correction codes, organizing processors in a computer, etc.) are trees (one piece and no circuits) and n-dimensional cubes.

Figure 1 shows five non-isomorphic (different structure) trees. Note that in these diagrams the lengths used to draw the segments (edges) joining the vertices (dots) do not matter for whether two graphs are the same or different (combinatorially equivalent).

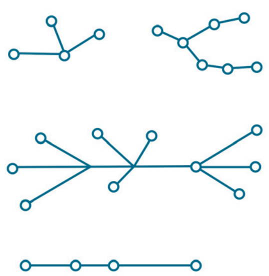


Figure 1. Four trees; graphs in one piece that have no cycles (circuits).

Trees have been used by computer scientists to organize information in searchable databases and also have proved a useful tool in seeing the connections between different species of viruses, such as those causing the Covid-19 epidemic that appeared dramatically in the United States in 2020. Trees also play a special role in understanding how to take a 3-dimensional polyhedron and make cuts along edges of the polyhedron to unfold it to a flat polygon, often informally known as a "net." It is still an unsolved problem as to whether every convex 3-dimensional polyhedron has a net. The cuts have to be made along edges of a tree that include all of the vertices of the vertex-edge graph of the polyhedron. Such a tree is known as a spanning tree of the graph. Higher dimensional cubes often called hypercubes have proved of use in understanding error correction systems. Figure 2 shows how to start with a zero dimensional cube and using the thick dark edges paste two copies together to get a 1-cube; two copies of a 1-cube can be used to make a 2-cube; two copies of the 2-cube can be pasted together to form a 3-cube, and so on. One can assign labels to the vertices of an n-cube by using all of the zero-one (0,1; binary) sequences of length n. The labels are chosen so that vertices joined by an edge differ in only one coordinate position.

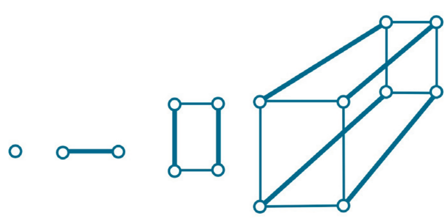


Figure 2. Cubes of dimensions 0 to 3. Note that one can take two copies of the prior cube and paste these copies together using the dark edges to get the next cube in the "series."

Figure 3 shows two 3-cubes assembled to form a 4-cube. Note that in some of these diagrams edges meet at points that are not vertices of the graph. A graph drawn in the plane with edges

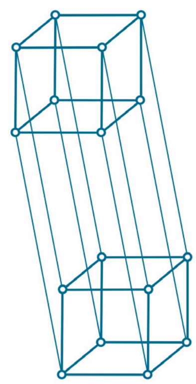


Figure 3 (A 4-dimensional cube can be constructed from two copies of 3-cube by joining corresponding vertices of the 3-cubes with edges. Can you find a different drawing with fewer or the fewest crossings for the 4-cube?)

meeting at vertices is called a plane graph, while graphs with the potential for such drawings are called planar. All trees are planar graphs. While the 3-cube can be drawn in a plane graph version as shown in Figure 4, starting with the 4-cube one cannot get plane drawings of such graphs. It is interesting to investigate how few "crossings" of edges one can get away with in drawings of cubes in the plane. The 3-cube in Figure 2 suggests the 3-dimensionality of the cube but there is a drawing of a 3-cube in the plane with 0 crossings (Figure 4) rather than the 2 that appear in Figure 2.

The 2-cube consists of one circuit (cycle) of length 4. The 3-cube has six 2-dimensional faces, its circuits of length 4, but it also has circuits of length 6 and 8. The circuits of length 8 (the largest possible on a 3-cube) visit each vertex once and only once and are known as Hamilton circuits. The *n*-cubes have no odd length circuits. The circuits of length 4 in such graphs correspond to the number of 2-dimensional faces of the higher dimension cubes (sometimes called hypercubes).

A nifty property shared by *n*-cubes and trees (with at least 2 vertices) is that they are bipartite graphs. Bipartite means that the vertices of such graphs can be put into two sets C and S so that edges of the graph only join vertices in C to S, never vertices in C to themselves or vertices in S to themselves. One can think of C and S as "colors" assigned to the vertices of the bipartite graph so that no two vertices of the same color are joined to each other. Note that for the *n*-cubes (n at least 1) the number of elements in the C and S sets must be the same size while for general trees this need not be the case. Trees with an odd number of vertices cannot have equal size C and S sets. Trees with an even number of vertices can have unequal or equal size sets C and S. I use the names C and S for circle labeled vertices (small circles for vertices) and square labeled vertices (small squares for vertices). See Figure 4(b) for the 3-cube drawn with vertices labeled in this way.

Warmup (and beyond) counting questions:

1. How many vertices does the 2-cube have? The 3-cube? The 4-cube? Can you find a general formula for the *n*-cube?

2. How many edges does the 2-cube have? The 3-cube? The 4-cube? Can you find a general formula for the *n*-cube?

3. How many circuits of length 4 does the 2-cube have? The 3-cube? The 4-cube? Note the 4-circuits of *n*-cube is each a 2-dimensional "face" of the cube. You should have found that the 4-cube has 24. Can you generate a formula for the number of 2-dimensional faces of an *n*-cube? Can you show that every *n*-cube (n at least 2) has a Hamilton circuit of its vertices (a circuit which passes through each vertex once and only once)? Omitting one edge from a Hamilton circuit of a cube gives rise to a path, a Hamilton path between two of the vertices of the cube. Cubes can have different "types" of Hamilton paths.

It is not difficult to see that the number of vertices and edges of a tree obeys the relationship: V(vertices) = E(edges) + 1. You can verify that one of the trees in Figure 1 has 12 vertices and 11 edges. If a vertex of a tree has i edges at the vertex it will be said to have degree *i* or to be *i*-valent and the number of such vertices will be denoted by $t(i)$. Often the 1-valent vertices of a tree are called the leaves of the tree. Since each edge of a tree is counted at the two vertices that are its distinct end points, the sum $(i)t(i)$ adds to twice the number of edges of the tree, and the sum of the $t(i)$ values adds to the number of its vertices. Using the equation $V = E + 1$, the valences of a tree obey the equation (*). The value m is the maximal valence of any vertex in the tree.

$$t(1) = 2 + \sum_{i=2}^{i=m} (i-2)t(i) \quad (*)$$

What is noteworthy is that there is no restriction on the number of 2-valent vertices that can occur in a tree. When a spanning tree of a connected (one piece) graph has no 2-valent vertices it is sometimes referred to in the research literature as a HIST tree or a (2')-tree (meaning no 2-valent vertices). Verify there are two trees in Figure 1 where the counts of valences of the vertices are given by: $t(1) = 3$ and $t(3) = 1$ and $t(1) = 3$, $t(2) = 3$, and $t(3) = 1$. Can you draw two additional trees not isomorphic to any tree in Figure 1 where $t(1) = 3$, $t(2) = 3$, and $t(3) = 1$? Note that since a 3-cube has all of its vertices of degree 3, any spanning tree, a subgraph which is a tree and which includes all of the 8 vertices of the cube, must have valences that obey these two equations:

$$t(1) = 2 + t(3) \quad (1)$$

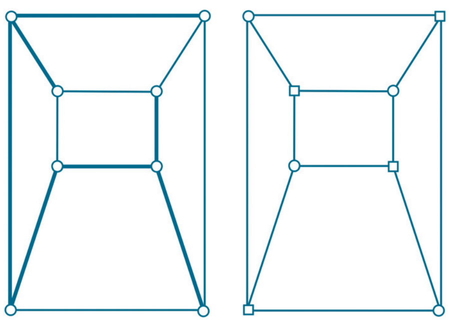
$$t(1) + t(2) + t(3) = 2^3 = 8 \quad (2)$$

From these two equations one can derive the fact that:

$$t(2) + 2t(3) = 6 \quad (3)$$

Thus, when $t(3) = 2$ the spanning tree would have $t(2) = 2$, and since the cube has 8 vertices the value of $t(1)$ has to be 4. In Figure 4 we can see that a 3-cube actually admits a spanning tree (dark edges) that has these valences. Notice that the spanning tree has three edges in common with two faces and two edges in common with four faces. Since there are six faces, we can associate this tree with the partition of 6, {4, 2}. Can you find spanning trees of the 3-cube that correspond to all of the other solutions of equation (1) and (2)?

It is interesting to note the pattern with which the dark edge-spanning tree in Figure 4 visits the six faces of the 3-cube, which are the length 4 circuits in the graph. Since a tree can't include all of the edges of a circuit, a tree will visit a 2-dimensional face of a cube of any dimension in either 0, 1, 2, or 3 edges. The number of visits that occur with these numbers of edge must add to 6, the number of faces of a 3-cube. This bears some similarity to counting the partitions of the six 4-circuits of the cube. A partition of the positive integer n is a way of writing n as the sum of nonnegative integers that add to n. Thus, the 11 partitions of 6 would be {6}, {5,1}, {4,2}, {4,1,1}, {3,3}, {3,2,1}, {3,1,1,1}, {2,2,2}, {2,2,1,1}, {2,1,1,1,1}, {1,1,1,1,1,1}. There is no simple formula for the number of partitions, which, being a set of numbers is unordered, but if one thinks about "ordered" partitions, sometimes called compositions, it turns out for a positive integer n the number of compositions is 2^{n-1}. Thus, for $n = 4$, {2,1,1} is a partition that "gives rise" to the compositions (2,1,1), (1,2,1), and (1,1,2). The partition {2,2} gives rise to only one composition, (2,2). So there are five partitions of 4, namely, {4}, {3,1}, {2,2}, {2,1,1} and (1,1,1,1} but there are eight compositions (4), (3,1), (1,3), (2,2) (2,1,1), (1,2,1), (1,1,2), (1,1,1,1). Sometimes a problem (finding a formula for the number partitions) can be very hard, but looking for a related formula for something that at first glance might be harder, in fact, turns out to be easier. Note that a spanning tree of a 3-cube can have no edges in common with some face of the cube.



(a) **(b)**

Figure 4. (a) A spanning tree of the 3-cube that has 3,3,2,2,2,2 as the number of edges that the tree has in common with the faces of the 3-cube. (b) A drawing of the 3-cube showing its bipartite structure, 4 vertices shown with small squares as vertices in the color set S (for squares), and 4 small circles as vertices in the color set C (for circles.)

Special classes of trees are:

a. Caterpillar: The tree has a path for which all of the edges of the tree have a vertex in common with this path. b. (1, k) tree; a tree all of whose vertices are either 1-valent or k-valent. c. A graph will be called a (2′)-tree if it has no vertices of valence 2. A tree without 2-valent vertices is sometimes called a HIT tree. Spanning trees with no 2-valent vertices are sometimes called HIST trees (standing for homeomorpically irreducible spanning trees).

There is no spanning tree for the solution: $t(1) = 5$, $t(2) = 0$, $t(3) = 3$ of the equations (1)-(2). Put differently there is no (1,3)-spanning tree of the 3-cube.

In Figure 1 only one tree is not a caterpillar (which one?) and the path (bottom tree) is a (1, k) tree for $k = 2$; there is also a (1, 3) tree there. The graph in the second row of Figure 1 is a (2′)-tree.

Research questions:

The interaction of cubes and spanning trees suggests what I think are an interesting collection of not fully explored problems.

1. For each n, determine the possible valences (degrees) of spanning trees for the n-cube. Can one always find a spanning tree of the n-cube for each possible solution?

Comment: For the 3-cube all the solutions are possible except the (2′)-case.

2. If for an n-cube a particular collection of valences can't be realized by a spanning tree, can one find a spanning tree of the $(n+1)$-cube with as many additional $t(2)$ vertices to satisfy the necessary condition equations?

3. For the trees which are $(1, k)$ trees that have the potential to be spanning trees of the k-dimensional cube, when does there exist such a spanning tree for the k-cube?

Comment: As a first step derive the equation for the number of 1-valent and k-valent vertices that such a tree would have to satisfy. Typically there will be non-isomorphic $(1, k)$ trees with particular numbers of vertices.

4. Do k-cubes (k at least 3) admit spanning trees without 2-valent vertices? If so, what can be said about the tree valence sequences for which this is possible?

5. Study the pattern of the number of edges that spanning trees and Hamiltonian circuits can have in common with the 4-circuits of n-cubes. Is it possible that a Hamiltonian circuit or spanning tree can touch each 4-circuit of an n-cube with exactly the same number of edges? How large can the number of faces of 4-circuits of an n-cube can there be that is not touched by any Hamiltonian circuit or spanning tree? Note: Can the notion of a partition of an integer be modified to help classify your results —remember that a spanning tree may not touch one or more 4-circuits of a n-cube?

References

Hoffmann Ostenhof, A., and K. Noguchi, and K. Ozeki. On homeomorphically irreducible spanning trees in cubic graphs, J. Graph Theory 89.(2018): 93-100.

West, D., Introduction to Graph Theory, (2nd. ed.), Prentice-Hall, 2001.

Joseph Malkevitch
Department of Mathematics and Computer Studies
York College (CUNY)
Jamaica, New York 11451