



Phylogenetic Trees

What They Are
Why We Do It
&
How To Do It

Presented by
Amy Harris
Dr Brad Morantz



Overview

- What is a phylogenetic tree
- Why do we do it
- How do we do it
- Methods and programs
- Parallels with Genetic Algorithms (time permitting)

Definition: Phylogenetic Tree



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A tree (graphical representation) that shows evolutionary relationships based upon common ancestry. Describes the relationship between a set of objects (species or taxa).
[Israngkul]



Phylogenetic Tree

- Finding a tree like structure that defines certain ancestral relationships between a related set of objects. [Reijmers et al, 1999]
- Composed of branches/edges and nodes
- Can be gene families, single gene from many taxa, or combination of both. [Baldauf, 2003]

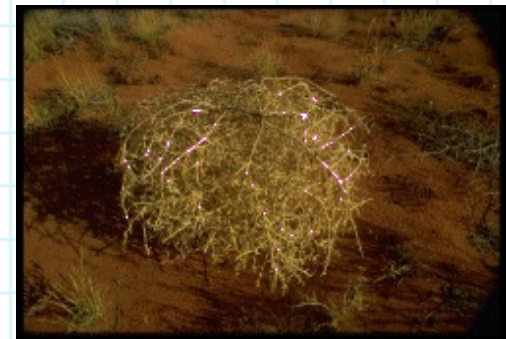


Terminology

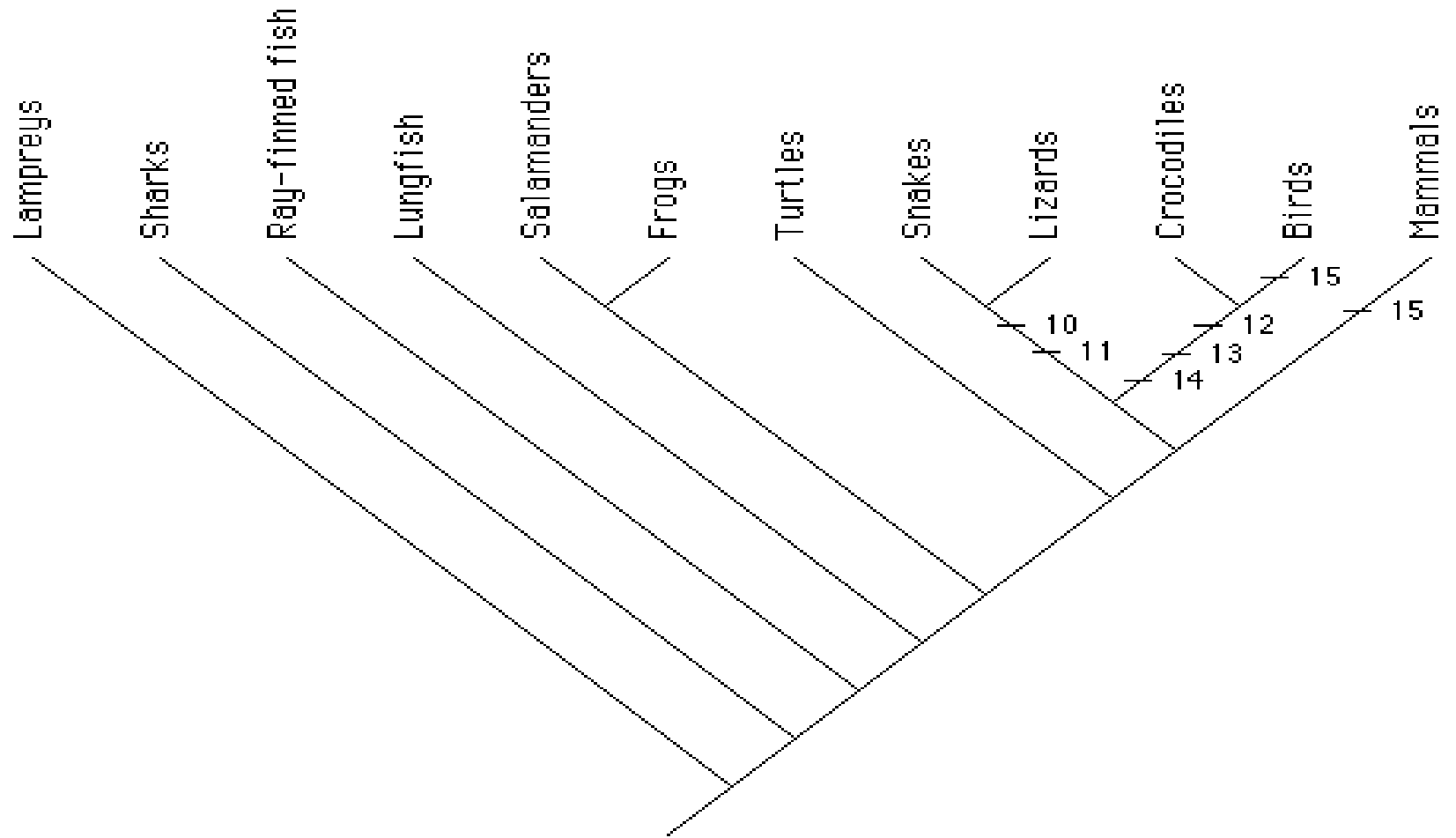
- Branches – connections between nodes
- Evolutionary tree – patterns of historical relationships between the data
- Leaves – terminal node; taxa at the end of the tree
- Nodes – represent the sequence for the given data; Internal nodes correspond to the hypothetical last common ancestor of everything arising from it. [Baldauf, 2003]
- Taxa (a car for hire) – individual groups
- Tree (number after two) - mathematical structure consisting of nodes which are connected by branches

Rooted vs Unrooted

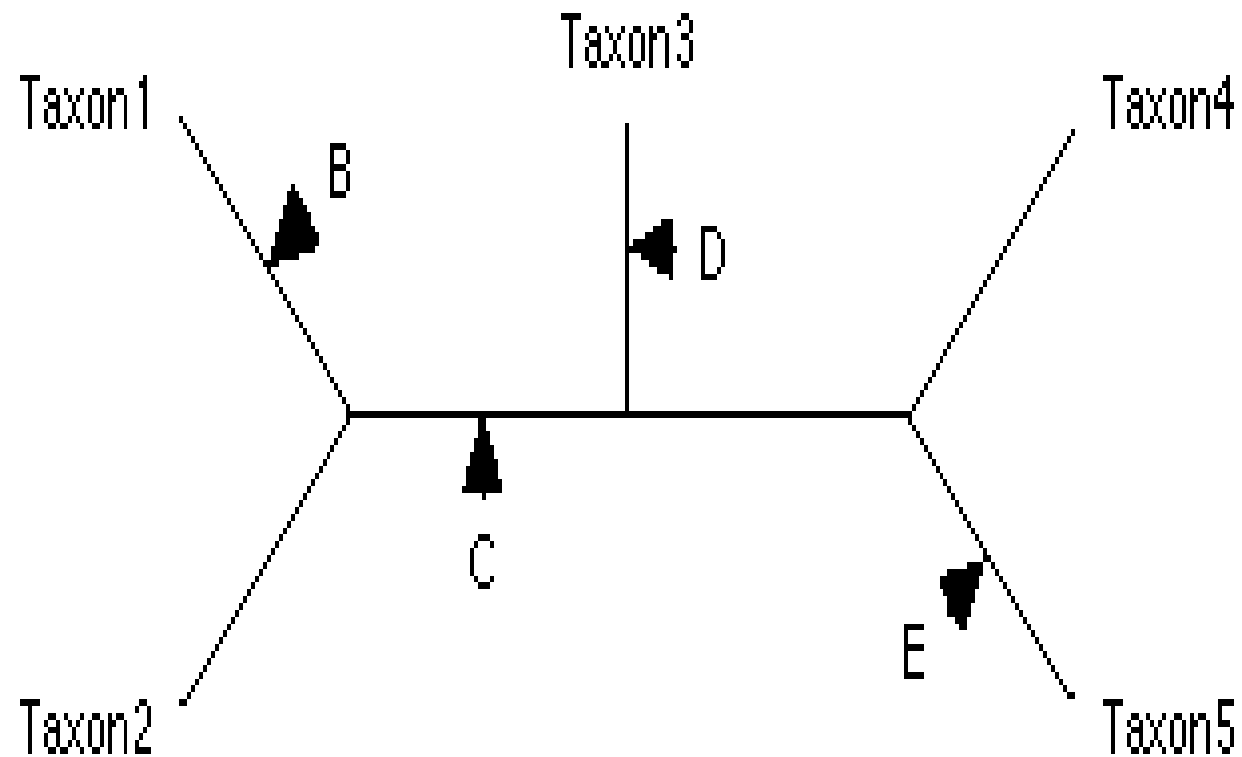
- Rooted tree
 - Directed tree
 - Has a path
 - Accepted common ancestor
 - Doesn't blow over in the wind
- Unrooted Tree
 - Typical results
 - Unknown common ancestor
 - Common in Arizona, blowing around plains



Rooted Phylogenetic Tree



Unrooted Phylogenetic Tree



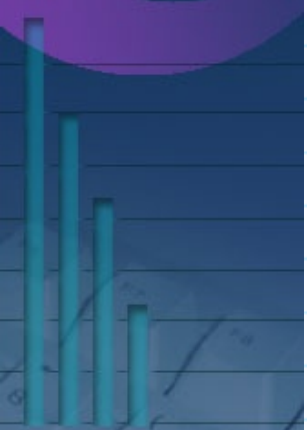
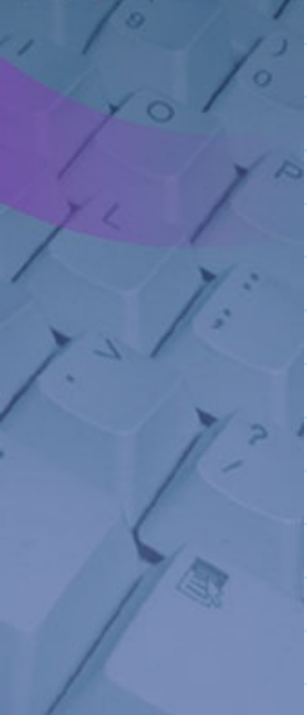


Combinatorial Explosion

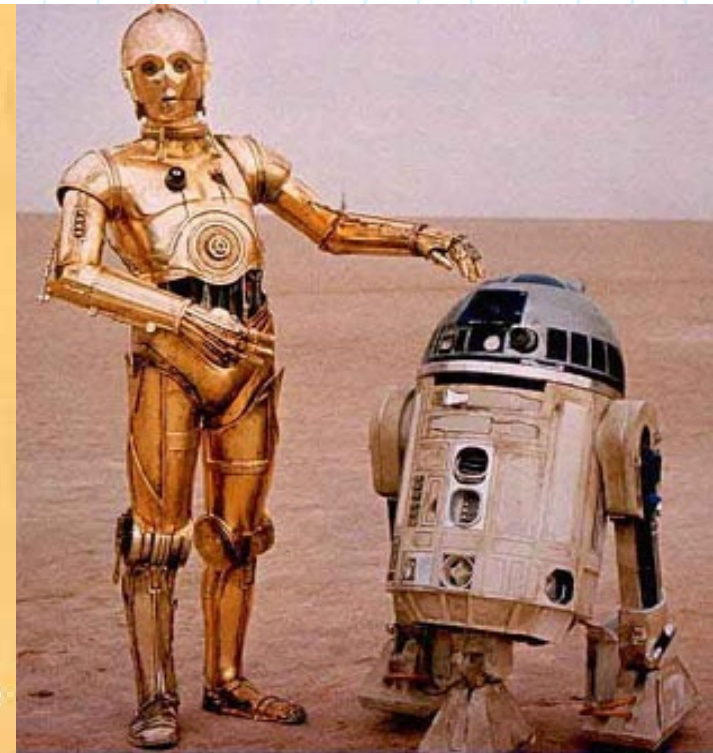
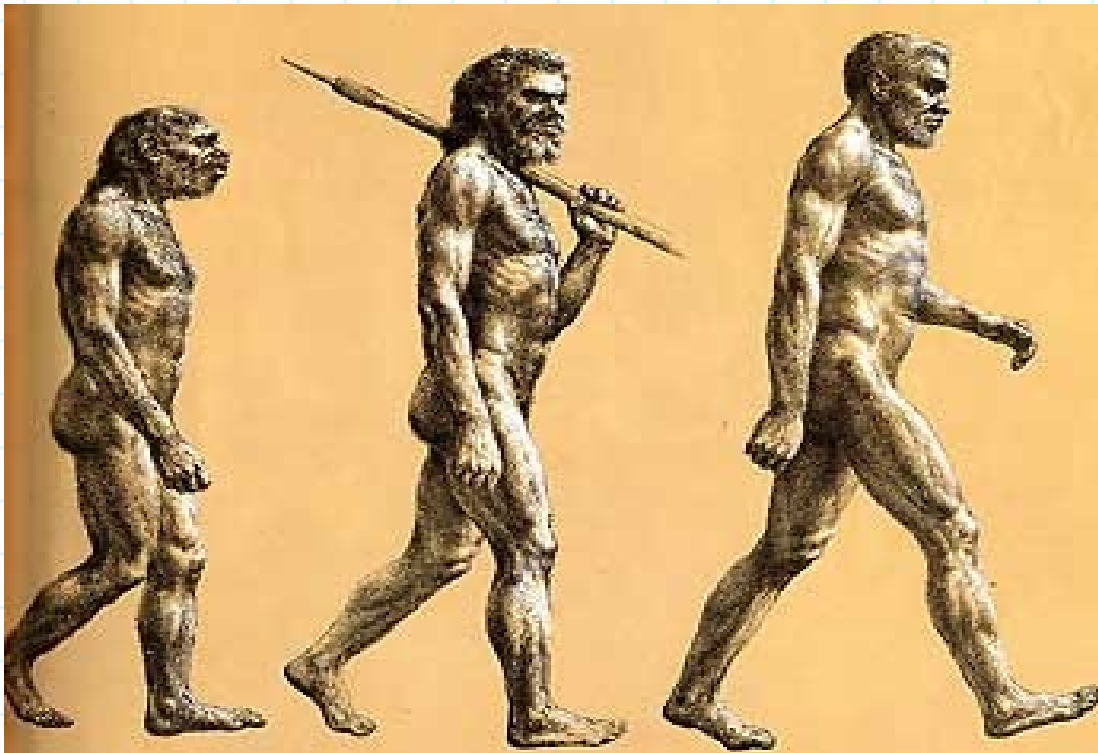
- Number of topologies =
 - Product $i = 3$ to x $(2i - 5)$
 - Ten objects yields 2,027,025 possible trees
 - 25 objects yields about 2.5×10^{28} trees
- Branches
 - $2x - 3$ branches
 - X are peripheral
 - $(X - 3)$ are interior



Why Do We Do It?

- Understand evolutionary history
 - Show visual representation of relationships and origins
 - Healthcare
 - Origins of diseases
 - Show how they are changing
 - Help produce cures and vaccines
 - Model allows calculations to determine distances
 - Forensics
 - Our history
- 
- 

Our Family



Terminal Node

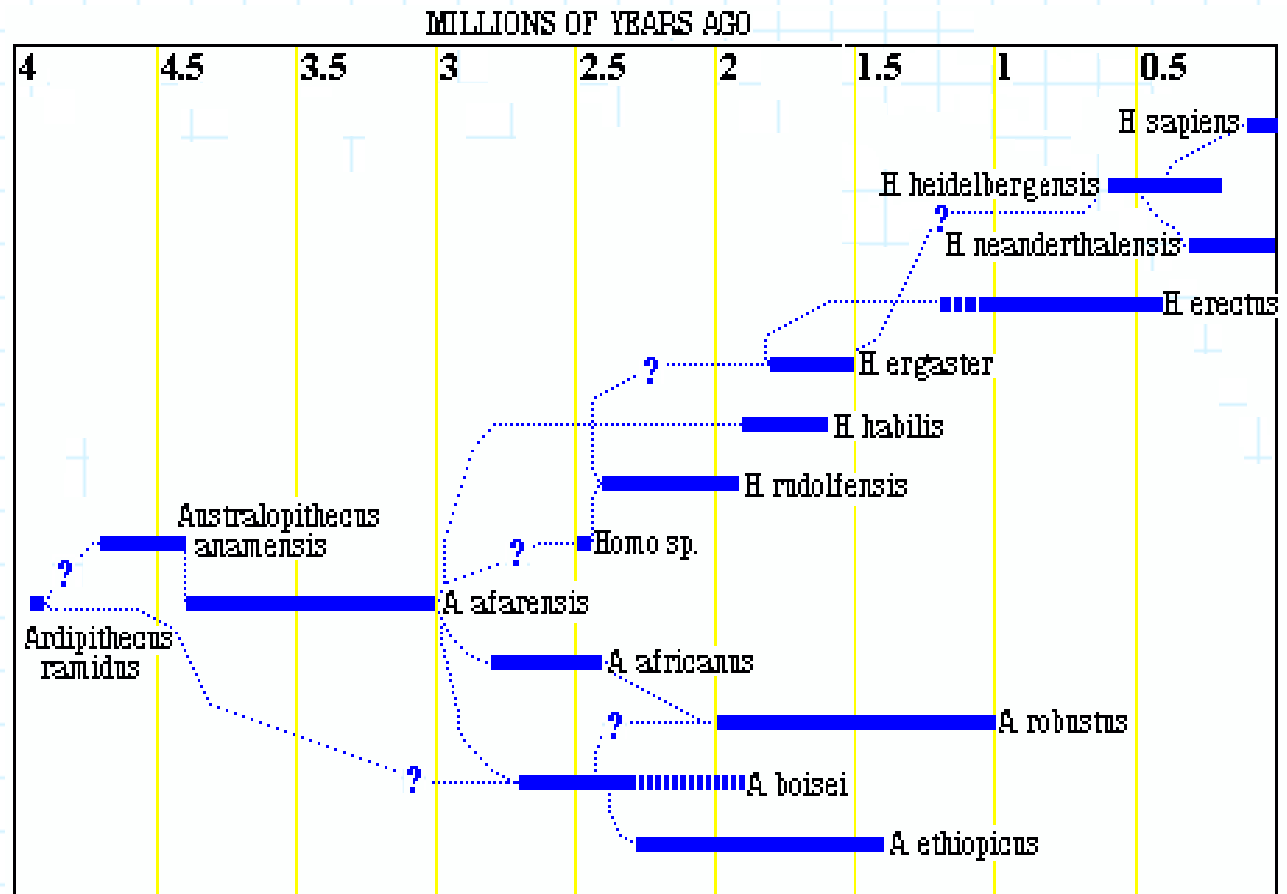


A hand holding a globe, with a bar chart and a keyboard visible in the background.

Evolution

- Theory that groups of organisms change over time so that descendants differ structurally and/or functionally from their ancestors. [Pevsner, 2003]
- Biological process by which organisms inherit morphological and physiological features that define a species. [Pevsner, 2003]
- Biological theory that postulating that the various types of animals and plants have their origin in other preexisting types and that distinguishable differences are due to modifications in successive generations. [Encyclopaedia Britannica, 2004]

Example





Ways to do it

- Parsimony
- Maximum Likelihood Estimator
- Distance based methods
- Clustering
- Genetic algorithm

* While there are numerous methods, these are among the most popular

Parsimony





Parsimony

- Character based
- Search for tree with fewest number character changes that account for observed differences
- Best one has the least amount of evolutionary events required to obtain the specific tree
- Advantages:
 - Simple, intuitive, logical, and applicable to most models
 - Can be used on a wide variety of data
 - More powerful approach than distance to describe hierarchical relationship of genes & proteins (Pevsner, 2003)
- Disadvantages;
 - No mathematical origins
 - Fooled by same multiple or circuitous changes



Parsimony Methods

- The best tree is the one that minimizes the total number of mutations at all sites [*Israngkul*]
- The assumption of physical systematics is that genes exist in a nested hierarchy of relatedness and this is reflected in a hierarchical distribution of shared characters in the sequence. (Pevsner, 2003)

Maximum Likely Hood





Maximum Likelihood Estimator

- Tree with highest probability of evolving from given data
- Mathematical Process
 - Complex Math – many have problems with this
- Advantages:
 - Can be used for various types of data including nucleotides and amino acids
 - Usually the most consistent
- Disadvantages:
 - Computationally intense
 - Can be fooled by multiple or circuitous changes

Distance Based Methods

- Uses distances between leaves
 - Upper triangular matrix of distances between taxa
- Percent similarity
- Metric
 - Number of changes
 - Distance score
- Produces edge weighted tree
- Least squares error
 - Can use Matlab



Distances

- Hamming distance
 - $n = \#$ sites different
 - $N =$ alignment length
 - $D = 100\% \times (n/N)$
 - ignore information of evolutionary relationship
- Jukes-Cantor
 - $D = -3/4 \ln (1-4P/3)$
- Kimura
 - Transitions more likely than transversions
 - Transitions given more weight

Distances

- The walk from the parking lot
- Now that's far!





Least Squares

- Start with distance matrix
- Pick tree type to start
- Calculate distances to minimize SSE
- Try other trees
- Time consuming
- Exhaustive search will yield optimal tree, but also may take l-o-n-g time

Example of Distance Matrix

	Human(A)	Chimp(B)	Gorilla(C)	Orang-utan(D)	Gibbon(E)
Human(A)	-	.09190	.1083	.1790	.2057
Chimp(B)	.0919/.0821	-	.1134	.1940	.2168
Gorilla(C)	.1057/.1083	.1161/.1330	-	.1882	.2170
Orang-utan(D)	.1806/.1838	.1910/.1838	.1895/.1838	-	.2172
Gibbon(E)	.2067/.2142	.2171/.2142	.2156/.2142	.2172/.2142	-



Clustering

- Genetic algorithm
- Neighbor joining
- UPGMA
- PAUP contains the last two

Clustering

- Neighbor joining
 - Uses distances between pairs of taxa
 - i.e. Number of nucleotide differences
 - Not individual characters
 - Builds shortest tree by complex methods
- UPGMA
 - Unweighted Pair Group Method w/ Arithmetic Mean
 - Starts with first two most similar nodes
 - Compares this average/composite to the next
 - Never uses original nodes again



Summary

- Real life is usually not the optimum tree
- The best model is one that is obtained by several methods



Comments

- Sometimes difficult because
 - Do not have complete fossil record
 - Parallel evolution
 - Character reversals
 - Circuitous changes
- Bifurcating vs polytomy split
- No animals, plants, or robots were hurt in the making of this presentation

References

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Genetic Algorithms

- Optimizing distance clustering (Reijmers et al)
- Optimal Distance method
- Not guaranteed the most optimal, only near optimal
- Exhaustive exploration not guaranteed
- Same solution may be checked multiple times
- Simulated time evolution (Brad's project for winter break)