Introduction to Bioinformatics

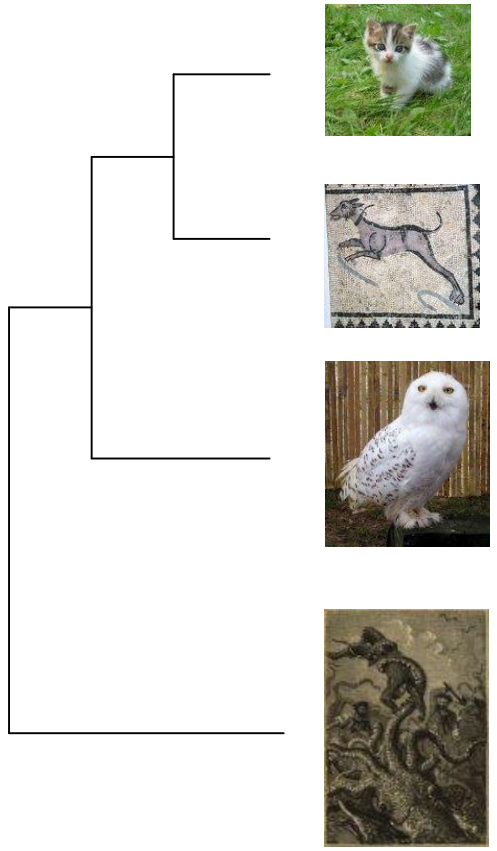
Phylogenetic trees

Inferring the Past: Phylogenetic Trees

- *The biological problem*
- Parsimony and distance methods
- Models for mutations and estimation of distances
- Maximum likelihood methods

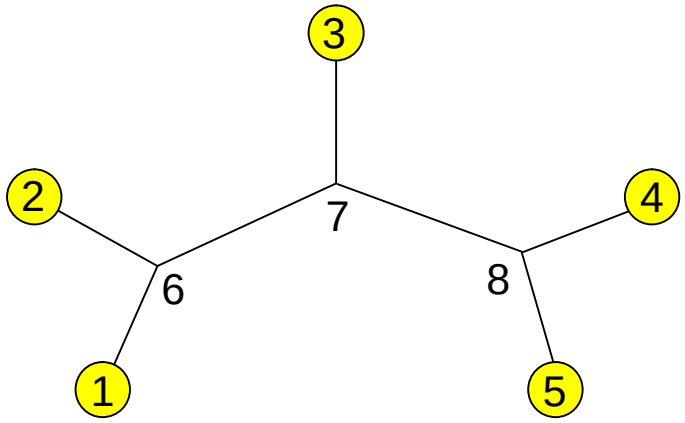
Phylogeny

- We want to study ancestor-descendant relationships, or *phylogeny*, among groups of organisms
- Groups are called *taxa* (singular: *taxon*)
- Organisms are usually called *operational taxonomic units* or *OTUs* in the context of phylogeny



Phylogenetic trees

- Leaves (external nodes) ~ species, observed (OTUs)
- Internal nodes ~ ancestral species/divergence events, not observed
- Unrooted tree does not specify ancestor-descendant relationships beyond the observation ”leaves are not ancestors”

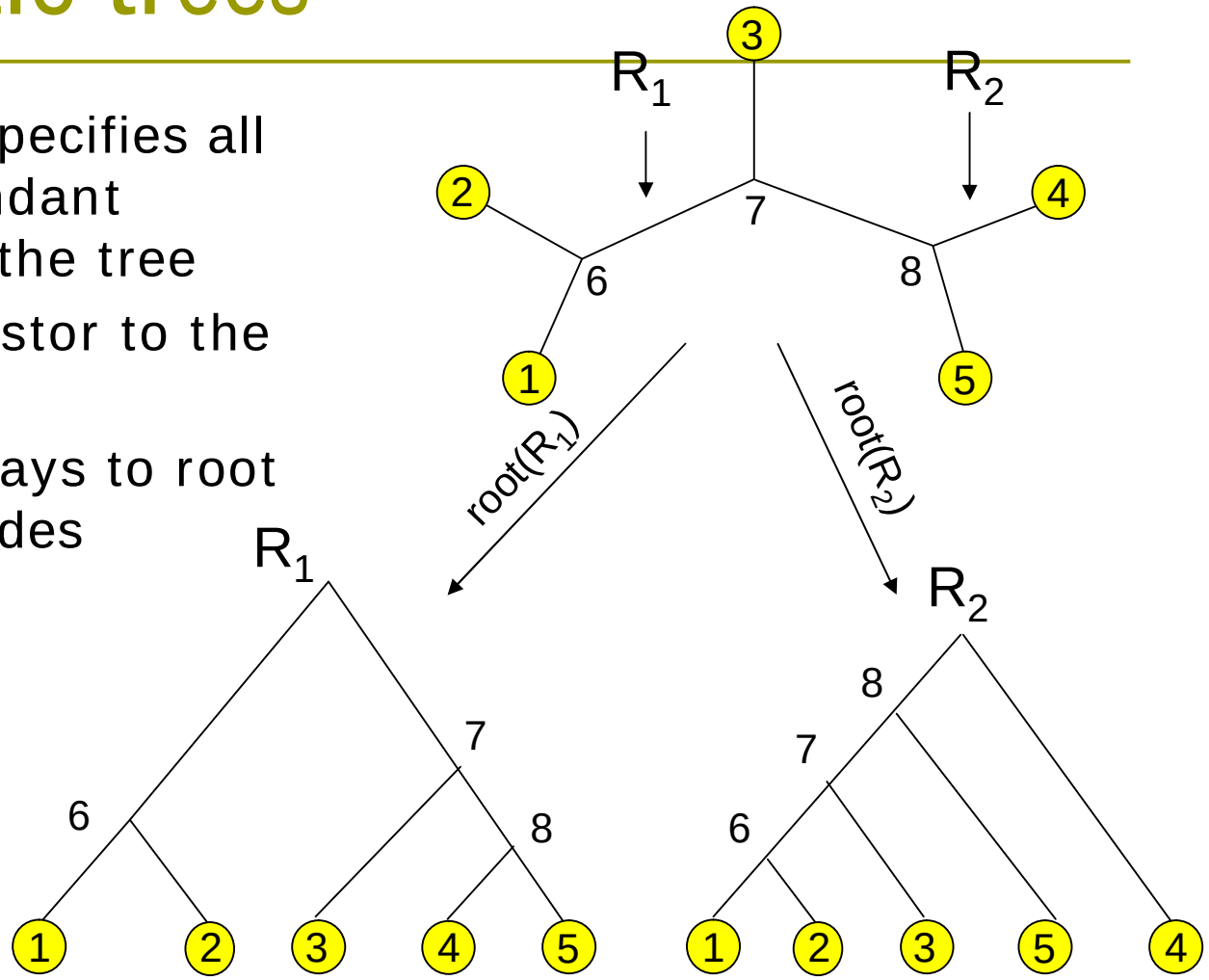


Unrooted tree with 5 leaves and 3 internal nodes.

Is node 7 ancestor of node 6?

Phylogenetic trees

- Rooting a tree specifies all ancestor-descendant relationships in the tree
- Root is the ancestor to the other species
- There are n-1 ways to root a tree with n nodes



Questions

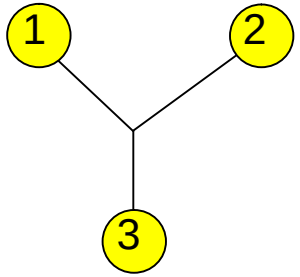
- Can we enumerate all possible phylogenetic trees for *n* species (or sequences?)
- How to score a phylogenetic tree with respect to data?
- How to find the best phylogenetic tree given data?

Finding the best phylogenetic tree: naive method

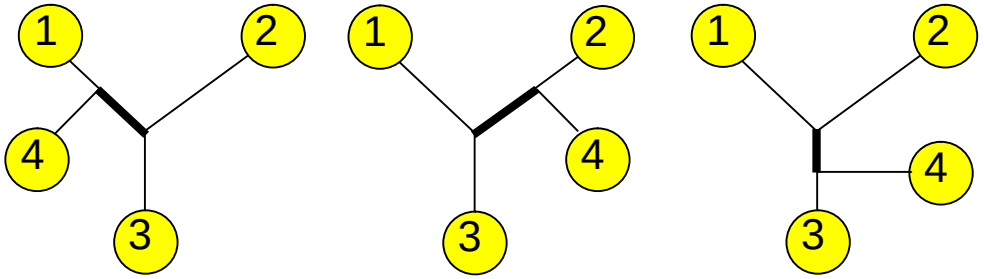
- How can we find the phylogenetic tree that best represents the data?
- Naive method: enumerate all possible trees
- How many different trees are there of *n* species?
- Denote this number by b_n

Enumerating unordered trees

- Start with the only unordered tree with 3 leaves ($b_3 = 1$)



- Consider all ways to add a leaf node to this tree



- Fourth node can be added to 3 different branches (edges), creating 1 new internal branch
- Total number of branches is n external and n – 3 internal branches
- Unrooted tree with n leaves has 2n – 3 branches

Enumerating unordered trees

- Thus, we get the number of unrooted trees

$$b_n = (2(n-1)-3)b_{n-1} = (2n-5)b_{n-1}$$
$$= (2n-5) * (2n-7) * \ldots * 3 * 1$$
$$= (2n-5)! / ((n-3)!2^{n-3}),\ n > 2$$

- Number of rooted trees b'_n is

$$b'_n = (2n-3)b_n = (2n-3)! / ((n-2)!2^{n-2}),\ n > 2$$

that is, the number of unrooted trees times the number of branches in the trees

Number of possible rooted and unrooted trees

n	B_n	b'_n
3	1	3
4	3	15
5	15	105
6	105	945
7	954	10395
8	10395	135135
9	135135	2027025
10	2027025	34459425
20	2.22E+020	8.20E+021
30	8.69E+036	4.95E+038

Too many trees?

- We can't construct and evaluate every phylogenetic tree even for a smallish number of species
- Better alternative is to
  - Devise a way to evaluate an individual tree against the data
  - Guide the search using the evaluation criteria to reduce the search space