A TREE IN A BRAIN TUMOR

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ABSTRACT. We use a *shelling procedure* to construct a semi-automated sphere packing treatment plan for brain tumors. We develop a new code to denote an unlabeled tree, and we use it to obtain a complete classification of unlabeled n-trees. We also produce a *Mathematica* program to list for each n, all *perfect sequences* corresponding to n-trees, as well as their graphs. We then develop an algorithm and a program to analyze the brain tumor shapes using trees and perfect sequences.

I. An Automated Sphere Packing Plan for Brain Tumors

The goal of stereotactic radiosurgery for a brain tumor is to deliver the desired dosage to the target, and only the target. This is not possible in reality. So they do the next best thing, which is to deliver enough dosage to the target, to avoid as much normal tissue as possible, and to deliver as little radiation as possible to whatever normal tissue must be affected. There are two additional important criteria–dose homogeneity and dose conformality. That is, we do not want 'hot spots,' which have been experimentally determined to cause complications; and we do want rapid falloff of dose levels outside the actual tumor. One of several such radiation surgery methods is called the 'Multiple Isocenter Method.' This involves filling the tumor image with spheres of different sizes, until the image is best filled up. This noninvasive method of surgery, namely by using radiation, relies on a piece of equipment called the *Linear Accelerator* (or simply, *Linac*). Most of the information in this section about treatment of a brain tumor is taken from Friedman et al.[4]. See [4] for further reference.

1. Making a Sphere by Arcs of Beams

According to [4], the linear accelerator is a complex machine capable of producing X-rays. A large amount of energy is generated by the power supply, which then powers the filament shown. This causes electrons to be emitted by the filament, which are in turn accelerated to higher energies using a (micro-)wave guide. The electrons are then changed in direction by the magnet so that they impact on a heavy metal alloy target. This results in X-ray production that can then be collimated or shaped by both primary and secondary collimators within the linear accelerator head. This beam is further collimated for radiosurgery by the tertiary radiosurgery collimator.

The Linac is mounted on a rotating gantry such that the beam has a center of rotation about 1.5m above the floor. Usually, the isocenter accuracy is defined within a 2mm sphere. Because stereotactic radiosurgery depends on optimized

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accuracy, an improved system was designed at the University of Florida, by adding a set of bearings to the stereotactic collimator system and under the patient table. As a result, this new system achieves mechanical accuracy within 0.2mm±0.1mm for defining the treatment isocenter of beam delivery.

The tertiary collimators are generally circular and allow improved centering of the treatment beam. The sizes of these collimators are from 5 to 40mm in 2- to 5-mm increments.

By varying the angle of the gantry and the angle of the table, one can deliver a radiation beam to the target from any angle within the range of the rotation. The shape of the common intersection of an arc of beams passing through one isocenter is a sphere. The neurosurgeons deliver a series of arcs (usually 5 or 9 arcs) to produce a single isocentered sphere shape. For an ellipsoidal target, they use fewer numbers of arcs to make a single isocentered ellipsoid shape.

So, if the target shape is very close to a sphere or an ellipsoid, then the treatment plan is relatively easy compared to an irregularly shaped target. In that case, we need to create a geometric treatment plan.

2. Sphere Packing Plan

As seen in the previous subsection, the physicians know how to irradiate-to-destroy tumors which are shaped like spheres or ellipsoids. For a non-spherical shape of tumor, they try to fill the target with several spheres of different sizes. This is called the 'sphere packing' treatment plan.

After finding a sphere packing plan, they treat each sphere separately as described in the previous subsection. So, multiple isocenter radiosurgery planning includes the problem of determining the best sphere packing arrangement with which to fill the target volume. General methods for this treatment plan are iteratively based, dosimetrically driven algorithms. But these methods require many computations in order to compute a radiosurgical plan dose distribution, and then to evaluate the quality of the dose distribution. So geometrically based radiosurgery optimization has been suggested as a possible alternative means.

However the method the physicians choose relies on human decisions and experience. Thus, for the same target, different surgeons may produce different plans. Even the same surgeon, doing the plan twice for the same target, may produce different plans. And the planning takes a long time, especially for a complicated target which needs more than 10 spheres. It might take as much as two hours of planning for a difficult case which needs about 20 spheres. During that time, the patient has to wait with the head ring attached to his or her head. And most importantly, even after spending the time to make a plan, many physicians without sufficient experience, are not sure if the plan is a 'good' one.

Therefore, we provide a semi-automated sphere packing method for the treatment plan (see [19]). This method shows potential to significantly aid the planning of difficult multiple isocenter cases. Based on tests with irregularly shaped phantom targets and with a representative sampling of clinical example cases, the method demonstrates the ability to generate radiosurgery plans comparable to, or of better quality than, multiple isocenter Linac radiosurgery plans found in other literature. At the same time, this program always produces the same treatment plan for the same tumor shape. So it can be used as a 'benchmark' to compare with other plans

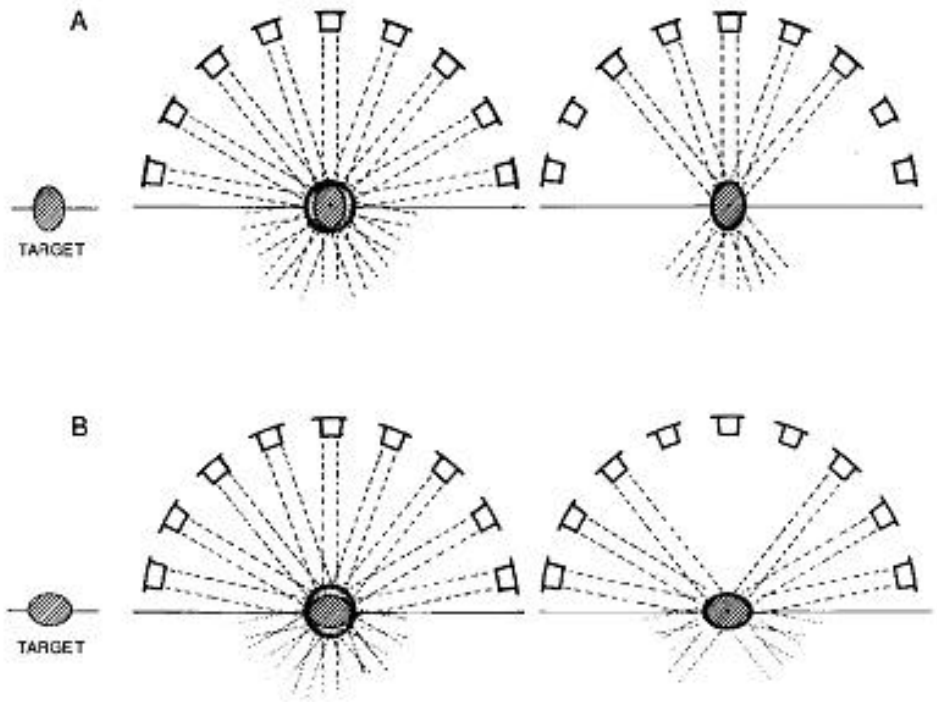

Figure I-1. Plan for a sphere shape and an ellipsoidal shape ([4])

for the given tumor shape. Moreover, this program provides the treatment plan in a relatively short time. For a very difficult case which needed more than 18 spheres, this program took less than 3 minutes instead of more than the 1.5 hours which were needed when the physicians created the plan using traditional methods.

In the following subsection, we explain the 'shelling procedure' which we used in this program to get the centers and sizes of spheres for the sphere packing plan.

3. Shelling Procedure

The shelling procedure is best illustrated in Figure I-2 to I-10. The major steps of this shelling procedure are as follows.

Step 1 Transfer the data of the boundary of the target to the three dimensional array and assign a status value for each voxel. (See Figure I-2 and I-3).

Step 2 Shell the target voxels (See Figure I-4).

We program a prodecure to count the number of layers of the largest sphere(s), and identify the deepest voxel(s). Occasionaly, several voxels remain at the deepest level. When this occurs, the *score function* is requested which is derived by Thomas Wagner. (see [19])

Step 3 Remove the largest sphere (as chosen by the score function, if use)

We think of the largest radius sphere as being removed, and repeat the process inductively. (See Figures I-5 to I-10.)

For further detailed information about the score function and the automated sphere packing plan, we refer the reader to [18] and [19].

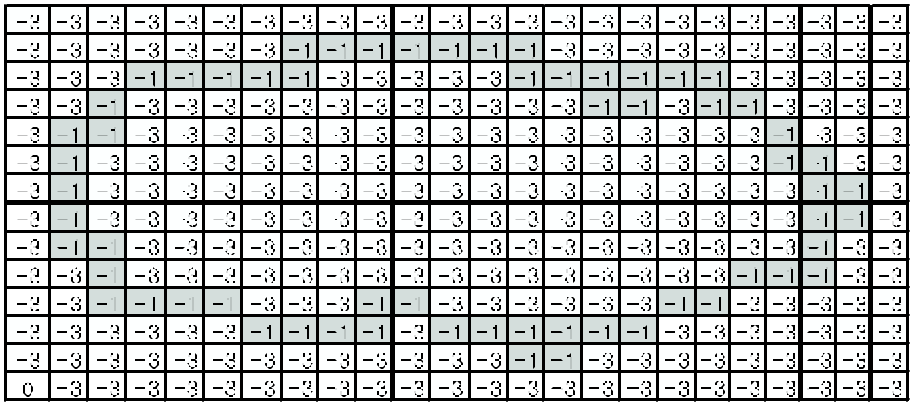

Figure I-2. Status values for the boundary and the initial voxel

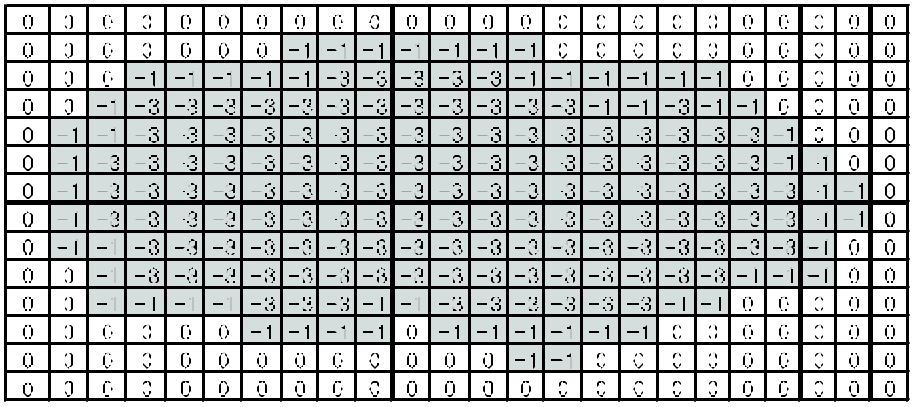

Figure I-3. Status values for the normal voxels

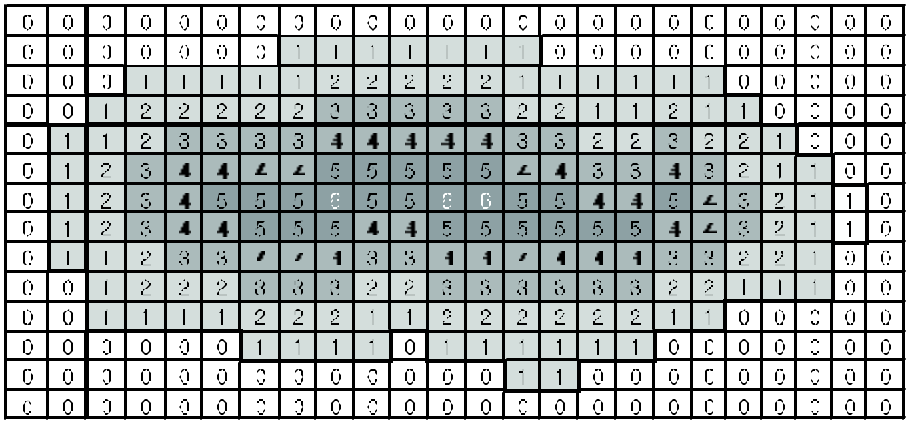

Figure I-4. Shelling the target voxels

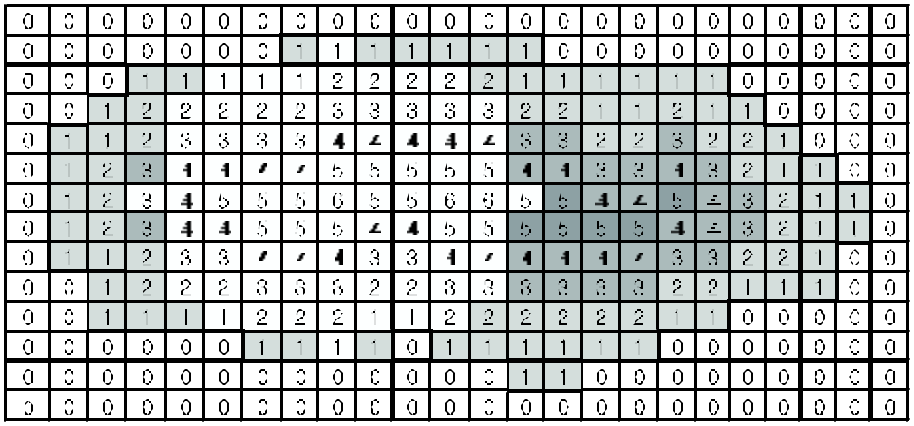

Figure I-5. Choosing the largest sphere

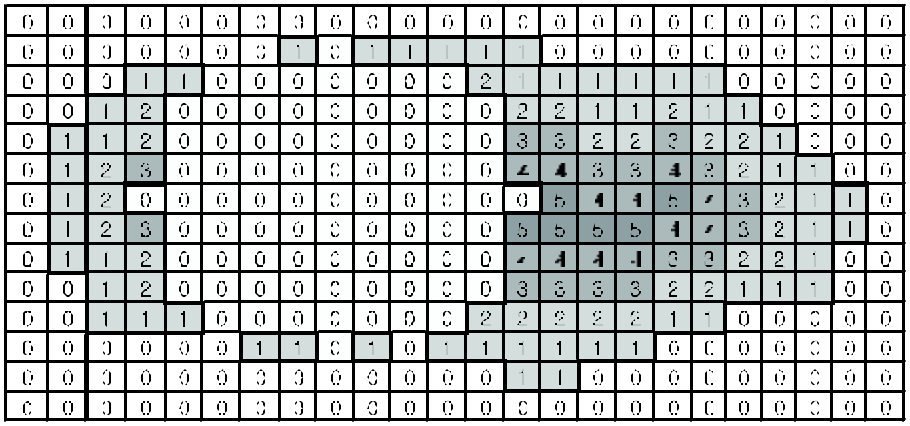

Figure I-6. Removing the largest sphere

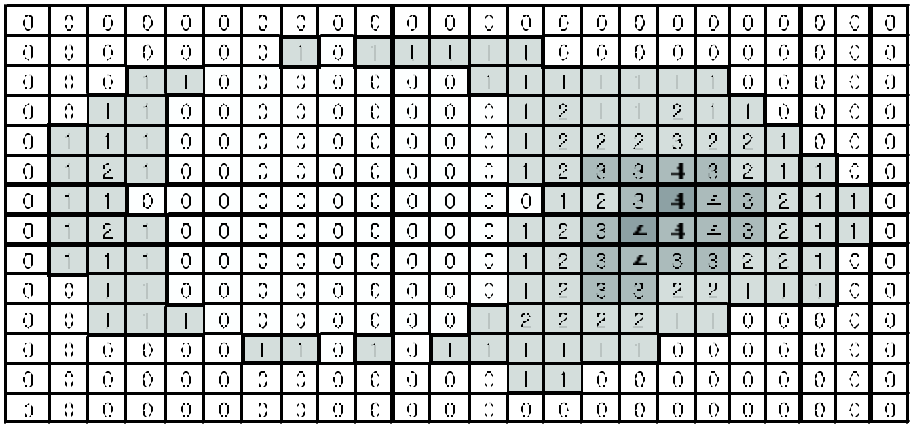

Figure I-7. Shelling the remaining target voxels

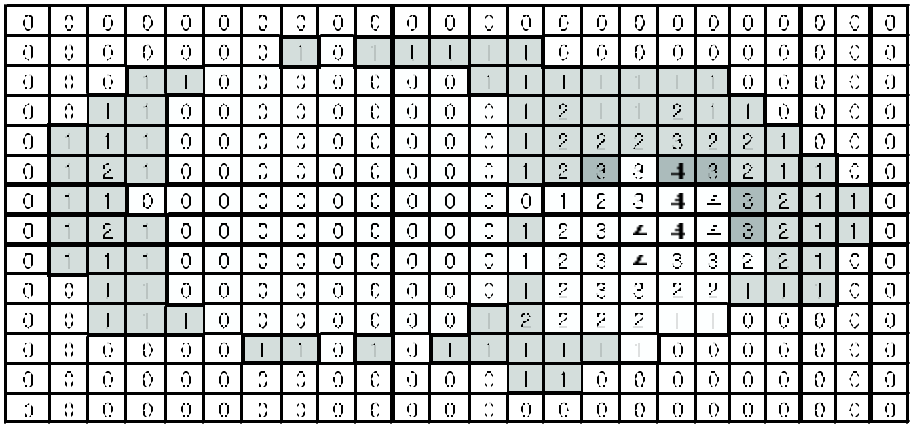

Figure I-8. Choosing the largest sphere of the remaining target

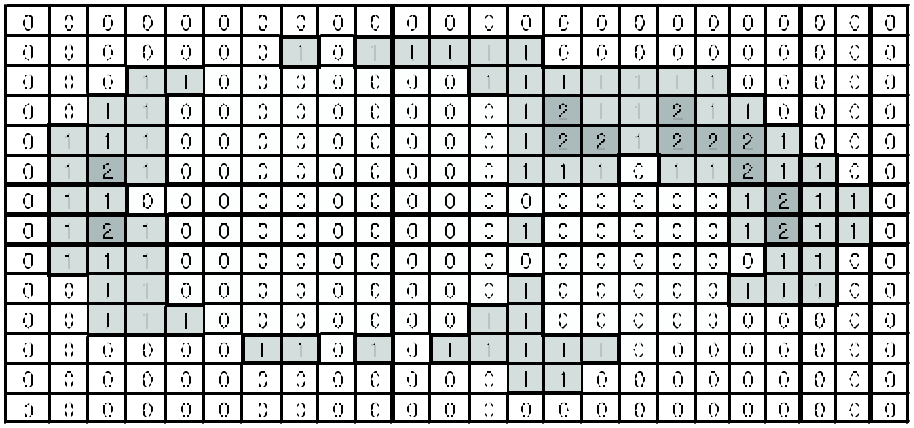

Figure I-9. Removing the second sphere

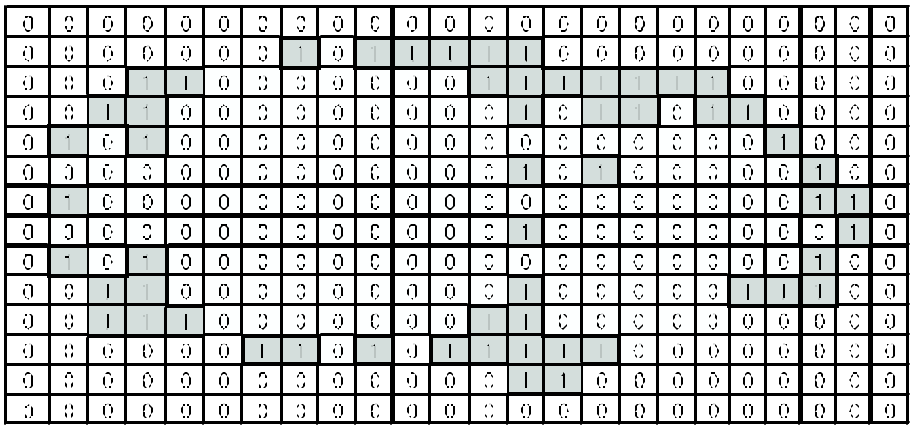

Figure I-10. Removing all the spheres

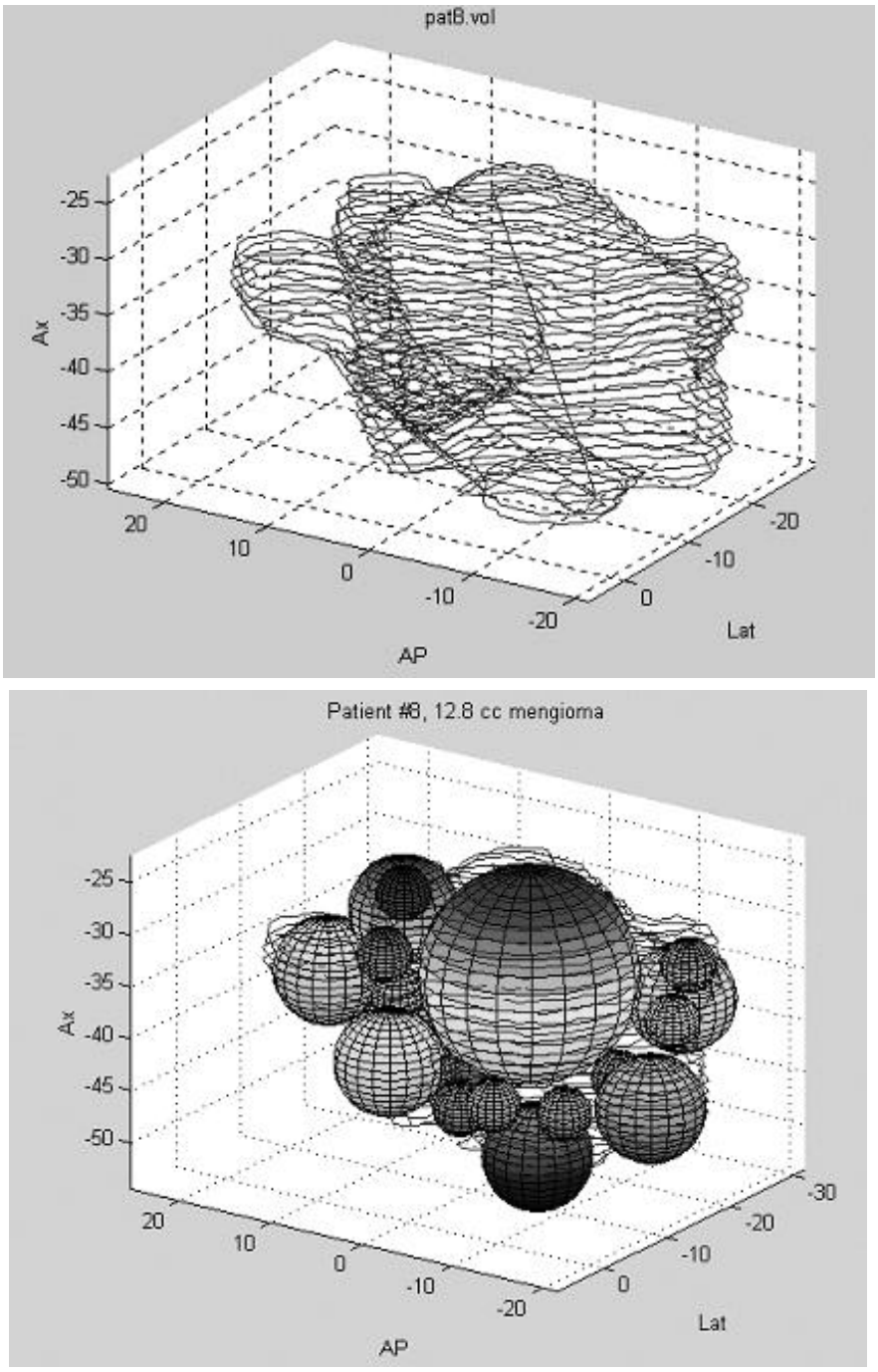

Figure I-11. A sphere packing plan for a brain tumor ([19])

II. A Classification of Unlabeled Trees

In this section, we obtain a new code to denote an unlabeled tree. By means of this code, we classify unlabeled n-trees. In particular, we call a tree an *n-tree* if and only if it is a tree with n vertices (that is, $(n-1)$ edges). Our code assigns a unique, ordered, 'perfect sequence', $pf(T) = \langle d_1, d_2, \ldots, d_n \rangle$, to each unlabeled n-tree, T. And, conversely, given an ordered sequence of n integers satisfying certain properties, it is the perfect sequence of exactly one unlabeled n-tree.

Our work includes an algorithm and a *Mathematica* program that produce a list of all the perfect sequences for all possible n-trees, thus also producing the number of n-trees, for any given n. Some examples are given below.

However, we do not have a *simple formula* that tells us how many unlabeled n-trees there are. This remains an open problem.

1. Perfect Sequence for a Tree

Let T be the unlabeled tree below, but we labeled the vertices of T as shown to construct a degree sequence.

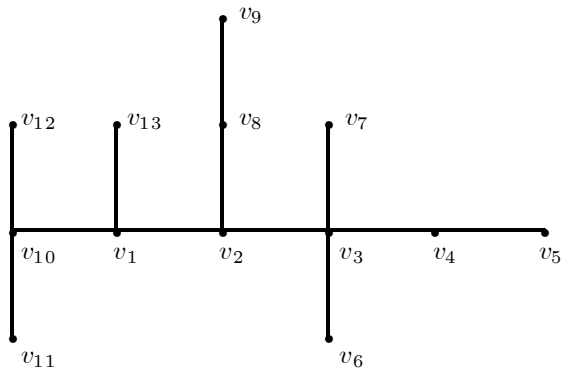

Figure II-5

For the chosen vertex sequence $V = \langle v_1, v_2, ..., v_{13} \rangle$, we can get the degree sequence, $D = \langle 3, 2, 3, 1, 0, 0, 0, 1, 0, 2, 0, 0, 0 \rangle$.

(a) Let $D = \langle 3, 2, 3, 1, 0, 0, 0, 1, 0, 2, 0, 0, 0 \rangle = \langle d_1, d_2, ..., d_{13} \rangle$. Then d_i equals (the degree of v_i) - 1, except the first term in which d_1 = the degree of v_1. Clearly, $\sum_{i=1}^{13} d_i = 12$, which is the number of edges in T.

(b) Every pair of consecutive terms in the sequence are connected in T except for the end vertices. We choose one of the closest vertices to the end vertex, that is not selected yet in the sequence. For example, since the vertex v_5 is an end vertex, we don't have any remaining unselected vertex connected to v_5. Then there are two (closest to v_5,) unselected vertices, v_6 and v_7. We could choose either of them for the next term after v_5.

We showed that, for a given tree T, there exist many vertex sequences, therefore degree sequences, depending on the starting vertex and choice among the adjacent vertices for each successive vertex. Therefore the degree sequence set $\mathcal{D}$ for the given tree T contains many different degree sequences which denote the same tree T. We need a way to choose one degree sequence representing the tree T. So we define an order on the set of all finite, nonnegative, integer sequences, and then we define a *perfect sequence* to be the unique maximum element under this order.

Theorem 1 [Tree Classification Theorem] *For any positive integer n, let $\mathcal{T}(n)$ be the set of unlabeled n-trees and $\mathcal{P}(n)$ the set of perfect sequences of length n. Then there is a one-to-one correspondence between $\mathcal{T}(n)$ and $\mathcal{P}(n)$.*

2. Some Program Results

Our notation for a degree sequence is $\langle d_1, d_2, \ldots, d_n \rangle$. But the *Mathematica* program produces the sequence notation with { and }. So in this subsection, any set notation actually denotes the degree sequence. Note that an n-tree has n vertices, so there are n-1 edges.

```
     n=3          total number of degree sequences : 1
{2, 0, 0}
```



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     n=4          total number of degree sequences : 2
{3, 0, 0, 0},         {2, 1, 0, 0}
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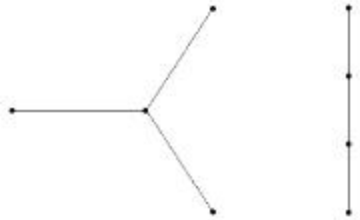

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     n=5          total number of degree sequences : 3
{4, 0, 0, 0, 0},     {3, 1, 0, 0, 0},     {2, 1, 1, 0, 0}
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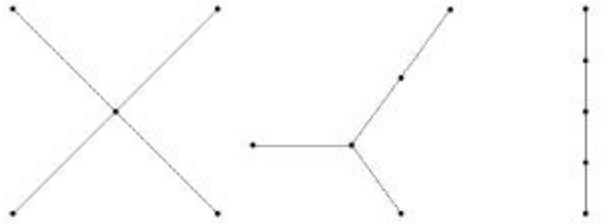

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     n=6          total number of degree sequences : 6
{5, 0, 0, 0, 0, 0},  {4, 1, 0, 0, 0, 0},  {3, 2, 0, 0, 0, 0},
{3, 1, 0, 1, 0, 0},  {3, 1, 1, 0, 0, 0},  {2, 1, 1, 1, 0, 0}
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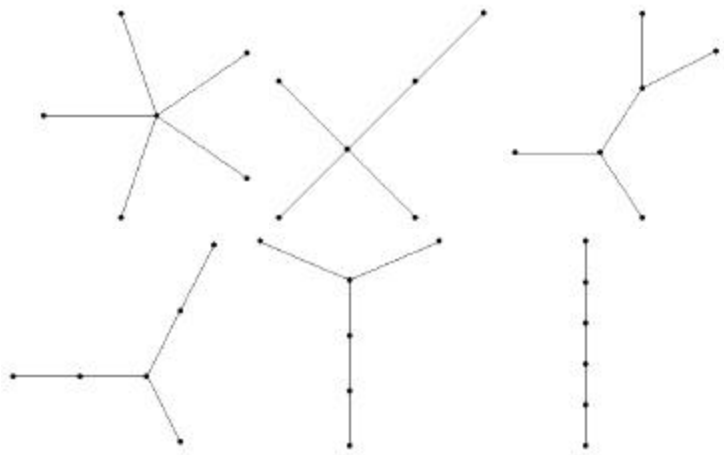

III. A Tree for a Brain Tumor

In section I, an automated sphere packing treatment plan for a given brain tumor is developed.

From that plan, we can assign a unique corresponding graph by matching a sphere with a vertex and matching the adjacency of two spheres with an edge. Then, by using the notion of *cutvertex* (a separating vertex), we give an order to the vertex set. We use this order to decide which edges to choose in order to obtain a *unique maximal tree* contained in the graph. We assume that a brain tumor is connected, so the graph representation for any brain tumor is a connected graph.

1. Cutvertex and Block

Let G be a graph with 14 vertices and 18 edges as in the Figure III-1 below.

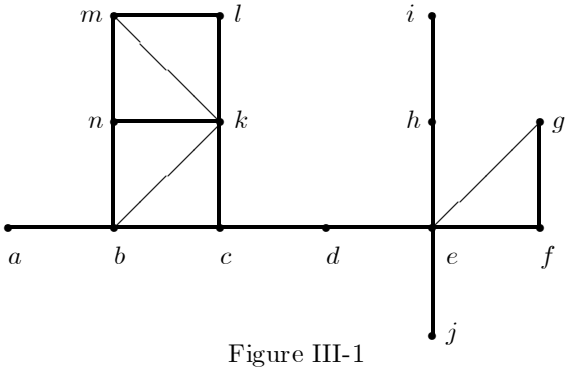

Figure III-1

There are 3 cutvertices, b, c, e. So the given graph G can be separated into 6 blocks as follows:

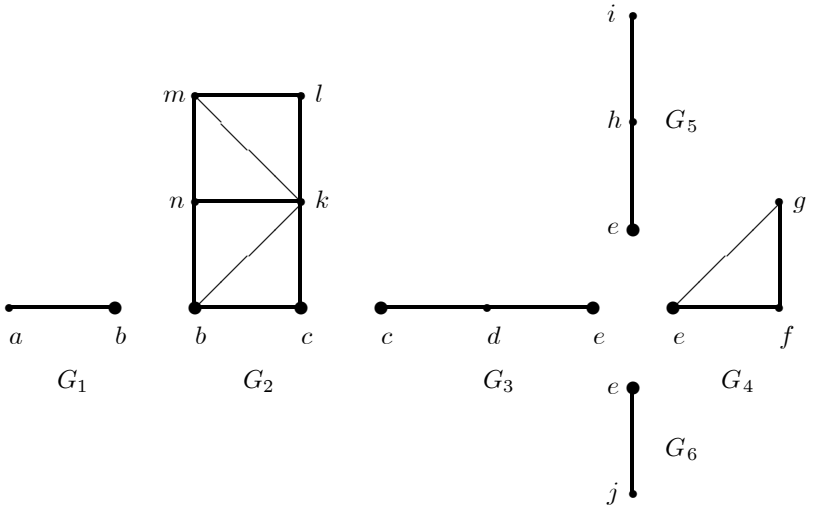

Figure III-2

2. Order in the Vertex Set

To get a maximal tree from a graph we may need to delete some edges in the graph. Thus we need to label each vertex in order to choose certain edges to delete, even though we are dealing with an unlabeled graph in this article. So there is no specific meaning for this labeling except that it is only used to choose a maximal tree for the graph.

Example III-1. Let P be the sphere packing treatment plan (see Figure III-3) for a given brain tumor, shown below.

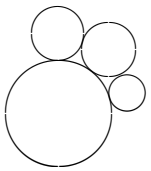

Figure III-3

Then there is a unique graph G for the sphere packing plan. The graph is given below in Figure III-4.

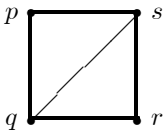

Figure III-4

There are two different isomorphism classes, namely T_1 and T_2, of maximal trees for the graph G. That is, we could choose either of these for a maximal tree to assign the graph G. Since, in our algorithm, we want to get the same maximal

tree for a given graph every time, we need certain rules to get the same tree. (See Figure III-5.)

Figure III-5

In this section, we assume that the graph comes from a sphere packing treatment plan. That is, the main shape of the brain tumor depends on the size of spheres and the connection between spheres. Even though we cannot keep the information about the size of spheres in the graph, it seems to us that the bigger the sphere is, the more it has a chance to get attached to more spheres. And we assume that the larger degree vertices play a more important role in classifying the tumor shapes into trees than the smaller degree vertices. That is, by choosing a largest degree vertex first, the shape of the tumor is apparently most closely preserved. Thus, in the previous example, we choose the vertex q or s as the starting vertex; then we pick all the incident edges (see Figure III-4). Then we get the tree T_1. Therefore we want to choose the tree T_1 for the maximal tree of G. Note that the tree T_2 produces a linear graph which does not show the shape of the tumor as closely as T_1.

But there are some vertices which are more important than the larger degree vertices. Recall the graph G in the subsection III-1. Then, in the block G_2, it is clear that the vertex k has the largest degree, 5. But the cutvertices, b and c, play a critical role in obtaining a maximal tree of G. So, to get a maximal tree for a graph G, we want to start at the cutvertices of G first, instead of the vertices with the largest degree. So we want to label the cutvertices first. On the other hand, there are different kinds of 'cutvertices' in some graphs. The following example shows such a case.

Example III-2 Let $G = \{V, E\}$ be the graph in Figure III-6.

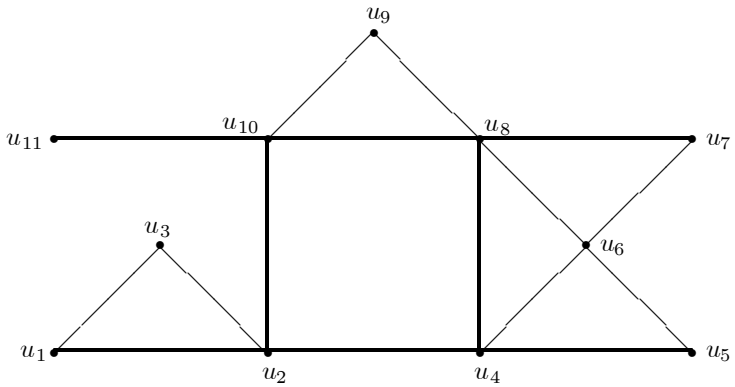

Figure III-6

Then there are two cutvertices of the graph G, namely u_2 and u_{10}. Using these two cutvertices, the graph G is separated into four subgraphs, namely G_1, G_2, G_3 and G_4. (See Figure III-7.)

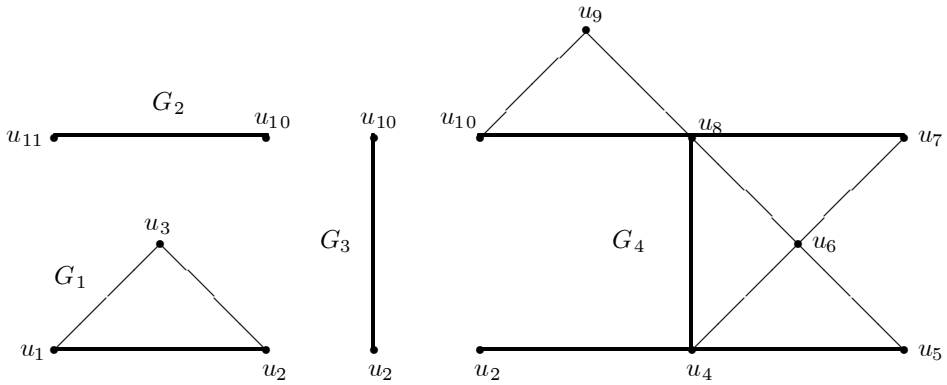

Figure III-7

Then the subgraphs G_1, G_2, and G_3 are blocks, but the subgraph G_4 contains its own cutvertices, u_4 and u_8, which are not cutvertices of the graph G. We separate the subgraph G_4 into four subgraphs by using its cutvertices u_4 and u_8. (See Figure III-8.) Note that there is no specific order in labeling the subgraphs. So at this moment, we relabel the subgraphs of G by H_1, H_2, ..., H_7.

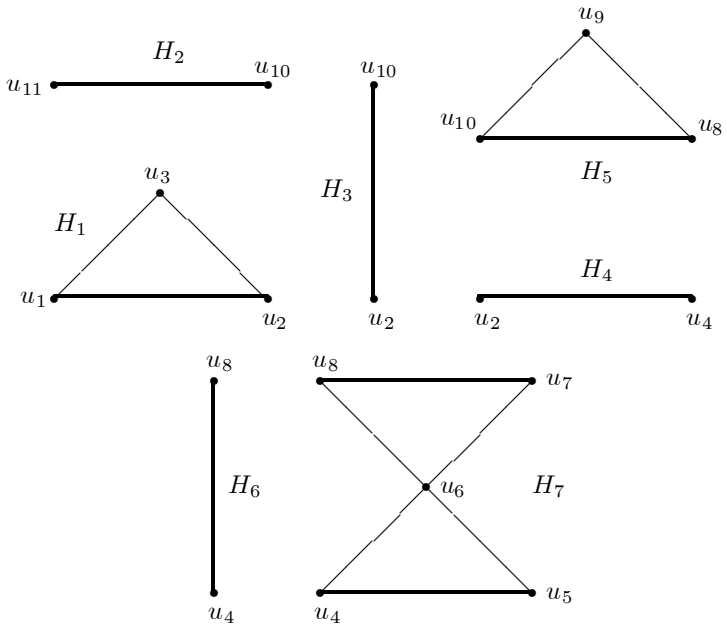

Figure III-8

Then, again, the subgraphs H_1, H_2, ..., H_6 are blocks, but the subgraph H_7 contains its own cutvertex, u_6, which is neither a cutvertex of the graph G

nor a cutvertex of the subgraph G_4. We separate this subgraph H_7 into two subgraphs by using u_6. (See Figure III-9.) And we relabel the subgraphs of G by $B_1,\ B_2,\ \ldots\ ,\ B_8$.

Therefore $\{u_2, u_{10}\}$ is the set of cutvertices of the graph G. But $\{u_4, u_8\}$ is the set of the cutvertices of a subgraph which is produced after the first separation using the cutvertices of the graph, and u_6 is the cutvertex of a subgraph which is produced after the second separation.

For the purpose of labeling the vertices in a graph, we separate these cutvertex sets for different levels, from each other.

Let G be the graph assigned for a given sphere packing plan P. Then the vertex set $V(G)$ of the graph G is the union of two disjoint subsets, namely $C_1(G)$ and $C_1^c(G)$, where $C_1(G) = \{v \in V(G) |\ v$ is a cutvertex of $G\}$ and $C_1^c(G) = V(G) - C_1(G)$. We call $C_1(G)$ the *first step cutvertex set* of G. For every $i = 2,3,\ldots,|V(G)|$, we define a subset $C_i(G)$ of $C_{i-1}^c(G)$ as the collection of the vertices of $C_{i-1}^c(G)$, which are cutvertices of a subgraph produced after the $(i-1)$-th separation using the elements of $C_{i-1}(G)$. Then we call $C_i(G)$ the *i-th step cutvertex set* of G, and let $C_i^c(G) = C_{i-1}^c(G) - C_i(G)$. We assume that there are finitely many vertices in a given graph. If there exists at least one cutvertex, then there exists an integer $1 \le k \le n$ such that $C_i(G) \neq \emptyset$ for every $i \le k$, and $C_i(G) = \emptyset$ for every $i \ge k+1$. Then we call k the *separation step constant* of the graph G, and let $C^c(G) = (C_k)^c(G)$.

If there is no cutvertex of G then the graph is a block, and we say that the separation step constant of G is 0.

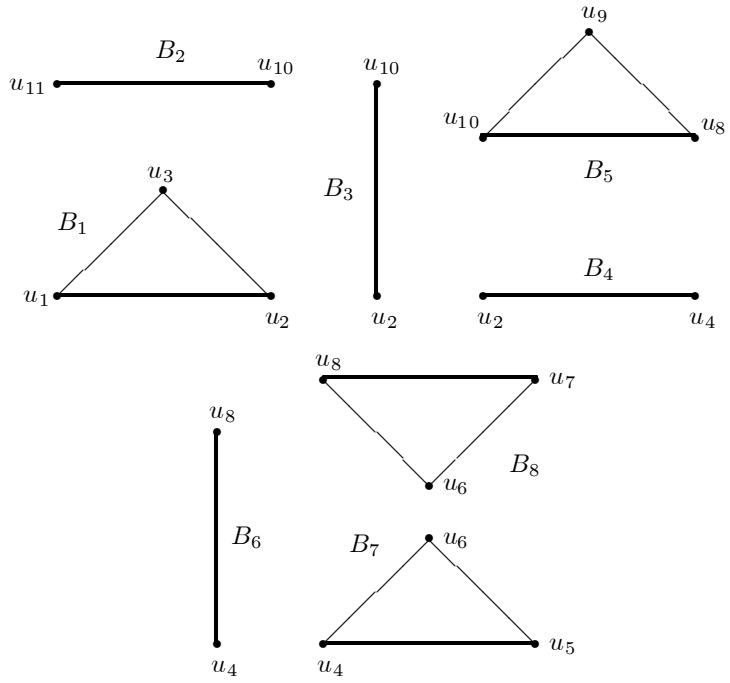

Figure III-9.

It is clear that for any two different spheres, at least one of the center coordinates is different. Thus any two distinct spheres can always be compared by the above order. Therefore the above order for the vertices of the graph is well defined.

3. Maximal Tree from a Graph

In this section, we illustrate, by means of an example, how to select a unique maximal tree from the graph which is produced for a given brain tumor by using an example. For the detailed algorithm, refer to [23].

Example III-3 Let G be the graph in Figure III-1, with a new labeling. Then $C_1(G) = \{b, c, e\}$ and $C_1^c(G) = \{a, d, f, g, h, i, j, k, l, m, n\}$. In $C_1(G)$, we have that $d(e) = 5$, $d(b) = 4$ and $d(c) = 3$. On the other hand, in $C_1^c(G)$, we have that $d(k) = 5$, $d(m) = d(n) = 3$, $d(d) = d(f) = d(g) = d(h) = d(l) = 2$, $d(a) = d(i) = d(j) = 1$. And $C_2 = \emptyset$. Thus we order the vertices as follows; $v_1 = e$, $v_2 = b$, $v_3 = c$ and $v_4 = k$, $\{v_5, v_6\} = \{m, n\}$, $\{v_7, v_8, v_9, v_{10}, v_{11}\} = \{d, f, g, h, l\}$, $\{v_{12}, v_{13}, v_{14}\} = \{a, i, j\}$. Assume that $v_5 = m$, $v_6 = n$, $v_7 = d$, $v_8 = f$, $v_9 = g$, $v_{10} = h$, $v_{11} = l$, $v_{12} = a$, $v_{13} = i$, $v_{14} = j$, which are decided by the sizes and centers of the corresponding spheres. (See Figure III-16.)

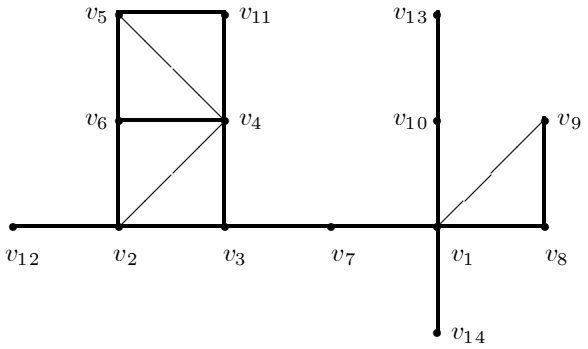

Figure III-16

For the cutvertex v_1, we keep the 5 edges attached to v_1. (See Figure III-17.)

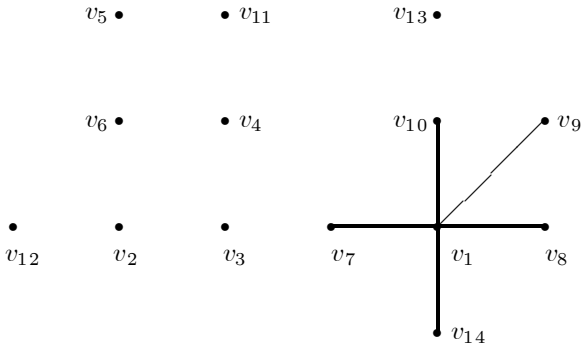

Figure III-17

Since v_2 is not adjacent to the vertex v_1, we keep all the edges attached to v_2. (See Figure III-18.)

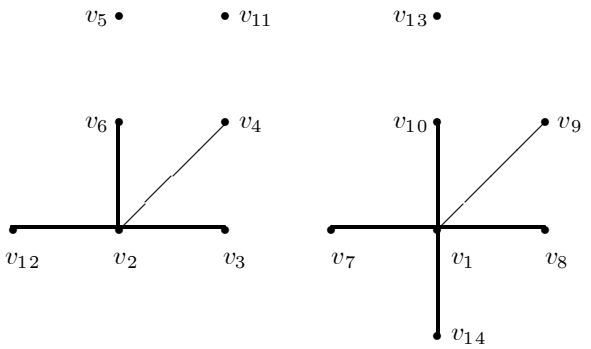

Figure III-18

Since v_3 is an adjacent vertices of v_2, the edge $\{v_3, v_4\}$ makes a circular form. Thus we keep the edge $\{v_3, v_7\}$ only. (See Figure III-19.)

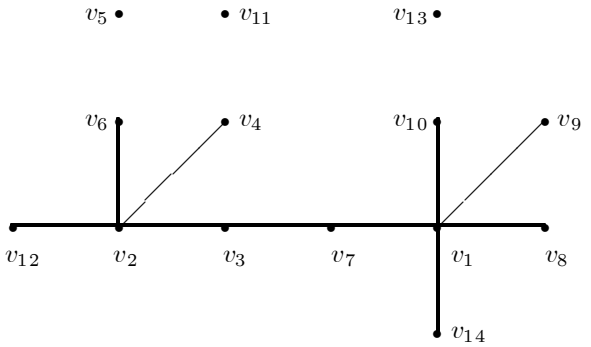

Figure III-19

For the vertex v_4, by the same reasoning, we keep only 2 edges, $\{v_4, v_5\}$ and $\{v_4, v_{11}\}$. (See Figure III-20.)

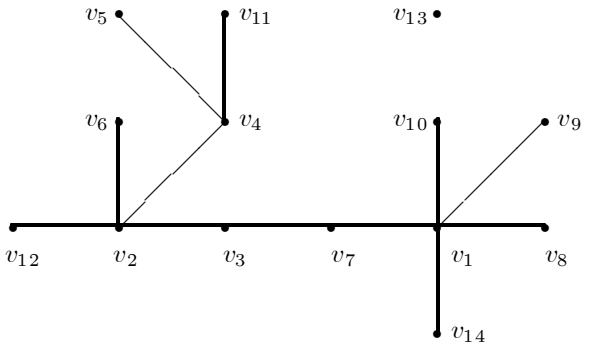

Figure III-20

For the vertices v_5, v_6, v_7, v_8, v_9, there is no 'new' edge. For the vertex v_{10}, we could keep the edge $\{v_{10}, v_{13}\}$. At this moment, the total number of edges in this

tree is 13 which is one less of the number of vertices. Therefore we have a maximal tree for the given graph. (See Figure III-21.)

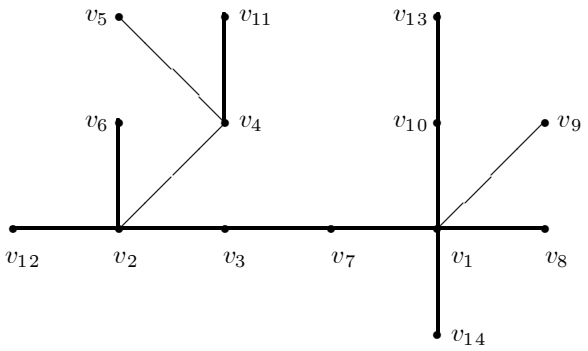

Figure III-21

For this resulting tree T, we choose the vertex sequence

$$\langle v_1, v_7, v_3, v_2, v_4, v_5, v_{11}, v_6, v_{12}, v_{10}, v_{13}, v_8, v_9, v_{14} \rangle .$$

Then $P = \langle 5, 1, 1, 3, 2, 0, 0, 0, 0, 1, 0, 0, 0, 0 \rangle$ is the *perfect degree sequence* of T.

If we are interested only in the shape of a brain tumor, without regard to physical consequences (for example, location near an eye or the brain stem, etc), then we can fully automate our program from section I, to obtain a unique tree.

For any brain tumor, we have a unique sphere packing plan by the automated program in [21] and [22], and it can be represented by a graph. Then we have a unique *perfect sequence* for the graph. That is, we can assign exactly one perfect sequence to each brain tumor. So, if two perfect sequences are distinct, then their corresponding trees, and therefore their respective corresponding graphs and sphere packings, are also distinct. That is, if two tumors are represented by distinct perfect sequences, then their corresponding trees are not isomorphic. And their respective graphs and sphere packing plans are not isomorphic. Thus, we may consider their shapes to be distinct. Therefore we have the following:

Theorem 2 *The perfect sequences are invariants of the shapes of arbitrary brain tumors.*

This work is a summary of the author's dissertation, under the direction of Beverly L. Brechner. Various parts of this work were in collaboration with different subgroups of the following people: Beverly L. Brechner, Frank Bova, Yen Chen, Mattew Harvey, Tomas Wagner, as well as additional faculty from the Brain Institute at University of Florida. This work is motivated by questions radised by Dr. Frank Bova of the McKnight Brain Institute at the University of Florida. Dr. Bova led a joint medical and mathematics research group, which included all of the mentioned people above. For more detailed results see references [19], [21], [22], [23], [24].

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