Research: You Might Get STD Through Swimming in the Arctic Ocean, Here's How

9 March 2020, 3:24 am EDT By Jamie P. Tech Times

Sexually-transmitted diseases or STDs can now be transferred to a person even without having sexual intercourse. Worse, the research found out that it can also be acquired through simply swimming in an ocean. How can this be possible?

How do you get STD? By swimming in the Arctic ocean, apparently

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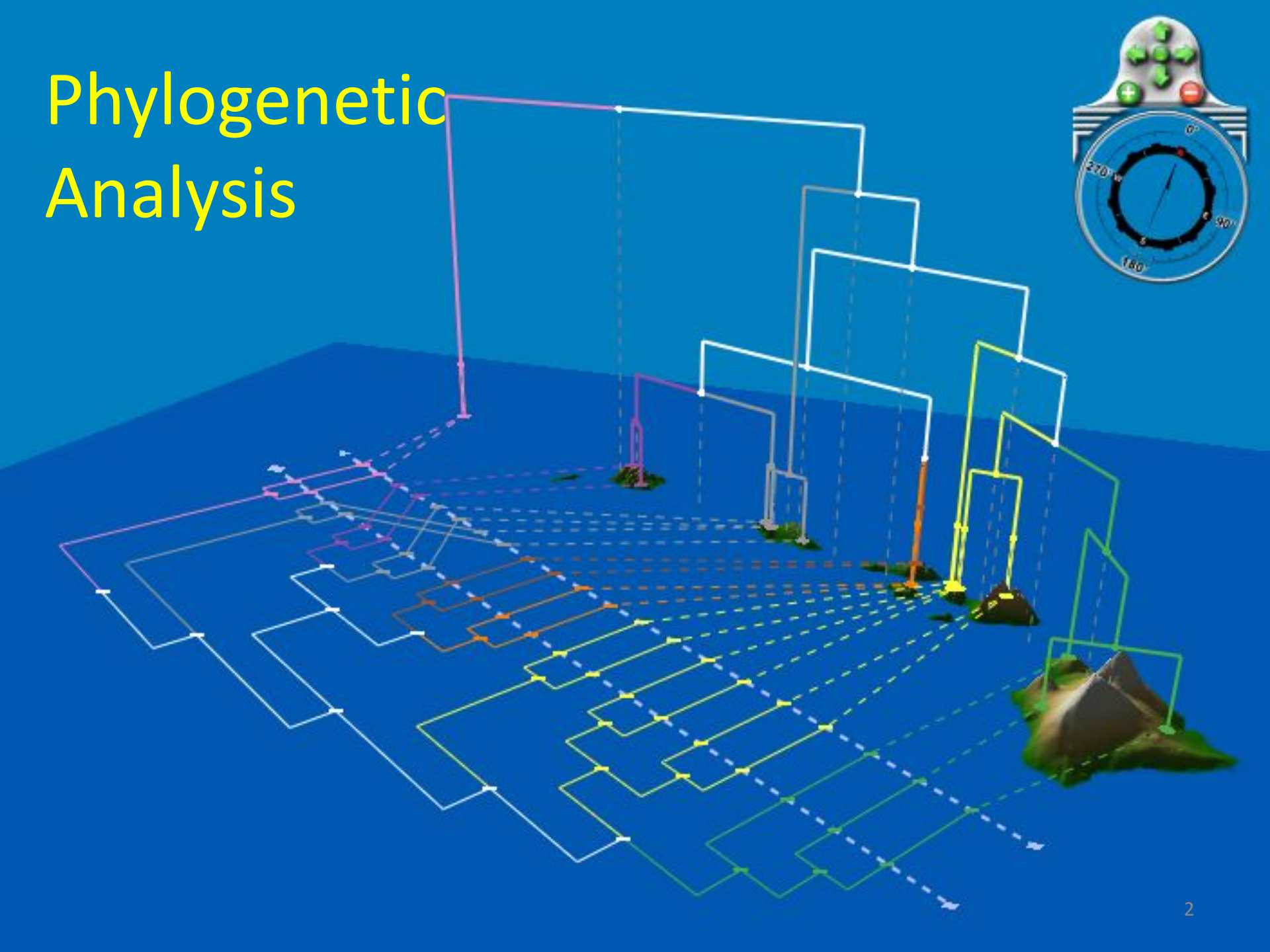
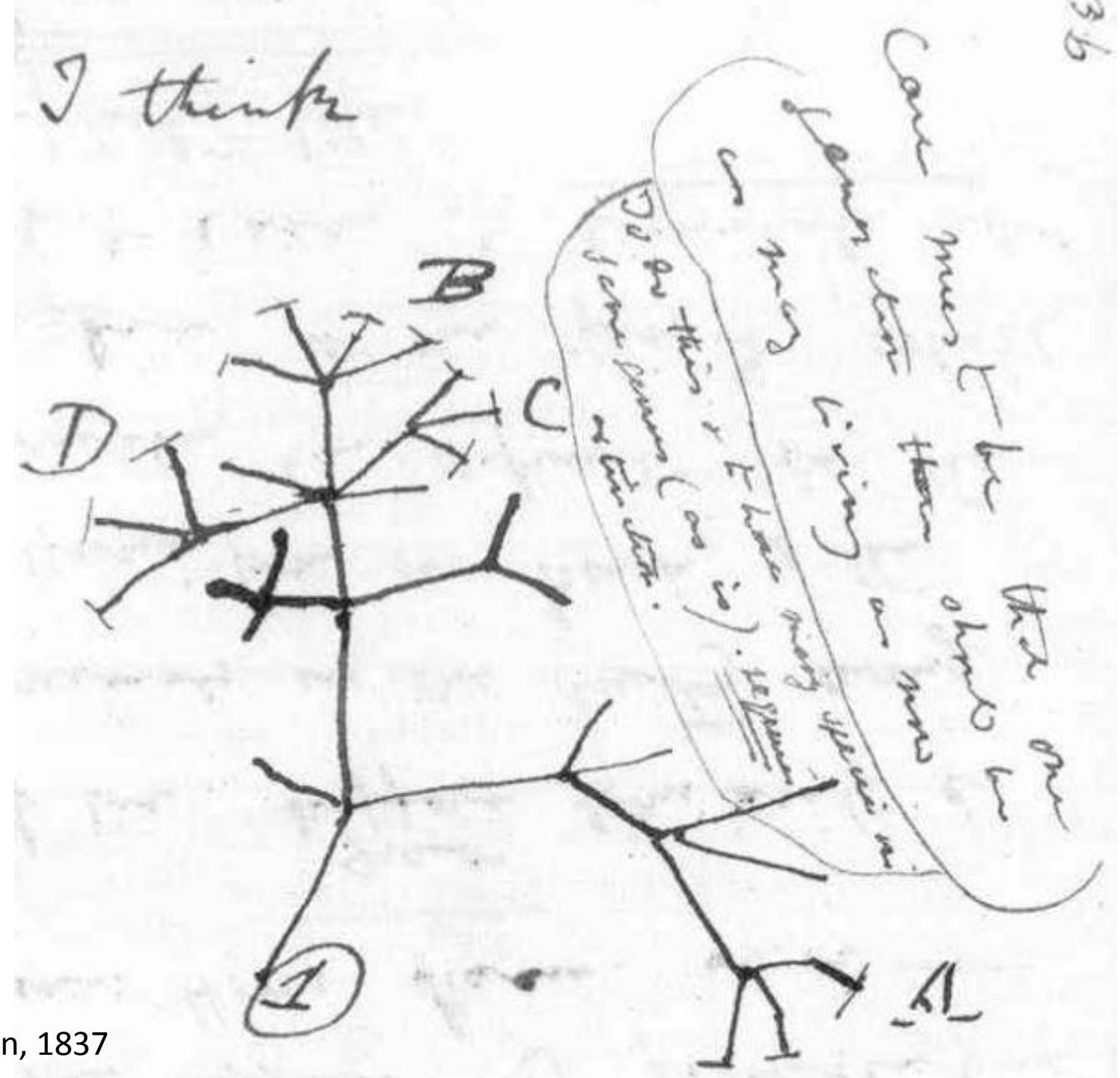
Phylogenetic Analysis



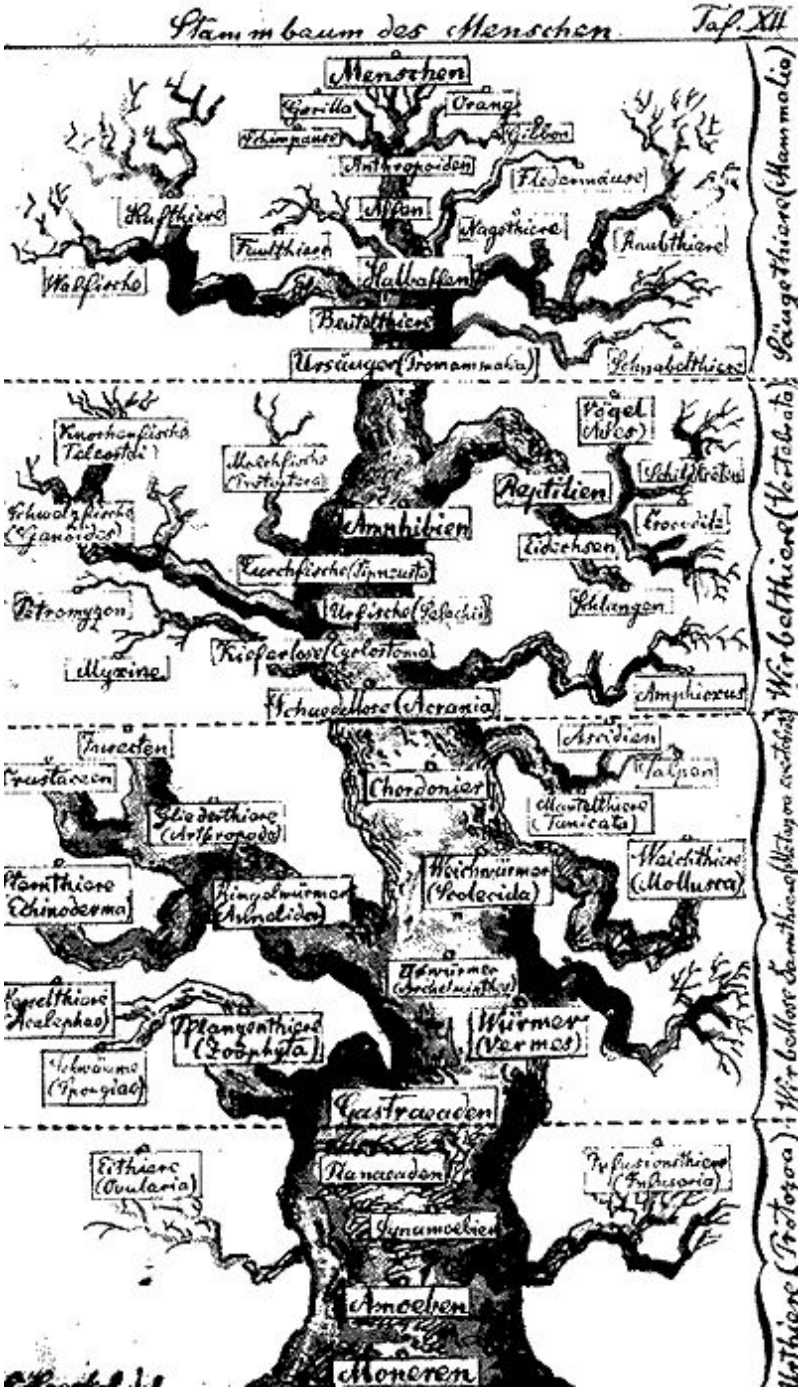
The Point

Use the relationships among one or (ideally) many **homologous characters** to reconstruct an evolutionary tree

Often means aligned sequences (with homologous residues in columns)

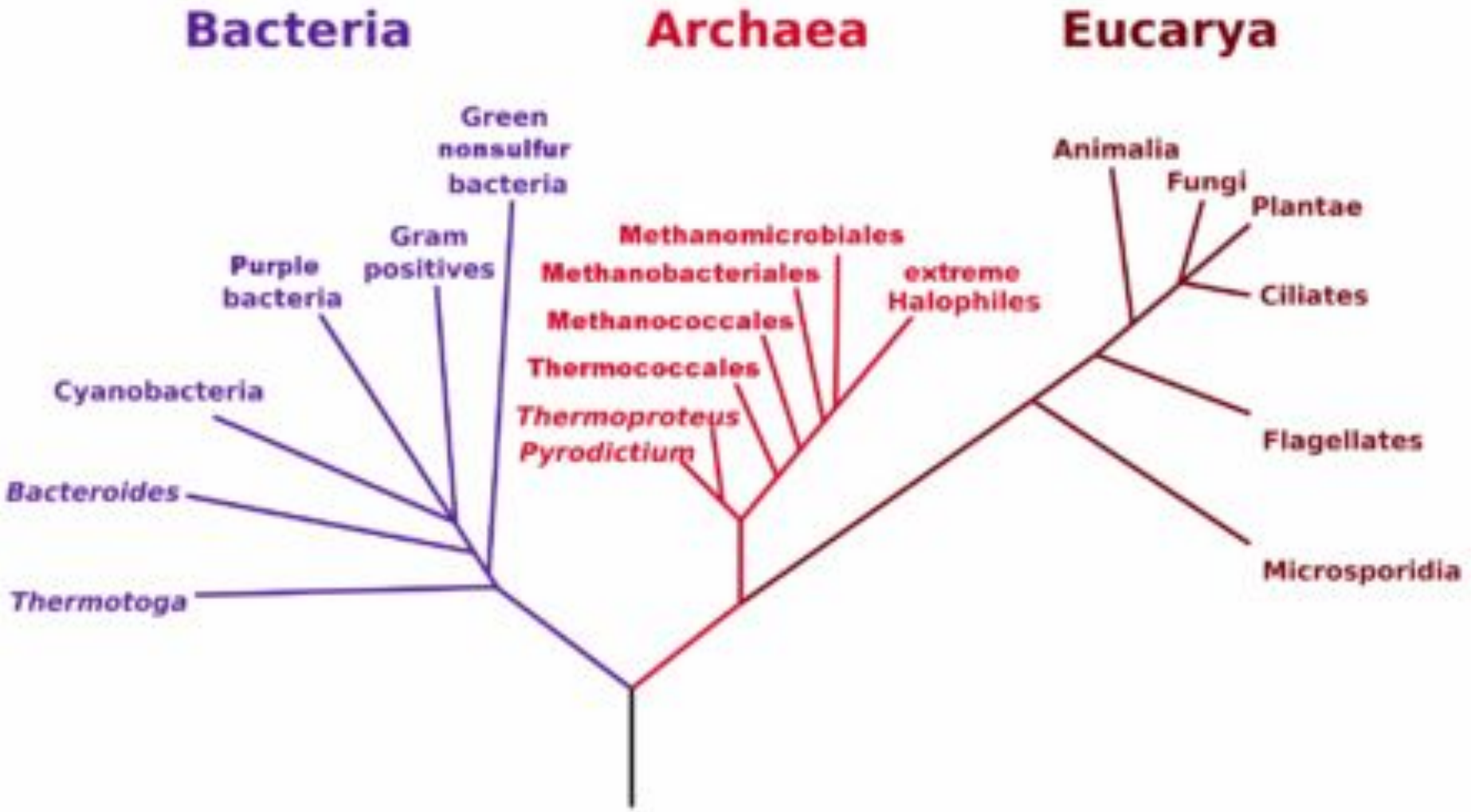


Darwin, 1837

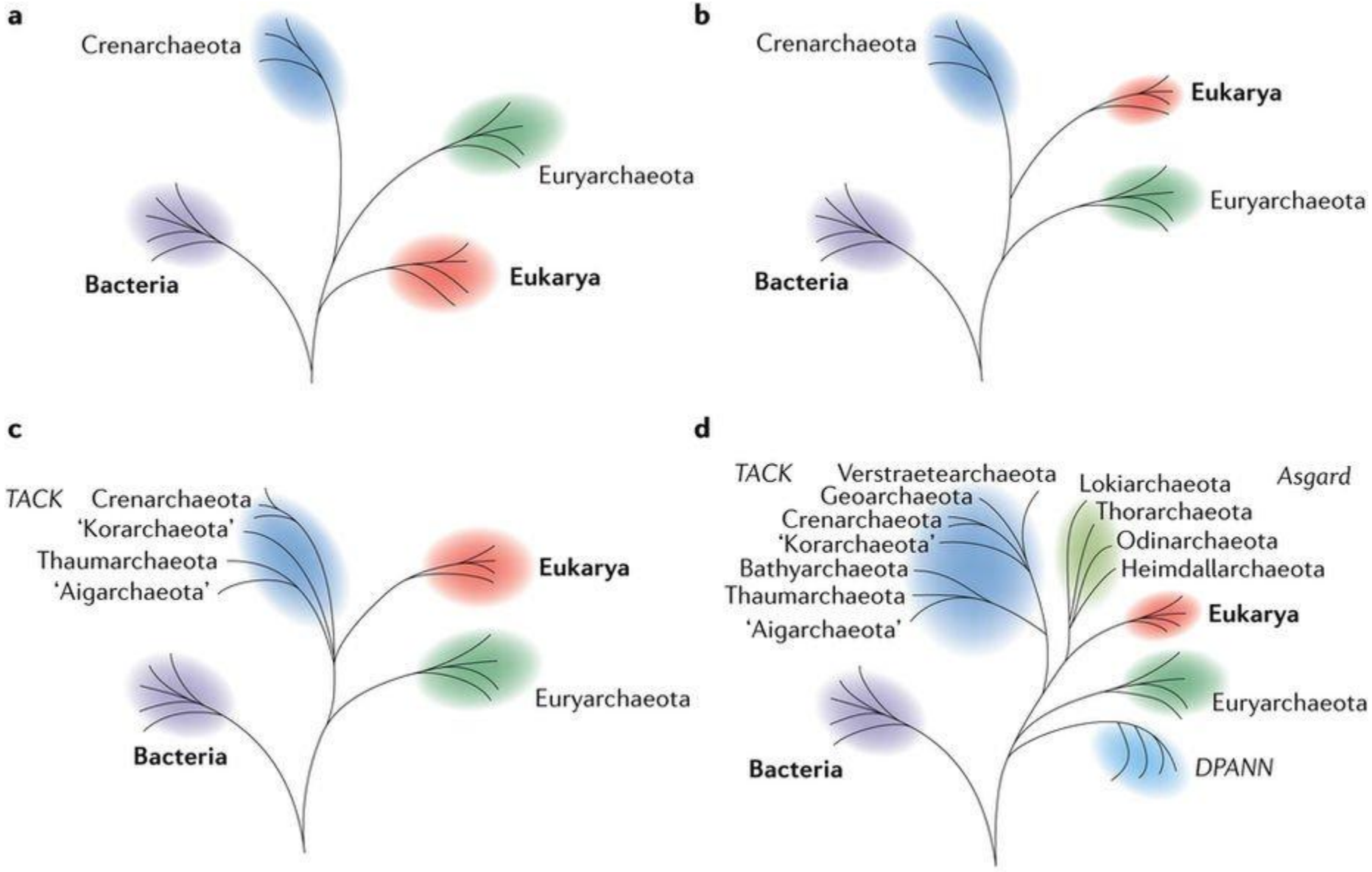


Haeckel, 1874
"Pedigree of Man"

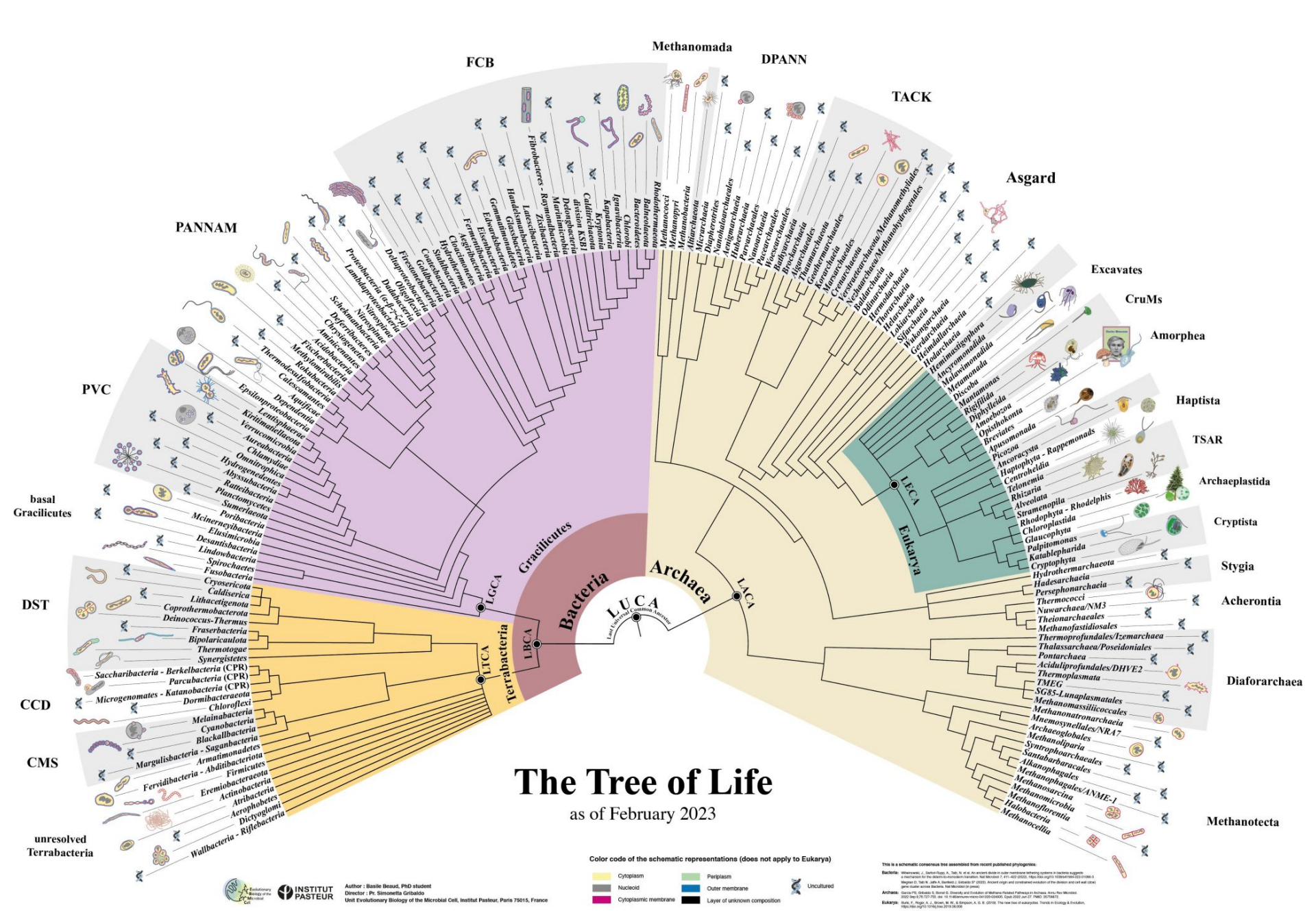
Phylogenetic Tree of Life

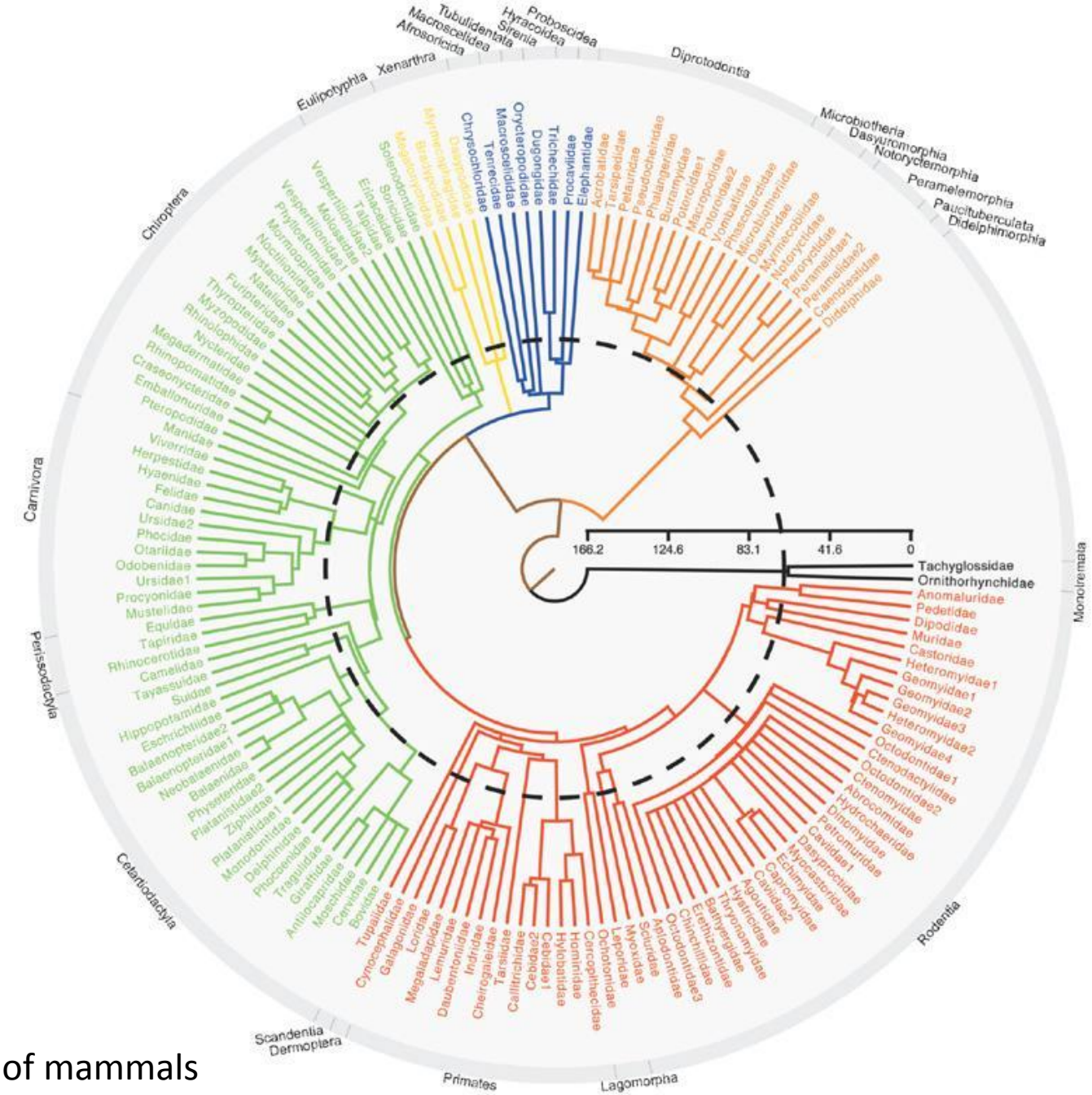


Fox and Woese (1977) and many, many others

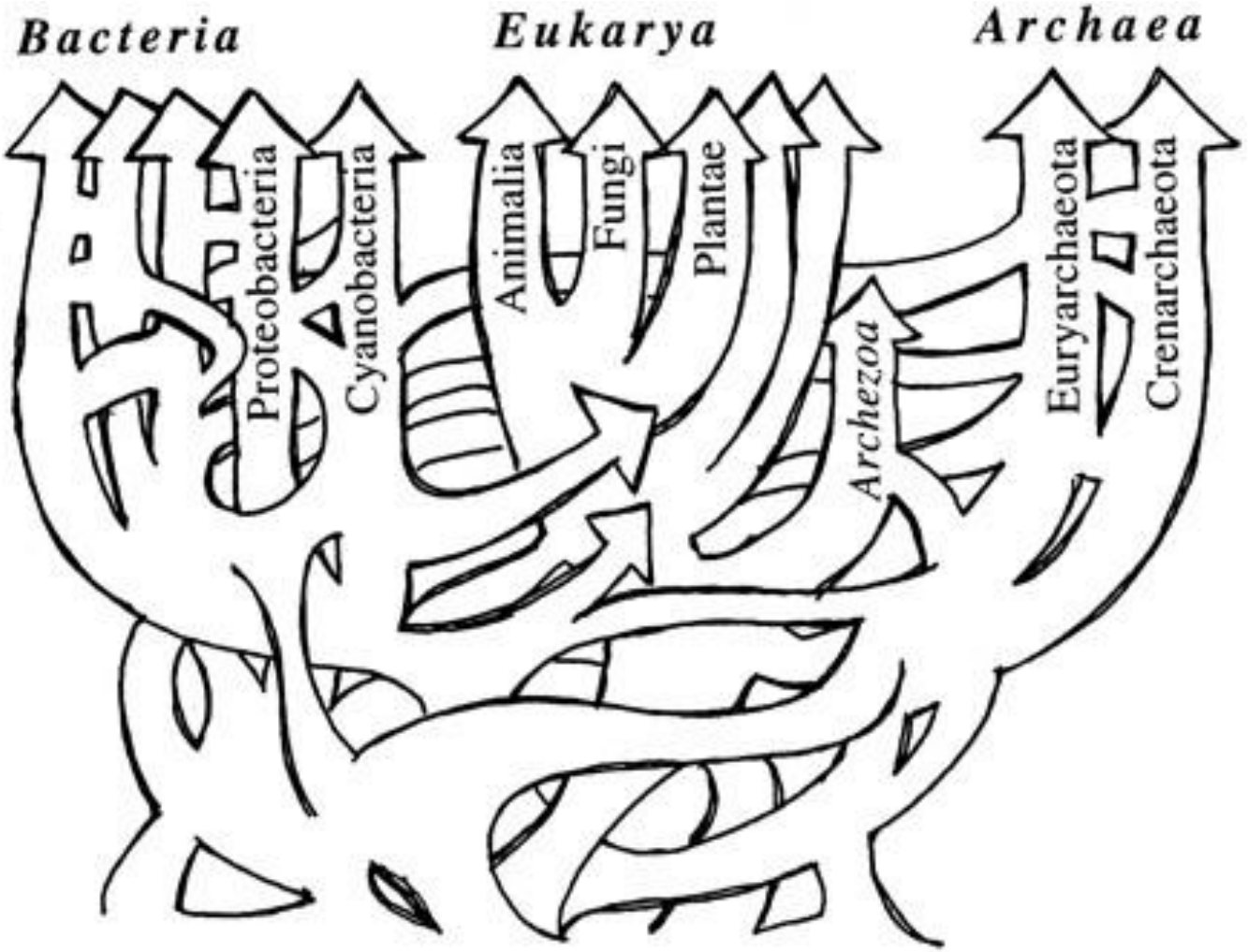


Eme et al (2017) *Nat Rev Microbiol*

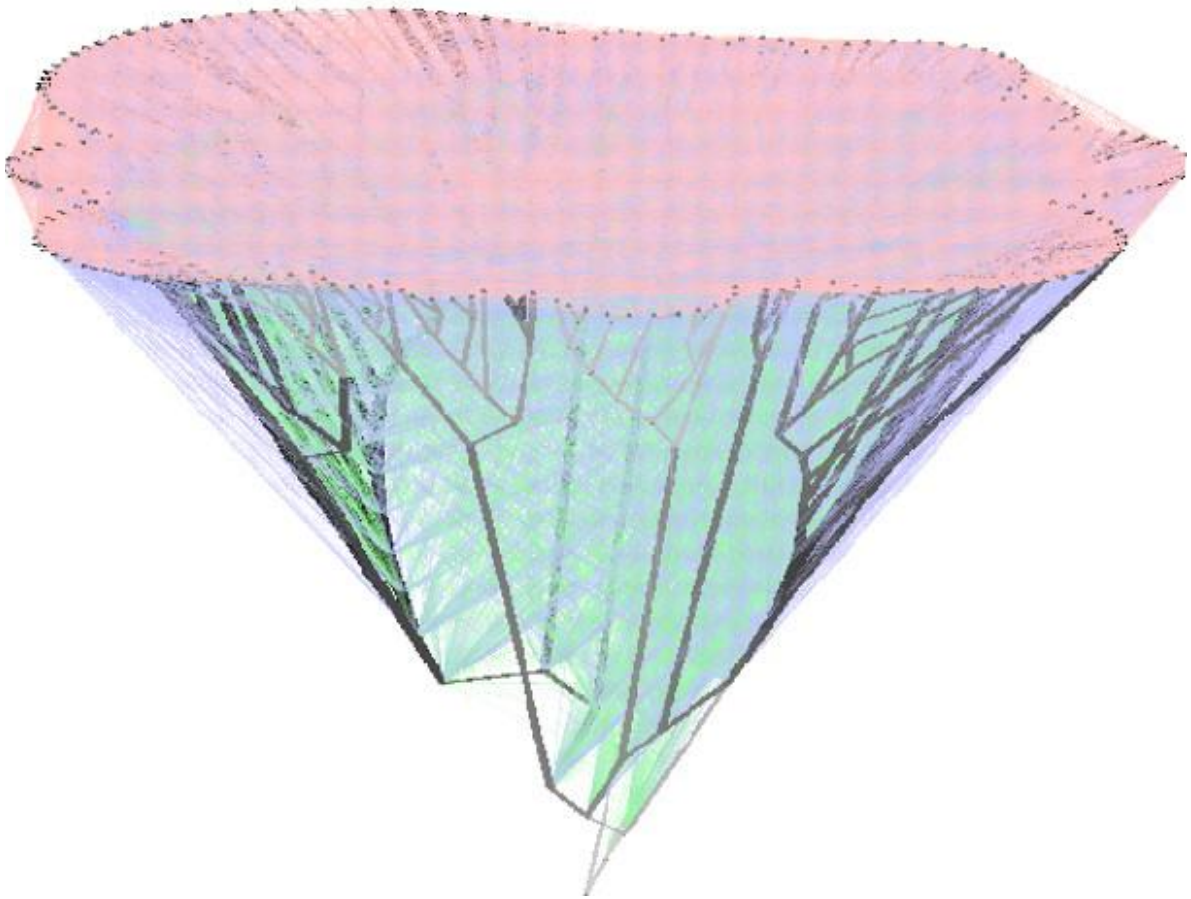

The Tree of Life
as of February 2023
LUCA
Last Universal Common Ancestor
Bacteria
Archaea
Gracilicutes
Terrabacteria
LGCA
LBCA
LTCA
LACA
LECA
Eukarya
Methanomada
FCB
DPANN
TACK
Asgard
PANNAM
PVC
basal Gracilicutes
DST
CCD
CMS
unresolved Terrabacteria
Excavates
CruMs
Amorphea
Haptista
TSAR
Archaeplastida
Cryptista
Stygia
Acherontia
Diaforarchaea
Methanotecta
Color code of the schematic representations (does not apply to Eukarya)
Cytoplasm
Nucleoid
Cytoplasmic membrane
Periplasm
Outer membrane
Layer of unknown composition
Uncultured
Author : Basile Beaud, PhD student
Director : Pr. Simonetta Gribaldo
Unit Evolutionary Biology of the Microbial Cell, Institut Pasteur, Paris 75015, France
INSTITUT PASTEUR



(Super)tree of mammals
Bininda-Emonds et al., *Nature* (2007)



The tree of life is a network
Doolittle (1999) *Sci Am*



Bacterial evolution is a mess of a network
Dagan et al.(2008) *PNAS*

The problem

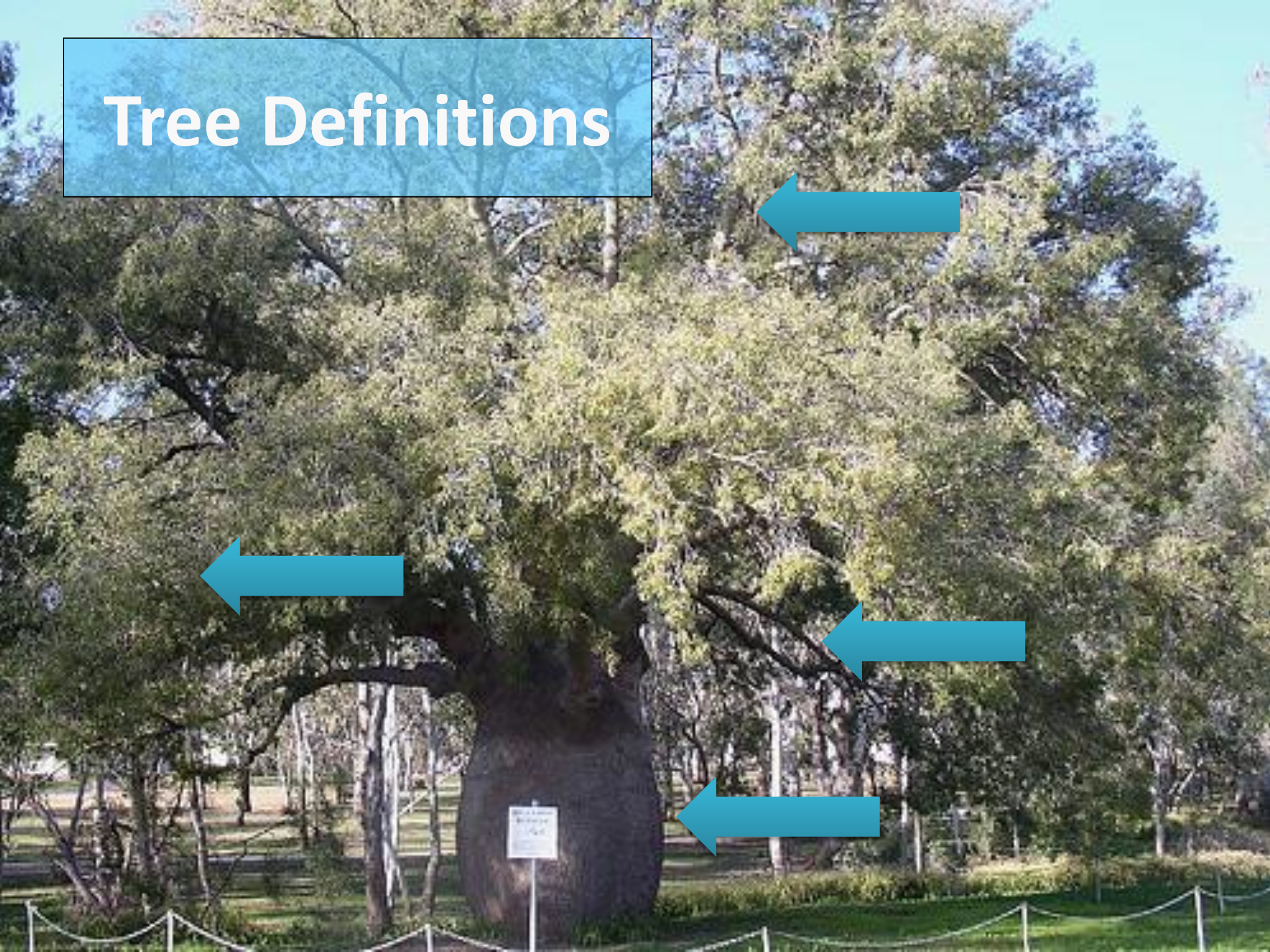
- **How** to build trees properly is not necessarily obvious, and depends on a large number of factors
- **Modeling** sequence similarity is challenging – evolution deals us a confusing hand
- **Searching** tree space can be a nightmare (again, exact vs. heuristic approaches)
- Many problems in evolution **cannot be effectively represented using trees**

Phylogenetics is multidisciplinary

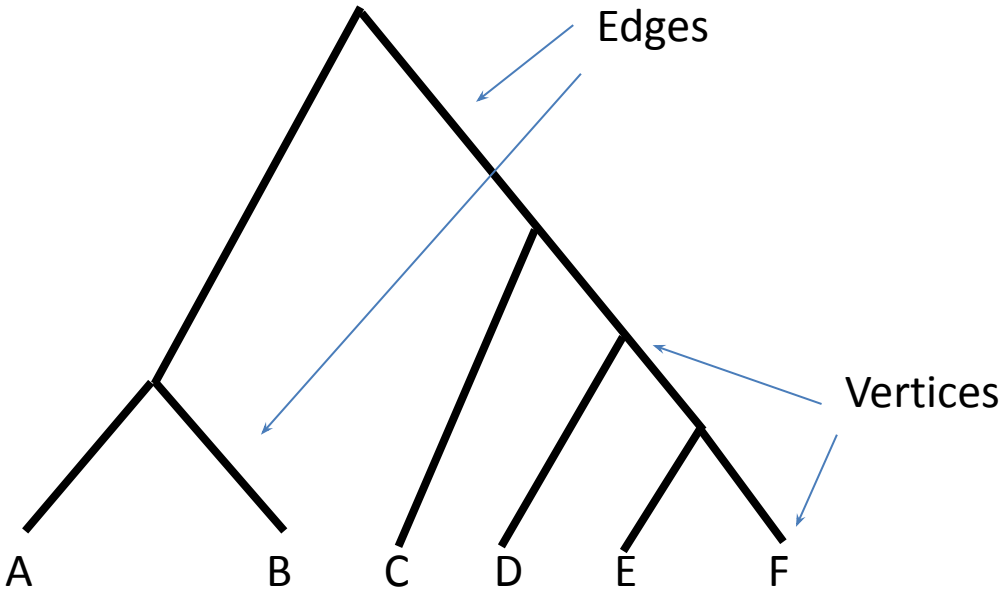
- First tree - Chemist (Linus Pauling)
- 1950s - Physicist (Margaret Dayhoff)
- 1960s - Statisticians
- 1970s - Computer Scientists
- Throughout - Biologists

- Lots of redundant terminology!

Tree Definitions

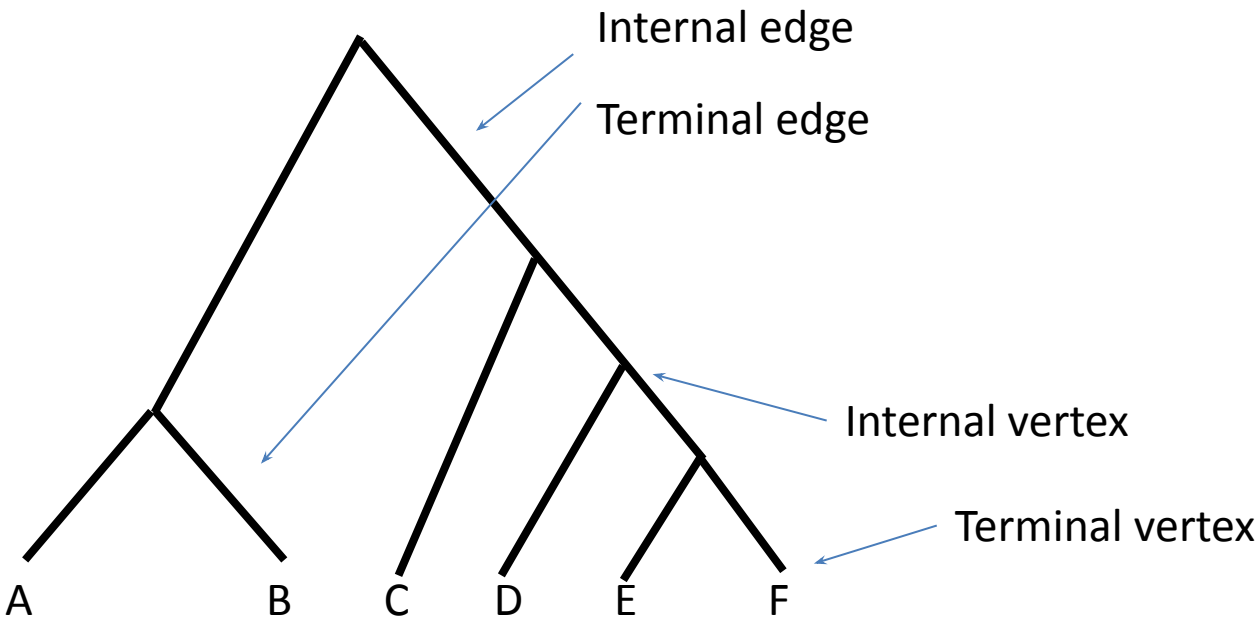


Tree Anatomy



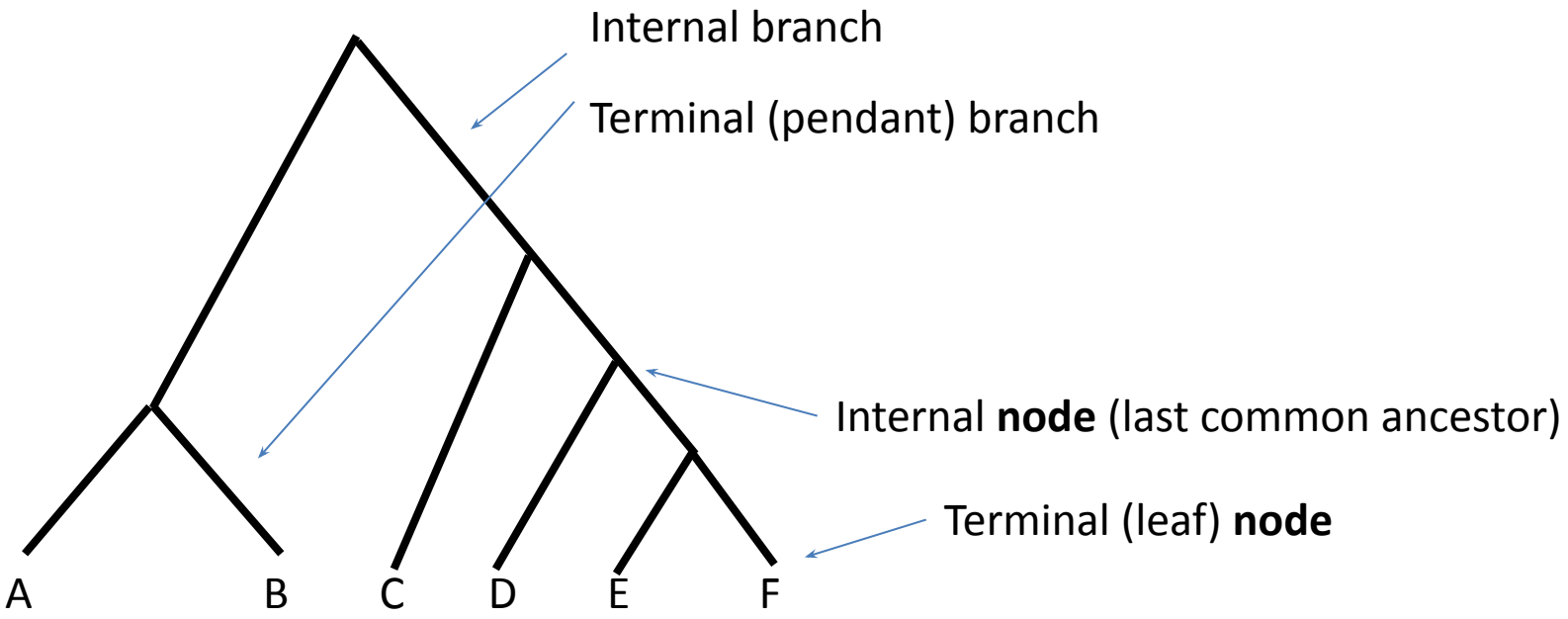
Trees can be described using the same terminology as graphs

Tree Anatomy



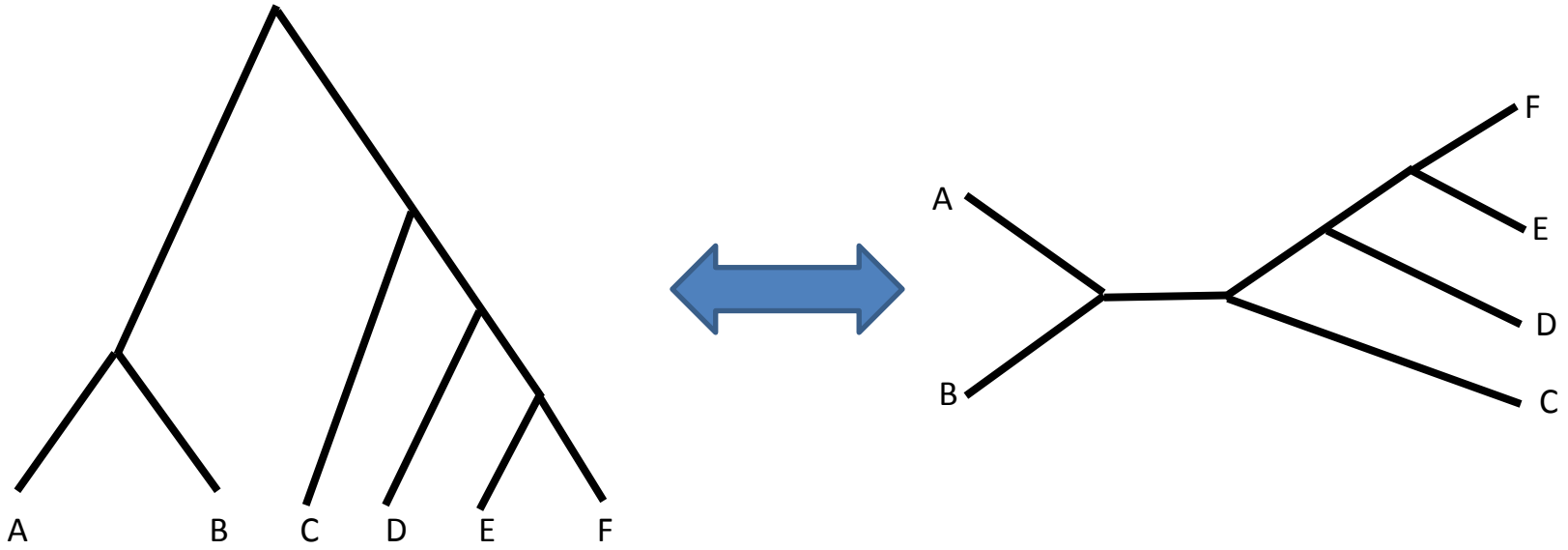
We distinguish between **internal** and **terminal** features

Tree Anatomy



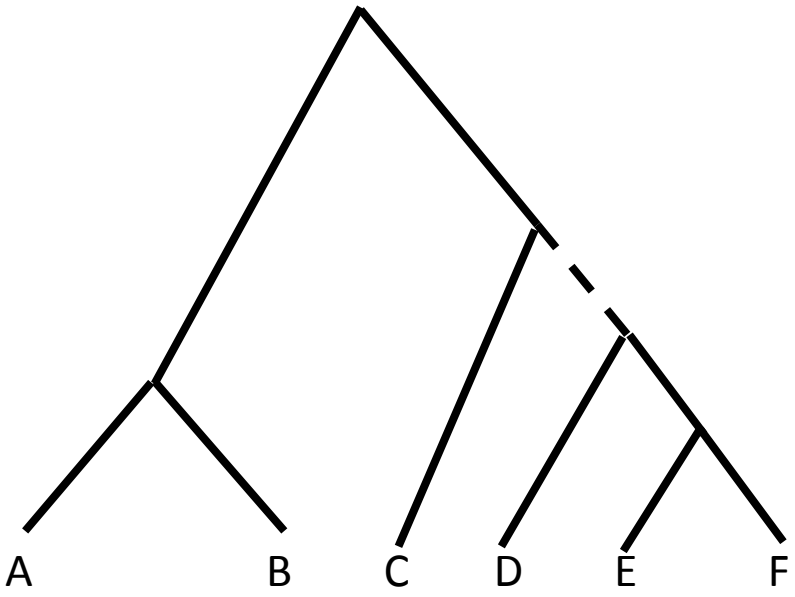
Some terms are used interchangeably

Rooted vs Unrooted Trees



Most methods (including parsimony) generate **unrooted** trees

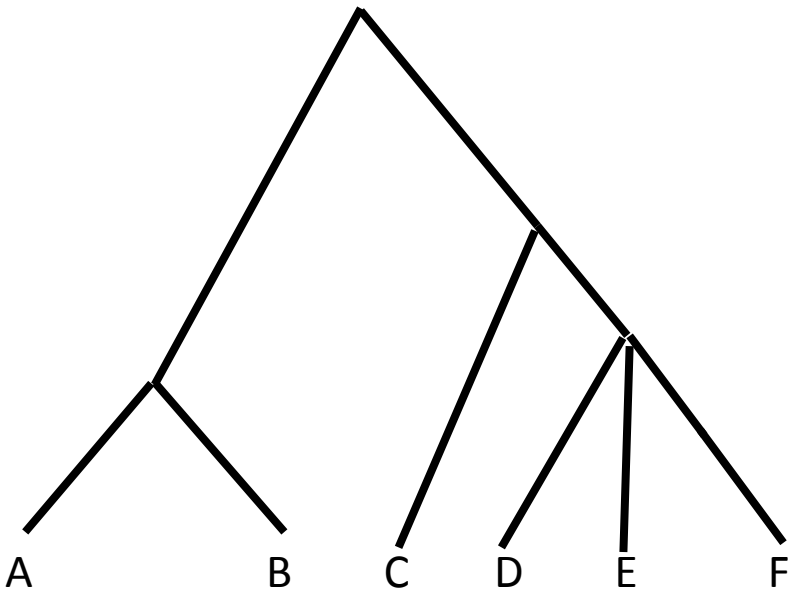
Tree splits (bipartitions)



(ABC | DEF)

Splits are *compatible* if they can appear in the same tree

Multifurcating Nodes

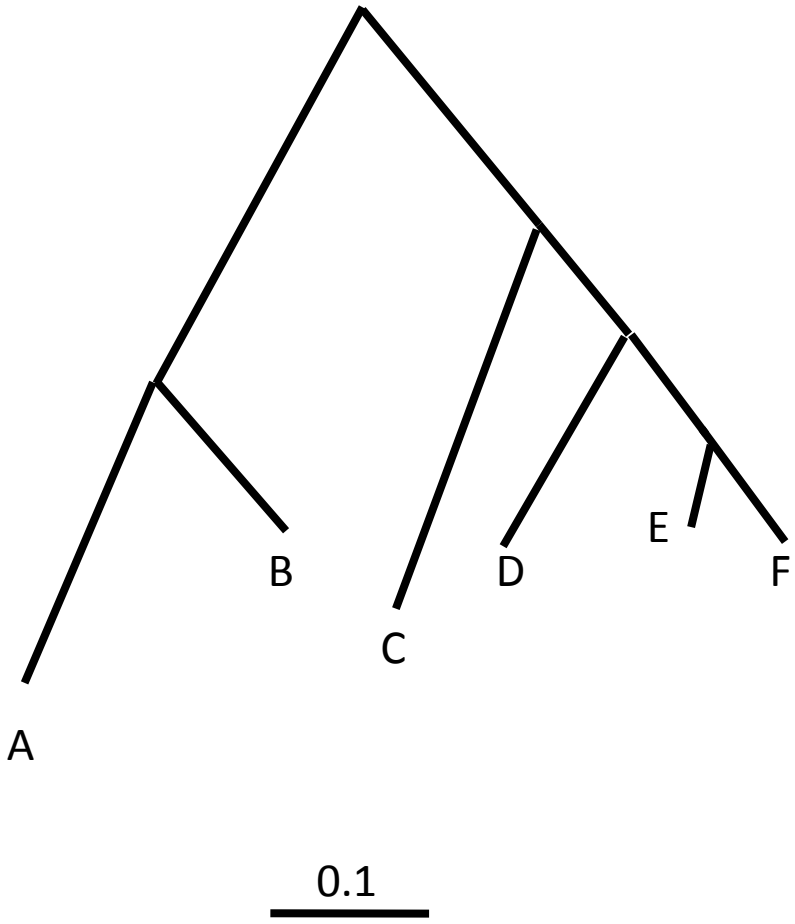


We may *collapse* a node in the tree for one of two reasons:

- 'Hard' polytomy (really a 3-way split)
- Lack of statistical support for any pairwise grouping

Most phylogenetic methods produce only **binary** trees
(but you can roll back relationships that lack support)

Branch lengths

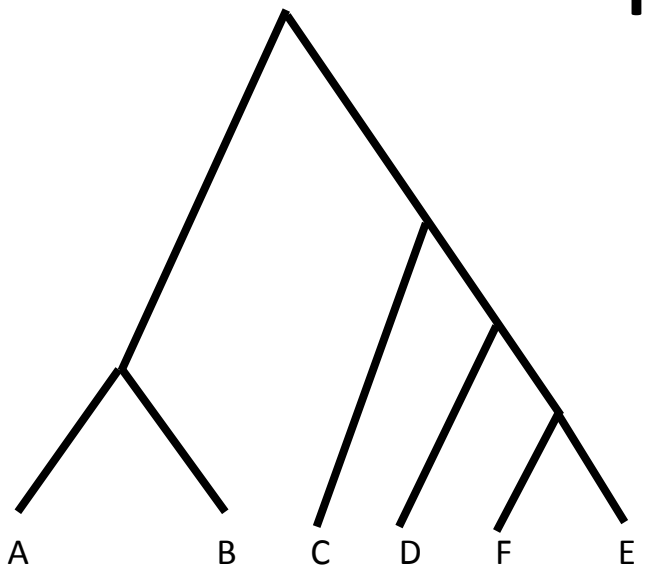


What (if anything) do branch lengths represent?

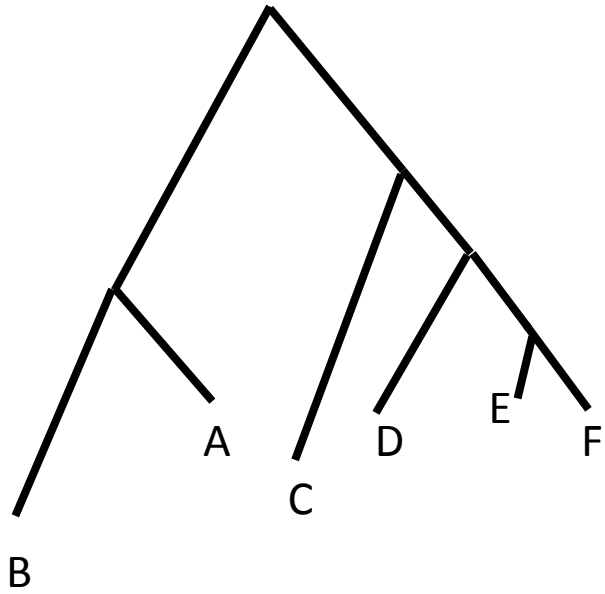
- Time?
- Sequence change?

Some methods (notably parsimony) do not produce meaningful branch lengths

Tree Shape



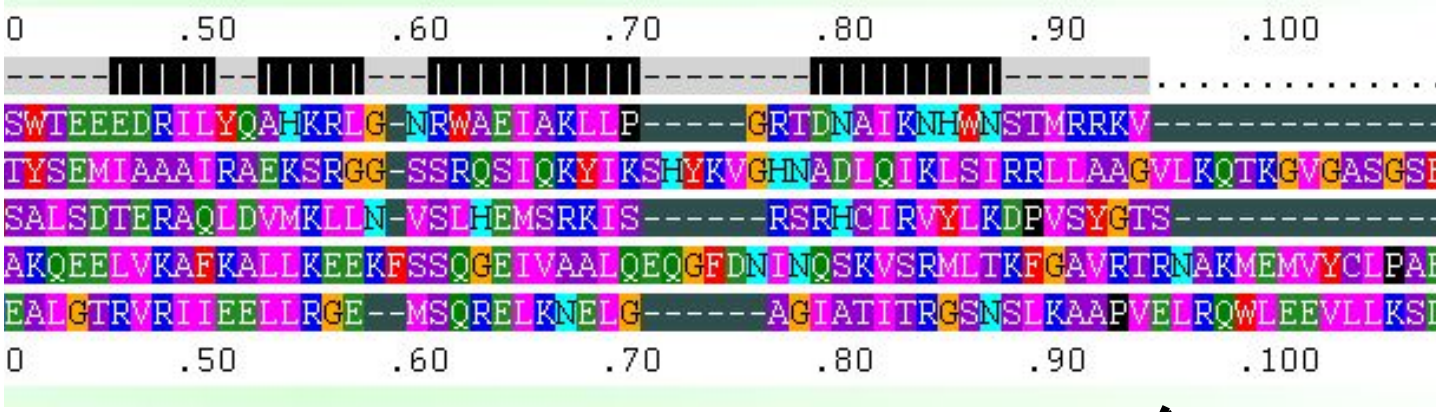
In general (and for the purposes of this course), the *shape* of a tree refers to its branching order, **not** to branch lengths

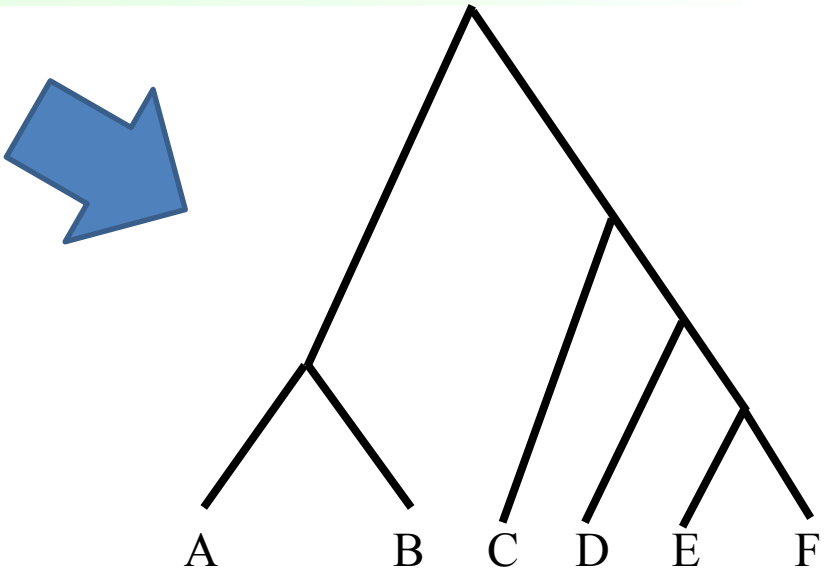


So the two trees on the left have the same shape

Shape can be described completely using a **split decomposition** of the tree

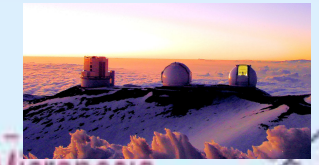
Nextstrain Intermission





But nucleotides and amino acids are not the only type of character that can be compared!

The Polynesian Triangle



Hawai'i

Formosan

WMP

SHWNG

Micronesia

Nuclear Micronesian

Oceanic

CMP

Madagascar

Wallacea

Rugby Playing Nations

Polynesia

Rapa Nui

Aotearoa

Words as homologous characters

Nature, 2000

Language trees support the express-train sequence of Austronesian expansion

Russell D. Gray & Fiona M. Jordan

Department of Psychology, University of Auckland, Auckland 92019, New Zealand

Meaning	Tonga	Niue	Samoa	E. Uvea	E. Futuna	Mangareva	Marquesas	Hawaii	Tahiti	Tuamotu	Rarotonga
Canoe	vaka	vaka	va'a	vaka	vaka	vaka	vaka	wa'a	va'a	vaka	vaka
Two	ua	ua	lua	lua	lua	rua	'ua	lua	rua	rua	rua
Five	nima	lima	lima	nima	lima	rima	'ima	lima	rima	rima	rima
Woman	fefine	fifine	fafine	fafine	fafine	ahine	vehine	wahine	vahine	vahiine	va'ine
Rainbow	*'umata*	*tangaloa*	nuanua	nuanua	nuanua	anuanua	aanuanua	aanuenue	aanuanua	anuanua	aanuanua

No collinearity constraint
(but who cares?)

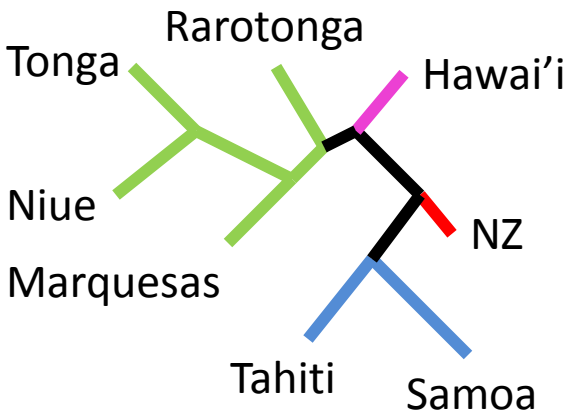
Character Convexity

Island	Canoe
Tonga	Vaka
Niue	Vaka
Rarotonga	Vaka
Marquesas	Vaka
Hawai'i	Wa'a
Tahiti	Va'a
Samoa	Va'a
NZ	Waka

Choose a tree at random (for now)

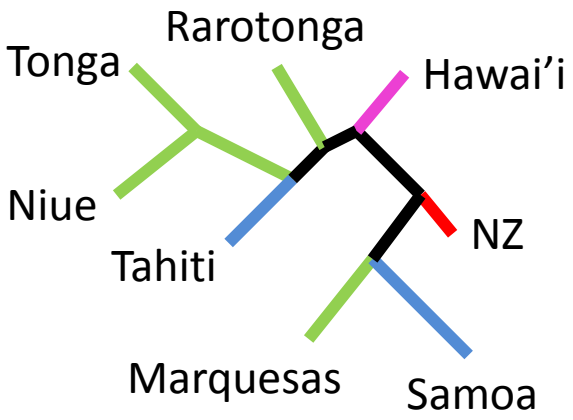
A character is *convex* on that tree if all states of that character can be partitioned to a separate 'region' of the tree

Think of it as a coloring problem!



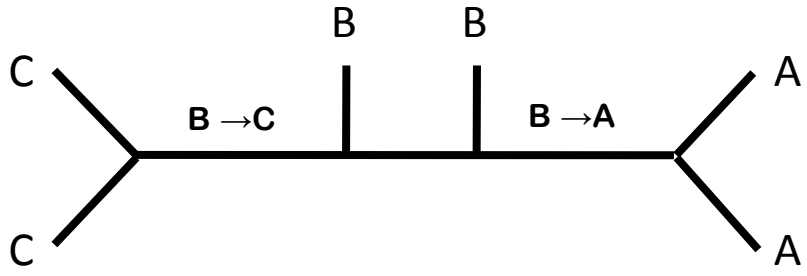
CONVEX

NOT CONVEX



What does convexity mean?

- If we have *n* states (waka, vaka, etc.) for a given character, then we only need the minimum possible *n* – 1 state changes within the tree

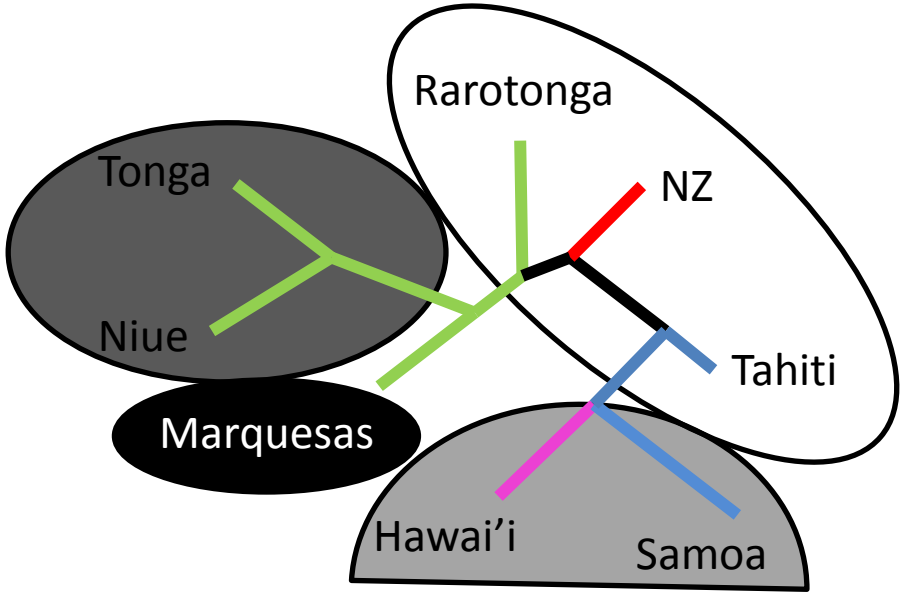


- The is the *most parsimonious* (simplest) situation

Character Compatibility

Island	Canoe	Two
Tonga	Vaka	Ua
Niue	Vaka	Ua
Rarotonga	Vaka	Rua
Marquesas	Vaka	‘ua
Hawai’i	Wa’a	Lua
Tahiti	Va’a	Rua
Samoa	Va’a	Lua
NZ	Waka	Rua

Two characters (words, alignment columns, etc.) are *compatible* if there exists at least one tree where both characters are convex



What is the “best” tree?

- Is it the **maximum compatibility** tree that maximizes the number of convex characters from the set C of characters?

maybe…but usually not

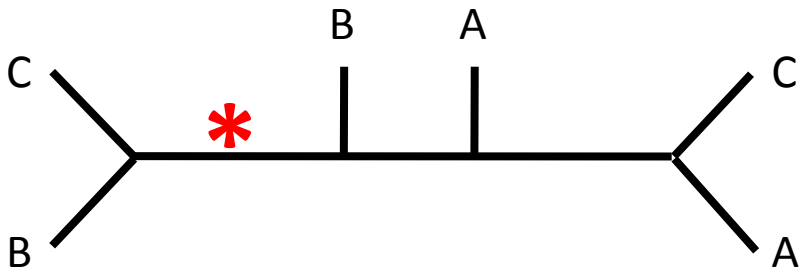
- What we typically want is the tree that minimizes the number of substitutions over *all* characters – this is the **maximum parsimony** tree

Parsimony Score

- The *parsimony score* (p) for a given character on a given tree T is the minimum number of changes needed to map character states onto leaves of the tree

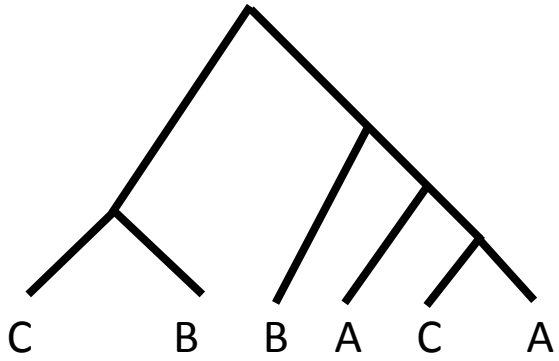
- How do we find this minimum for a single character?

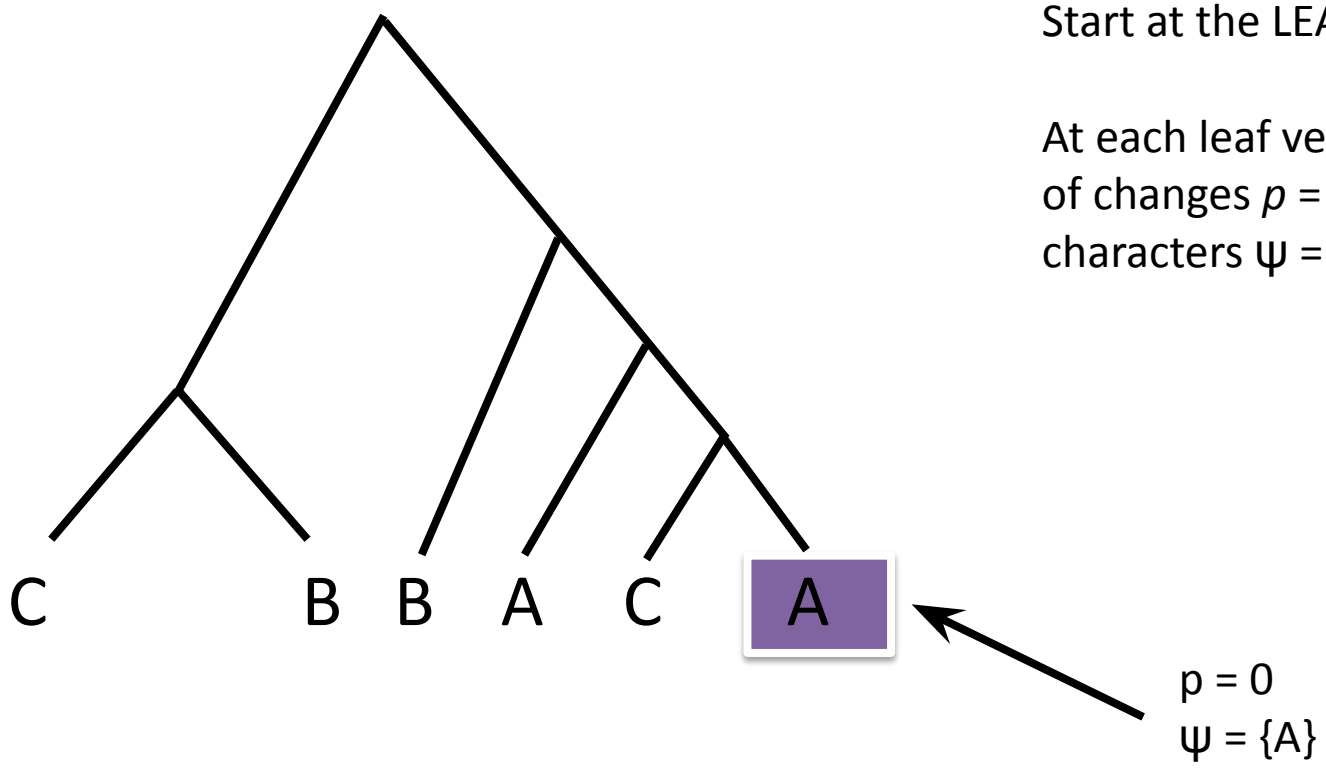
Fitch-Hartigan algorithm



One character, three states

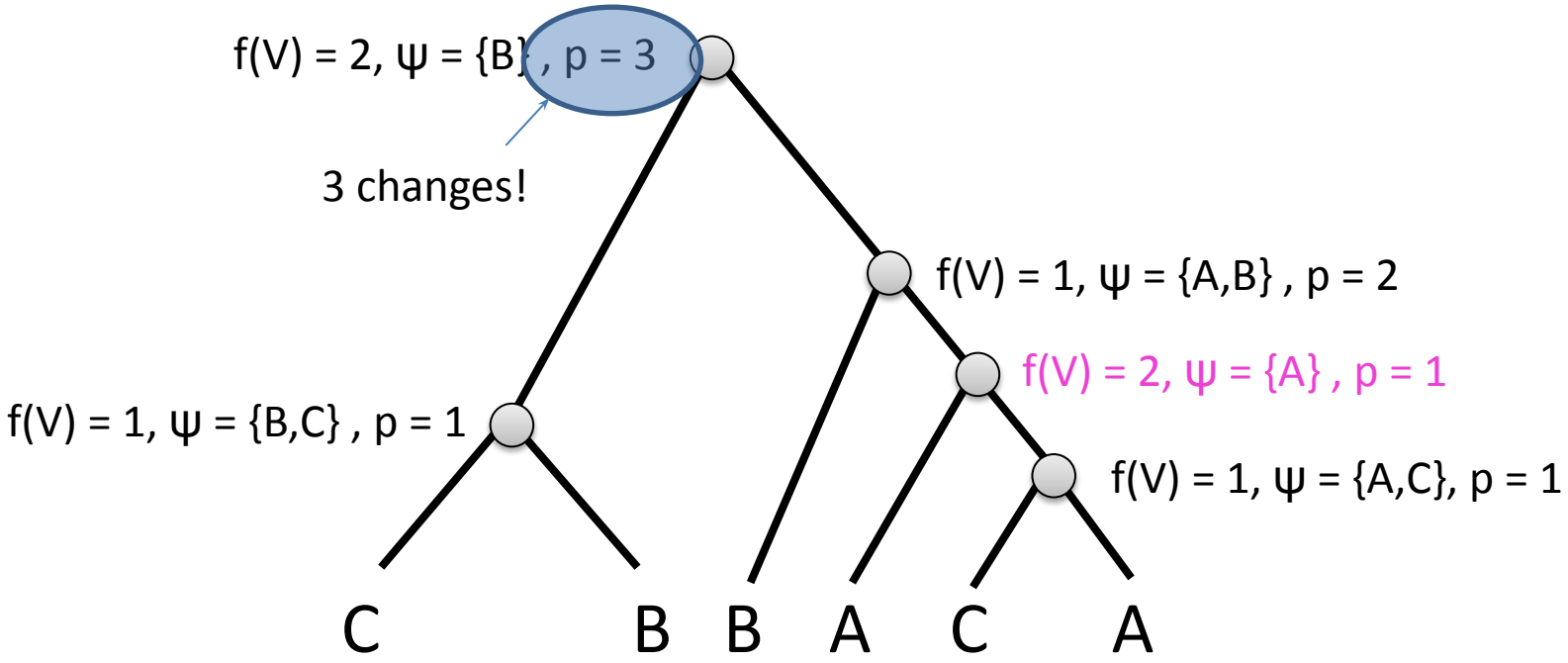
Introduce an arbitrary root to the tree if unrooted





Start at the LEAF vertices

At each leaf vertex, the count of changes $p = 0$ and the set of characters $\psi = \{X\}$



Mapping to internal vertices V:

f(V) is the maximum number of immediate children that contain any **particular** character state

→ *best guess for internal states*

ψ is the character or characters that cover f(V) children

→ *equally good internal state guesses*

p is equal to (p of all children) + (number of children) – f(V)

→ *number of required changes so far*

Total Parsimony Score

(for a given tree)

$$p_T = \sum_{c \in C} p_T(c)$$

(for all character columns)

The *maximum parsimony tree* is the tree that minimizes p_T

Note that it does **not** explicitly count convex characters!
They simply contribute the minimum possible changes given the number of states they contain

How well do the characters fit the tree?

We can use the **consistency index**

$$CI_{character} = m / s$$

Where m is the **minimum** number of steps

(= number of character states – 1)

And s is the **actual** number of steps (≥ m), from the F-H algorithm

$$0.0 < CI \leq 1.0$$

Maximum Parsimony

- There is no closed-form solution to find *T* such that p_T is minimal

- We must carry out a search through *tree space* – typically use a random starting tree T_0 and explore by permuting this tree

- Search strategies coming up next class!

Tree Searching

1. Choose a random starting tree T_0
2. n ← 0 *(this is the iteration number)*
3. Compute p_{T0}
4. While (patience remains)
    1. Permute T_n
    2. T_{n+1} = $\text{argmin}_p(T_n$, permuted $T_n)$
    3. n ← n+1
5. Output T_n

Problem

- There are a lot of trees!

- For *n* leaves, there are

1 x 3 x 5 x … x (2n - 3) rooted, bifurcating trees

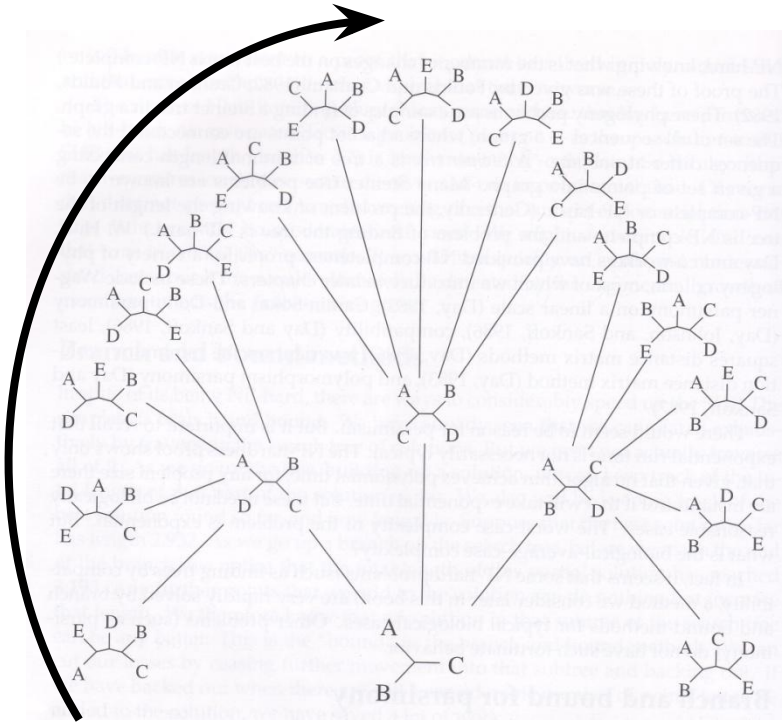
$$n_T = \frac{(2n-3)!}{2^{n-2}(n-2)!}$$

20 leaves $\longrightarrow$ 8,200,794,532,637,891,559,375 trees

Branch-and-Bound

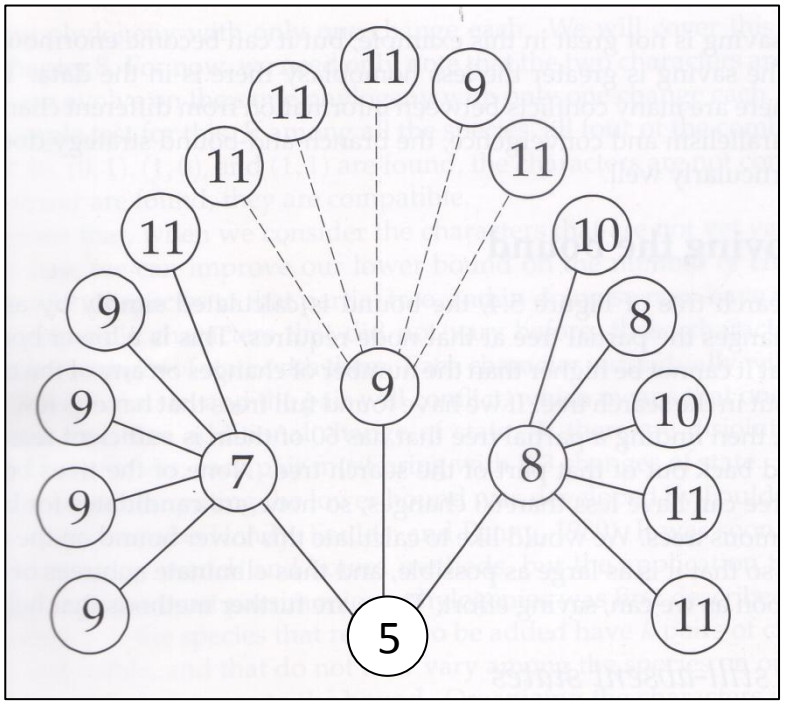
One way to restrict the search space is to explore it systematically, but identify and stop unproductive search paths

Species	Character					
	1	2	3	4	5	6
A	1	0	0	1	1	0
B	0	0	1	0	0	0
C	1	1	0	0	0	0
D	1	1	0	1	1	1
E	0	0	1	1	1	0



Tree building procedure

Felsenstein, 2004



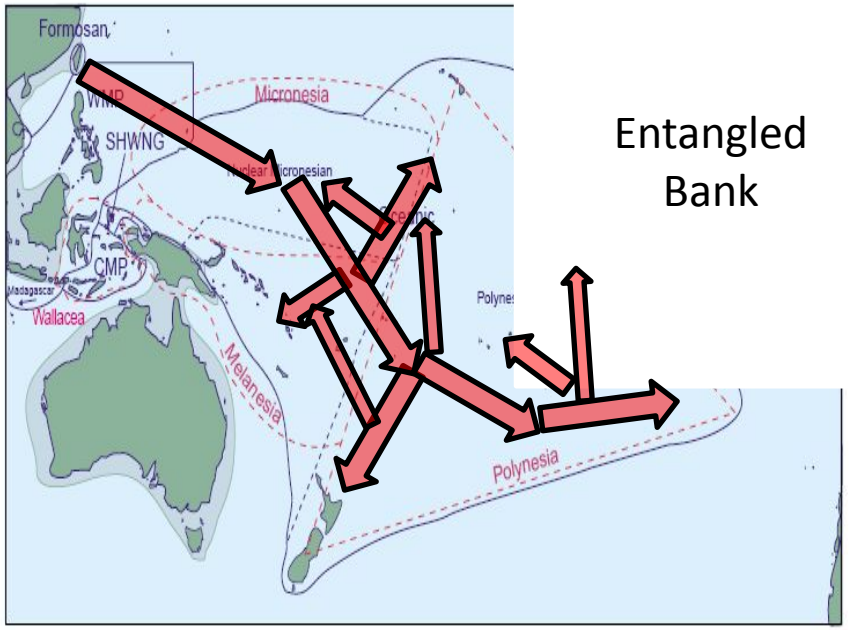
Number of substitutions required

Back to Polynesia

- Hypotheses about Polynesian expansion

- What are the predictions of these two models?

Express Train

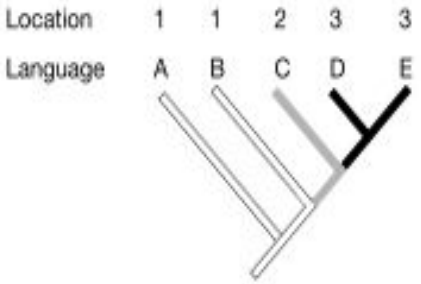


Entangled Bank

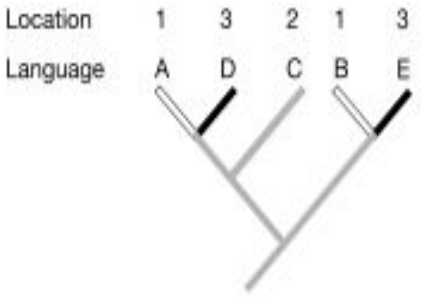
Predictions

- Express train: strong tree-like signal, congruent with geography. **High CI**

  (assuming enough time for language to evolve)

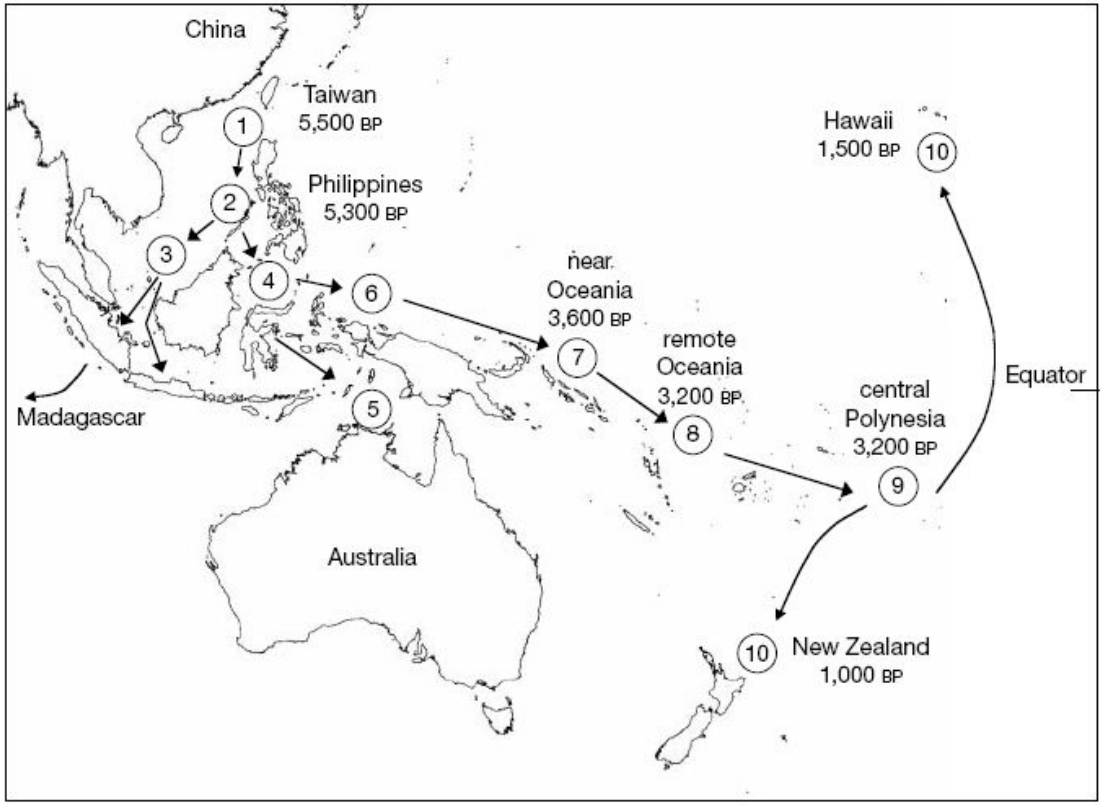


- Entangled bank: weaker signals, lots of sharing (travel / cultural exchange). **Low CI**

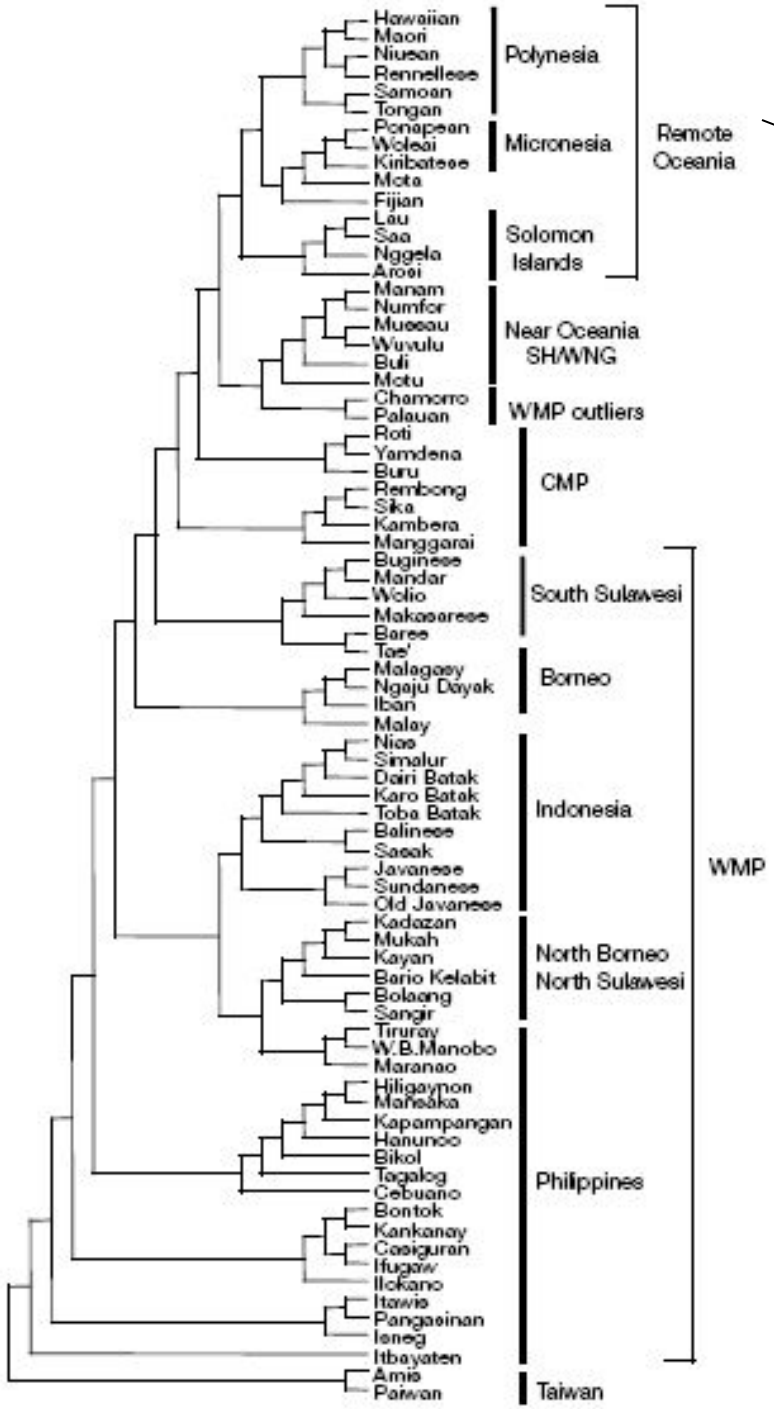


Analysis

- 77 Austronesian languages
- 5185 terms (no equivalent to NCBI!)



Express train model –
77 languages grouped into
10 categories (archaeological 'stations')



Relationships in the language tree are driven more by express-train predictions than by geographic proximity

Mininum number of transitions: 9 (= 10 – 1)

A total of **13** steps is needed to reconcile the 10 character states with the recovered tree (close to optimal)

CI = 9/13 = 0.69

What does a CI of 0.69 mean?

We can compare it to the CI of **random** trees to see whether the fit is better than expected

Randomized trees: Average of **49** steps (CI = 9/49 = 0.053)

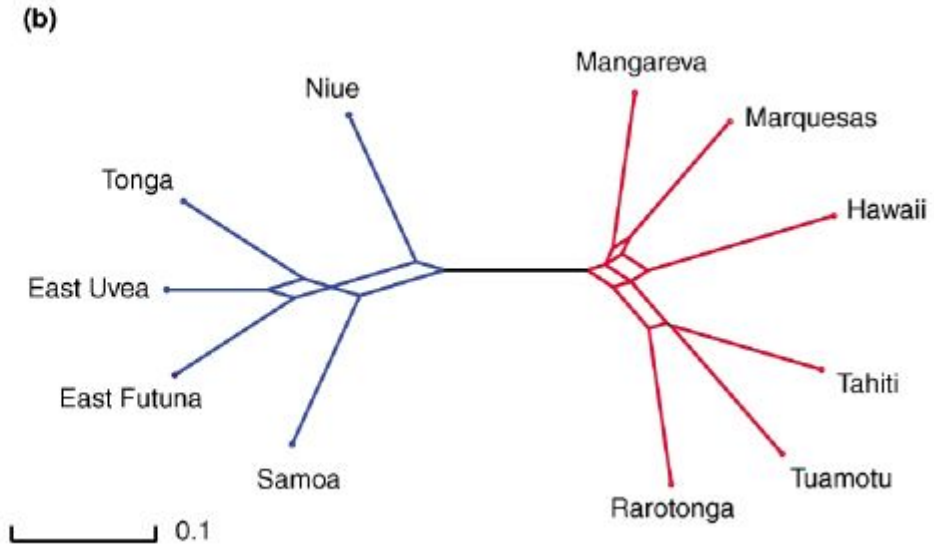
So there is **significant** tree-like signal, and the *shape* of the tree is consistent with express-train predictions

Review TRENDS in Ecology and Evolution Vol.18 No.10 October 2003 531

Untangling Oceanic settlement: the edge of the knowable

Matthew E. Hurles[1], Elizabeth Matisoo-Smith[2,3], Russell D. Gray[4] and David Penny[3,5]

West Polynesia
East Polynesia



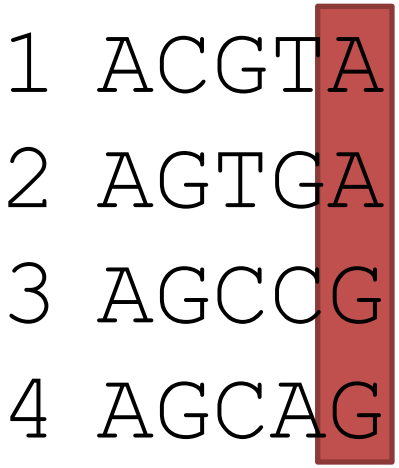
Splits graph

Significant signals that conflict with the canonical tree

Problems
with Parsimony

Not all alignment sites are informative

- Unless it can assign different scores to different trees, a given alignment column is not parsimoniously informative

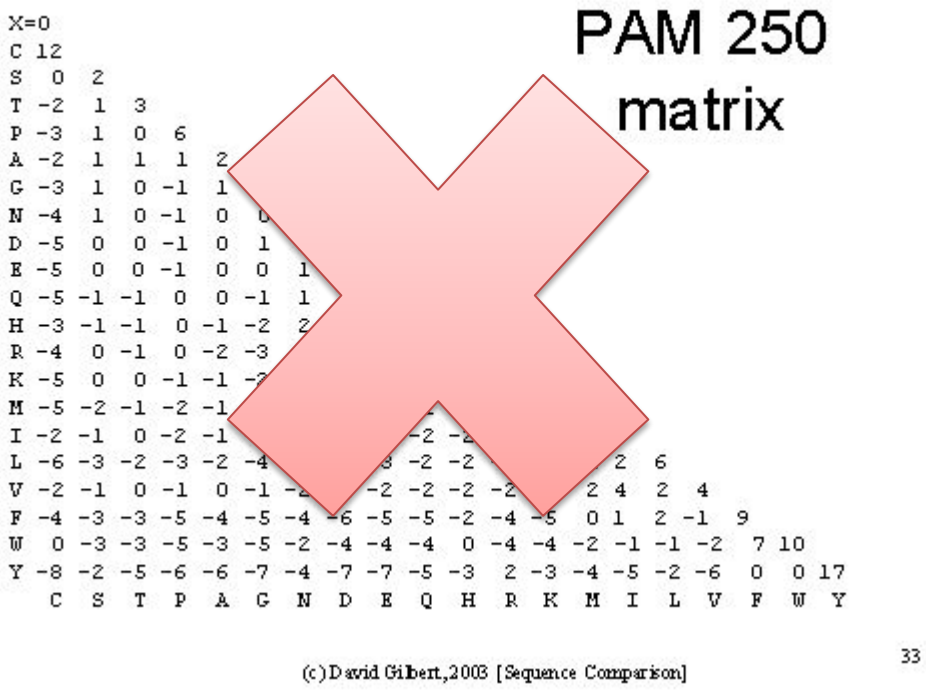


Favours ((1,2),(3,4))
over ((1,3),(2,4))
and ((1,4),(2,3))

Other sites say nothing!

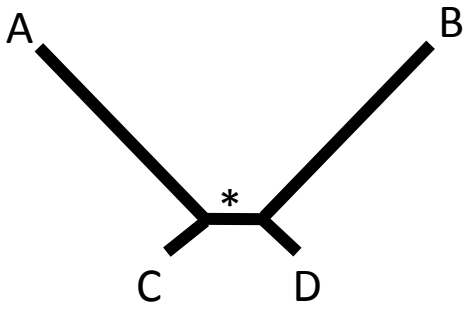
Parsimony treats all changes <u>equally</u>

- Parsimony is “model-free”, so there is no distinction between frequent and infrequent changes



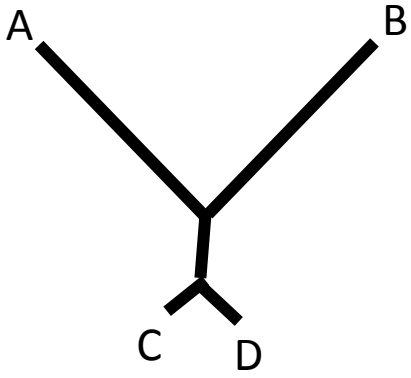
Long Branch Attraction

- Branches that accumulate many changes (e.g. parasites, mice) will share many homoplasies, and appear to be more similar than they really are



True tree

A	A**G**CAT**C**GAT
*	AATATACGA
B	C**G**TAC**C**CGA



Inferred tree

Parsimony: Summary

- Relatively easy (though potentially time-consuming) to use and understand
- The basic principle (the simplest explanation is the best) is attractive but not necessarily correct
- The lack of an explicit model can be an *advantage* or a serious *disadvantage*
- Throwing away uninformative alignment columns is not necessarily ideal