

## Bioinformatics – Lecture Notes

### Announcements

Next week is Spring Break (March 11-15). NO CLASS.

Class 15 – March 5, 2002 -

1. Evolutionary Problems – Clustering Methods – How do we determine the best fit phylogenetic data?

Cannot determine the minimum number of mutations for all possible tree topologies having  $n$  leaves since the number of binary trees is exponential. Instead we will use some concepts from graph theory

#### Definitions

*taxa* – entities whose distance from other entities can be measured

A *directed graph*  $G(V, E)$  consists of a set  $V$  of *nodes* or *vertices* and a set  $E \subseteq V \times V$  of *directed edges*. Then  $(i, j) \in E$  means that there is a directed edge from  $i$  to  $j$ .

A graph is *undirected* if the edge relation is *symmetric*, that is,  $(i, j) \in E$  iff  $(j, i) \in E$ .

A directed graph is *connected* if there is a directed path between any two nodes.

A directed graph is *acyclic* if it does not contain a cycle. (ie.  $(i, j)$ ,  $(j, k)$ , and  $(k, i)$  all belong to  $E$ .)

A *tree* is a undirected, connected, acyclic graph.

A *rooted tree* has a starting node called a *root*.

The *parent node* is immediately before a node on the path from the root.

The *child node* is a node that follows a node.

An *ancestor* is any node that came before a node on the path from a root.

A *leaf* or *external node* is a node that had no children.

Non-leaf nodes are called *internal nodes*.

The *depth* of a tree is one less than the maximal number of nodes on a path from the root to a leaf.

An *ordered tree* is a tree where the children of internal nodes are numbered.

A *binary tree* is a tree where each node has at most two children. Otherwise it is *multifurcating*.

Question: Draw all binary trees on 1, 2, and 3 taxa.

A *phylogenetic tree* on  $n$  taxa is a tree with leaves labeled by  $1, \dots, n$ .

Let  $T_1$ , and  $T_2$  be phylogenetic trees on  $n$  taxa. Then  $T_1=(V_1,E_1)$  and  $T_2=(V_2,E_2)$ ,  $E_1 \subseteq V_1 \times V_1$  and  $E_2 \subseteq V_2 \times V_2$ , and the leaves of both  $T_1$  and  $T_2$  are labeled  $1,2,\dots,n$ . A function  $f : V_1 \rightarrow V_2$  is an isomorphism from  $T_1$  to  $T_2$  if the following conditions are satisfied.

- 1)  $f$  is one-to-one and onto
- 2)  $x \in V_1$  is a leaf of  $T_1$  labeled by  $i$  iff  $f(x) \in V_2$  is a leaf of  $T_2$  labeled by  $i$ .
- 3)  $(x, y) \in E_1$  iff  $(f(x), f(y)) \in E_2$

- a) ultrameric trees
- b) additive metric
- c) estimating branch lengths