Phylogenetic Trees 2

Course “Discrete Biological Models” (Modelli Biologici Discreti)

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These slides are partially based on the lecture notes *Algorithms for Phylogenetic Reconstruction*, by Jens Stoye and others, Bielefeld University, 2009/2010.

Character data

Now the input data consists of states of characters for the given objects, e.g.

- morphological data, e.g. number of toes, reproductive method, type of hip bone, . . . or
- molecular data, e.g. what is the nucleotide in a certain position.

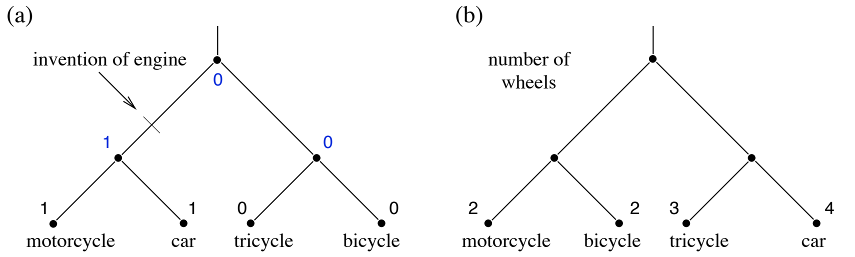
Character data

Example

	C_1 : # wheels	C_2 : existence of engine
bicycle	2	0
motorcycle	2	1
car	4	1
tricycle	3	0

- objects (species): Bicycle, motorcycle, tricycle, car
- characters: number of wheels; existence of an engine
- character states: $2, 3, 4$ for C_1;
  $0, 1$ for C_2 ($1 =$ YES, $0 =$ NO)
- This matrix M is called a character-state-matrix, of dimension $(n \times m)$, where for $1 \leq i \leq n, 1 \leq j \leq m$: $M_{ij} =$ state of character j for object i. (Here: $n = 4, m = 2$.)

Character data



Two different phylogenetic trees for the same set of objects.

Character data

We want to avoid

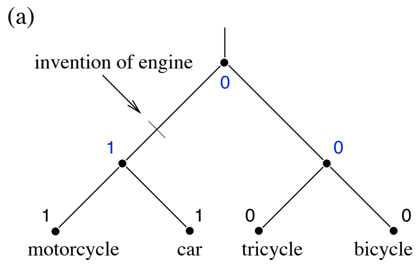
- parallel evolution (= convergence)
- reversals

Mathematical formulation: compatibility.

Compatibility

Definition

A character is compatible with a tree if all inner nodes of the tree can be labeled such that each character state induces one connected subtree.

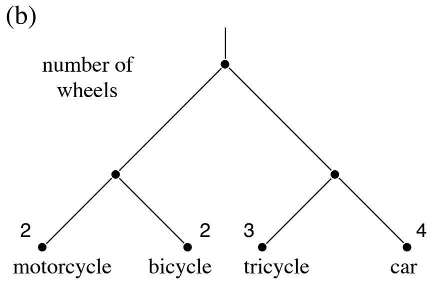


This tree is compatible with C_2, one possibility of labeling the inner nodes is shown.

Compatibility

Definition

A character is compatible with a tree if all inner nodes of the tree can be labeled such that each character state induces one connected subtree.

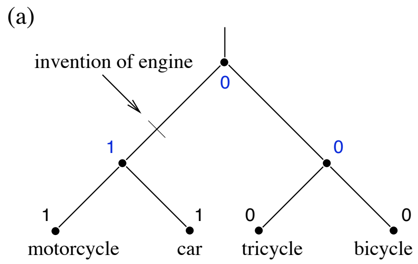


This tree is compatible with C_1. (We have to give a labeling of the inner nodes to prove this.) It is not compatible with C_2 (why?)

Compatibility

Definition

A character is compatible with a tree if all inner nodes of the tree can be labeled such that each character state induces one connected subtree.



This tree is also compatible with C_1: We have to give a labeling of the inner nodes (w.r.t. C_1) to prove this.

Compatibility

Exercise:
The objects $\alpha, \beta, \gamma, \delta$ share three characters C_1, C_2, C_3. The following matrix holds their states:

	C_1	C_2	C_3
α	a	c	f
β	a	d	g
γ	b	d	h
δ	b	e	f

(C_1 can have states a, b; C_2 states c, d, e; C_3 states f, g, h.)

Look at all possible tree topologies. Is there, among all these trees, a tree T such that all characters are compatible with T? (Hint: It is enough to consider unrooted trees.)

Compatibility

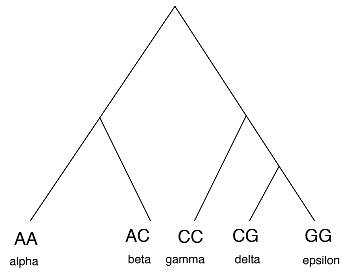
Note that the question whether a character is compatible with a tree is independent of the other characters. Moreover, often all characters have the same states (typically $\{A, C, G, T\}$). Thus the previous problem is equivalent to this one:

	C_1	C_2	C_3
α	A	C	A
β	A	G	C
γ	C	G	G
δ	C	T	A

Perfect Phylogeny

Definition
A tree T is called a perfect phylogeny (PP) for $\mathcal{C}$ if all characters $C \in \mathcal{C}$ are compatible with T.

Example

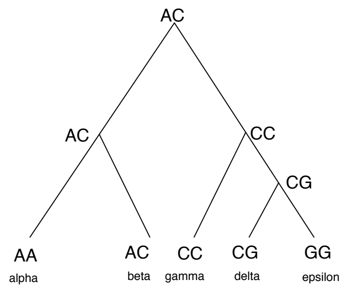


Why? We have to find a labeling of the inner nodes s.t. for both characters C_1 and C_2, each character induces a subtree.

Perfect Phylogeny

Definition
A tree T is called a perfect phylogeny (PP) for $\mathcal{C}$ if all characters $C \in \mathcal{C}$ are compatible with T.

Example



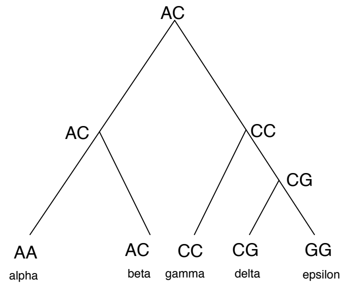
Our first tree for the vehicles was also a PP, as well as the solution to the exercise.

Perfect Phylogeny

- Ideally, we would like to find a PP for our input data.
- Deciding in general whether a PP exists is NP-hard.
- This is not really a problem, since most of the time, no PP exists anyway. Why: our input data has errors, our evolutionary model probably has errors, and, and, and . . .
- Therefore we usually want to find a best possible tree.

Parsimony

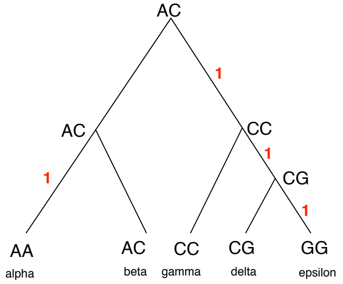
What is a best possible tree?



Why is this tree "perfect"?

Parsimony

What is a best possible tree?



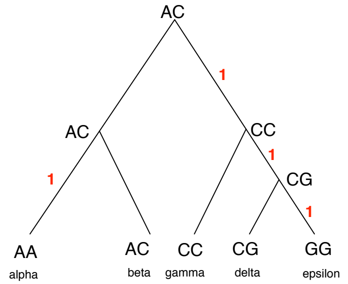
Why is this tree "perfect"?

Because it has few changes of states!
In red, we marked the edges where there are state changes (an evolutionary event happened), and how many (in this case, always 1).

Parsimony

Definition

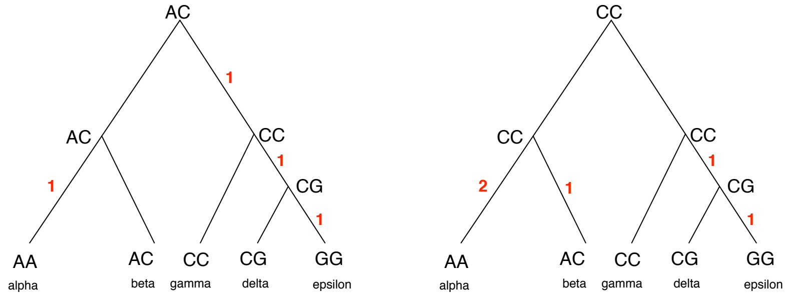
The parsimony cost of a phylogenetic tree with labeled inner nodes is the number of state changes along the edges (i.e. the sum of the edge costs, where the cost of an edge = number of characters whose state differs between child and parent).



The parsimony cost of this tree is 4.

Parsimony

Same tree, different labelings

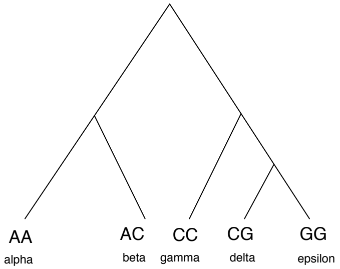


The parsimony cost of left tree is 4, of right tree it's 5.

Parsimony

Definition

The parsimony cost of a phylogenetic tree (without labels on the inner nodes) is the minimum of the parsimony cost over all possible labelings of the inner nodes.



The parsimony cost of this tree is 4, because the best labeling has cost 4.

Maximum Parsimony

Definition

The maximum parsimony problem is, given a character-state matrix, find a phylogenetic tree with lowest parsimony cost (= a “most parsimonious” tree).

- The underlying idea is (again) the Occam's razor principle: the simplest explanation is the best.
- When a PP exists, then it is also the most parsimonious tree.
- In general, this problem is NP-hard.

Summary for character data

- When the input is a character-state matrix, then we would like to find a tree which is compatible with each character.
- Such a tree is called a perfect phylogeny (PP).
- Usually, no PP exists, therefore in general . . .
- We are looking for a a most parsimonious tree (a tree with lowest parsimony cost).
- The parsimony cost is defined as the sum of the state changes on the edges over all possible labelings of the inner nodes.
- Recall: There are super-exponentially many trees on *n* taxa (both rooted and unrooted), so we can't try them all.
- The problem of finding a most parsimonious tree is NP-hard.