1. INTRODUCTION

We have the set \([n]\) and a dissimilarity map

\[ d : \frac{[n]}{2} \rightarrow \mathbb{R} \]

such that \(d(i,i) = 0\) for all \(1 \leq i \leq n\), and \(d(i,j) \geq 0\) for all \(1 \leq i,j \leq n\). We then define a polyhedron by the inequalities:

\[ P_d = \{ x \in \mathbb{R}^n | x_i + x_j \geq d_{ij} \text{ for } 1 \leq i \leq j \leq n \} , \]

and consider its bounded complex

\[ B_d = \{ x \in \mathbb{R}^n | x \text{ lies on a bounded face of } P_d \} . \]

**Theorem 1.1.** A metric \(d\) on \([n]\) is a tree-metric iff \(\text{dim}(B_d) = 1\). If \(d\) is a tree-metric, then The set \(B_d\) with the \(\| \cdot \|_\infty\) norm is the matric tree for \(d\) with the correspondence \([n] \ni i \leftrightarrow (d_{i1}, d_{i2}, \cdots, d_{in}) \in B_d\).

If we do have a tree-metric, then this gives us one way to construct the tree. The question is: What happens to the bounded complex if we don’t have a tree-metric? We want to study these polyhedral complexes.

2. IMPLEMENTATION

2.1. The Software POLYMAKE. POLYMAKE is a software for working with polytopes and polyhedra. It can be downloaded from "http://www.math.tu-berlin.de/polymake/". POLYMAKE allows us to input the inequalities that define a polyhedron and computes numerous properties of the polyhedron.

2.2. How the New Programs Work. POLYMAKE does not have built-in functions to work with bounded complexes. Julian Pfeifle and I implemented several programs to analyze and visualize the bounded complexes. We have done the following:

1. Build the bounded complex from the input polyhedron.

2. Label the points corresponding to the taxa.

Recall that in the tree-metric case, the correspondence between the taxa and the point on \(B_d\) is \([n] \ni i \leftrightarrow (d_{i1}, d_{i2}, \cdots, d_{in}) \in B_d\). If you fix \(i\), this point in \(\mathbb{R}^n\) is precisely the unique point that makes all the inequalities \(x_i + x_j \geq d_{ij}\) into equalities. In other words, the taxon \(i\) corresponds to the intersection of the hyperplanes defined by \(x_i + x_j = d_{ij}\) for all \(1 \leq j \leq n\). In the general case when our dissimilarity
map $d$ does not satisfy the four-point condition, their intersection may lie outside of $B_d$. So we look for vertices in the bounded complex that lie in the intersection of all but one hyperplanes and label them. If there aren’t any, then we look for vertices in the intersection of all but two hyperplanes.

3. Find a projection onto a three-dimensional subspace of $\mathbb{R}^n$ such that all the faces can be seen in the projection.

4. Visualize the (2-skelton of the) bounded complex.
Visualizing the honest projection usually does not turn out nice, so we used the spring embedder. Imagine putting a same charge to every vertex so that the vertices repell against each other, and a spring on every edges so that it pulls the vertices together. This process "unfold" the graph and gives a pretty picture. A drawback is that the edge length information is lost.

The source codes, instructions, and examples can be found at the web site "http://www.math.berkeley.edu/ jyu/polymakebounded_complex/bounded_complex.html".

3. An Example
Following is an input distance matrix of a set of phylogenetic data and Figure 3.1 is the corresponding visualization.

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<th>Zebrafish</th>
<th>Tetraodon</th>
<th>Fugu</th>
<th>Rat</th>
<th>Mouse</th>
<th>Rabbit</th>
<th>Horse</th>
<th>Pig</th>
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<td>0.38224</td>
<td>0.47441</td>
<td>0.47132</td>
<td>0.44783</td>
<td>0.43305</td>
<td>0.44488</td>
</tr>
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<td>0.43225</td>
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<td>0.41648</td>
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<td>0.42485</td>
</tr>
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<td>0.14313</td>
<td>0.35614</td>
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<td>0.34624</td>
<td>0.28836</td>
<td>0.19227</td>
<td>0</td>
</tr>
</tbody>
</table>

4. Some Results about the Bounded Complexes
From the experiments with polymake, I have the following proposition. I am writing up the details of the proof in a separate term paper.

For a dissimilarity map $d : \left( \begin{array}{c} \mathbb{N} \\ \leq \end{array} \right) \rightarrow \mathbb{R}$, define a polyhedron $P_d = \{ x \in \mathbb{R}^n \mid x_i + x_j \geq d_{ij} \}$, and let $B_d$ be the bounded complex of $P_d$.

**Proposition 4.1.**

1. The number of vertices in $B_d \leq 2^{n-1}$
2. The dimension of $B_d \leq \frac{n}{2}$.

In both cases, equality is achieved in a general case.

5. Further Questions
There is still much room for improvement in our program. The algorithms used are not very efficient and almost unusable if the number is taxa is over 12. There may also be a solution to the problem that our visualization does not reflect actual distances in the bounded complex. We should also look for the biological meanings of the pictures.
Figure 3.1. 5 mammals and 3 fishes

Figure 3.2. Metric on 5-taxa corresponding to the Thrackle triangulation

References