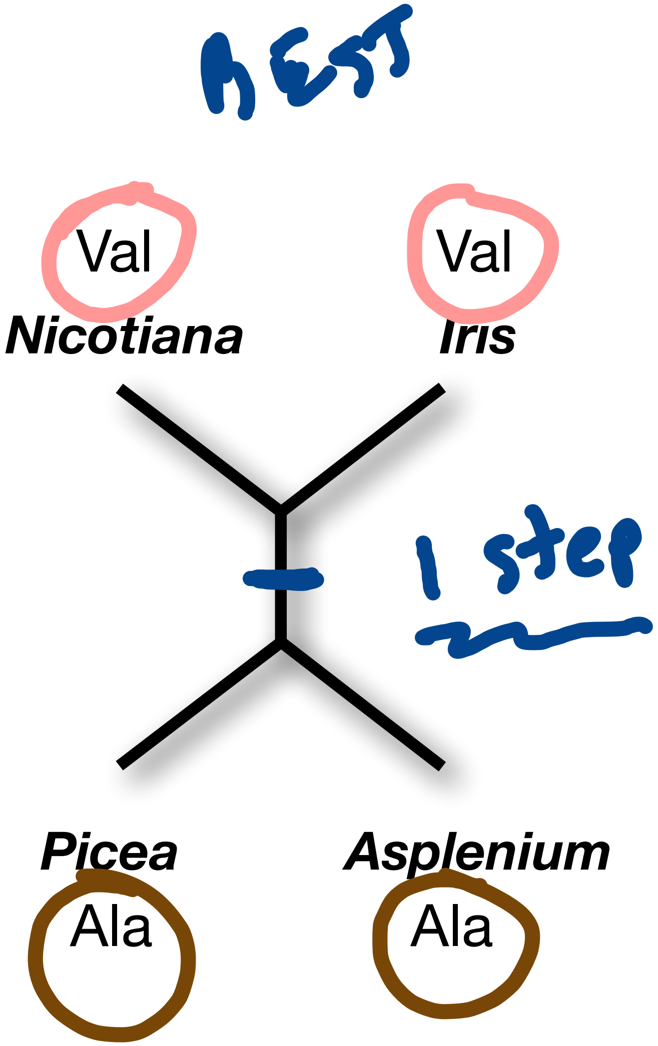
Optimality search combinations

Optimality Criteria	Search Strategies
Maximum Parsimony	Exhaustive Enumeration
Maximum Likelihood	Star Decomposition
Minimum Evolution	Stepwise Addition
Least Squares	Branch-and-Bound
	Branch Swapping

Parsimony criterion



BEST

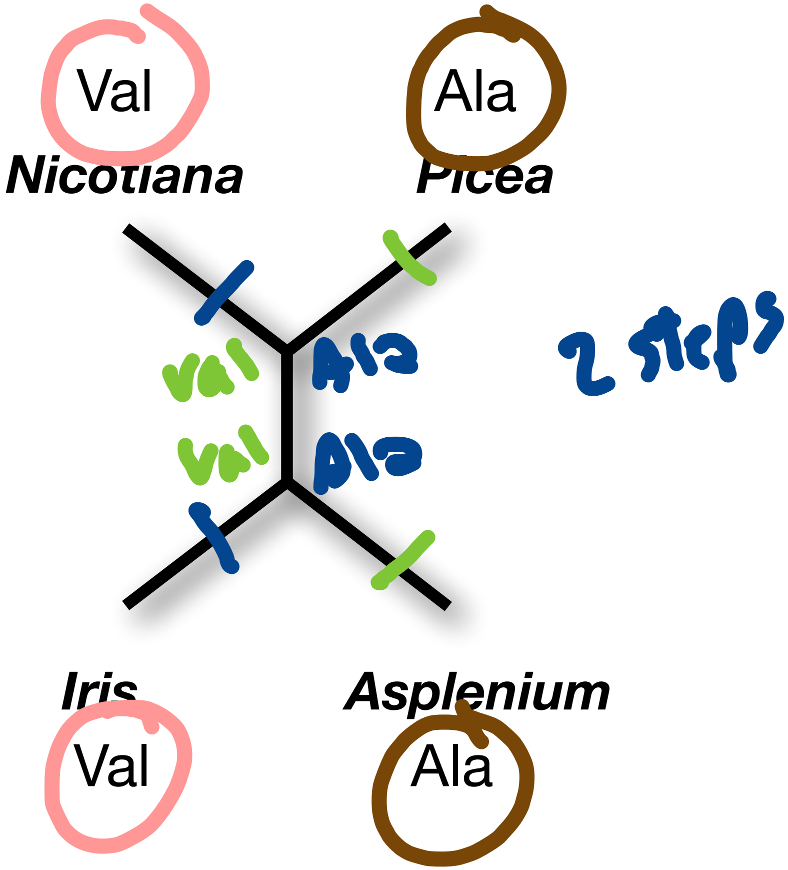
Val
Nicotiana

Val
Iris

1 step

Picea
Ala

Asplenium
Ala



Val
Nicotiana

Ala
Picea

Val
Val

Ala
Ala

2 steps

Iris
Val

Asplenium
Ala

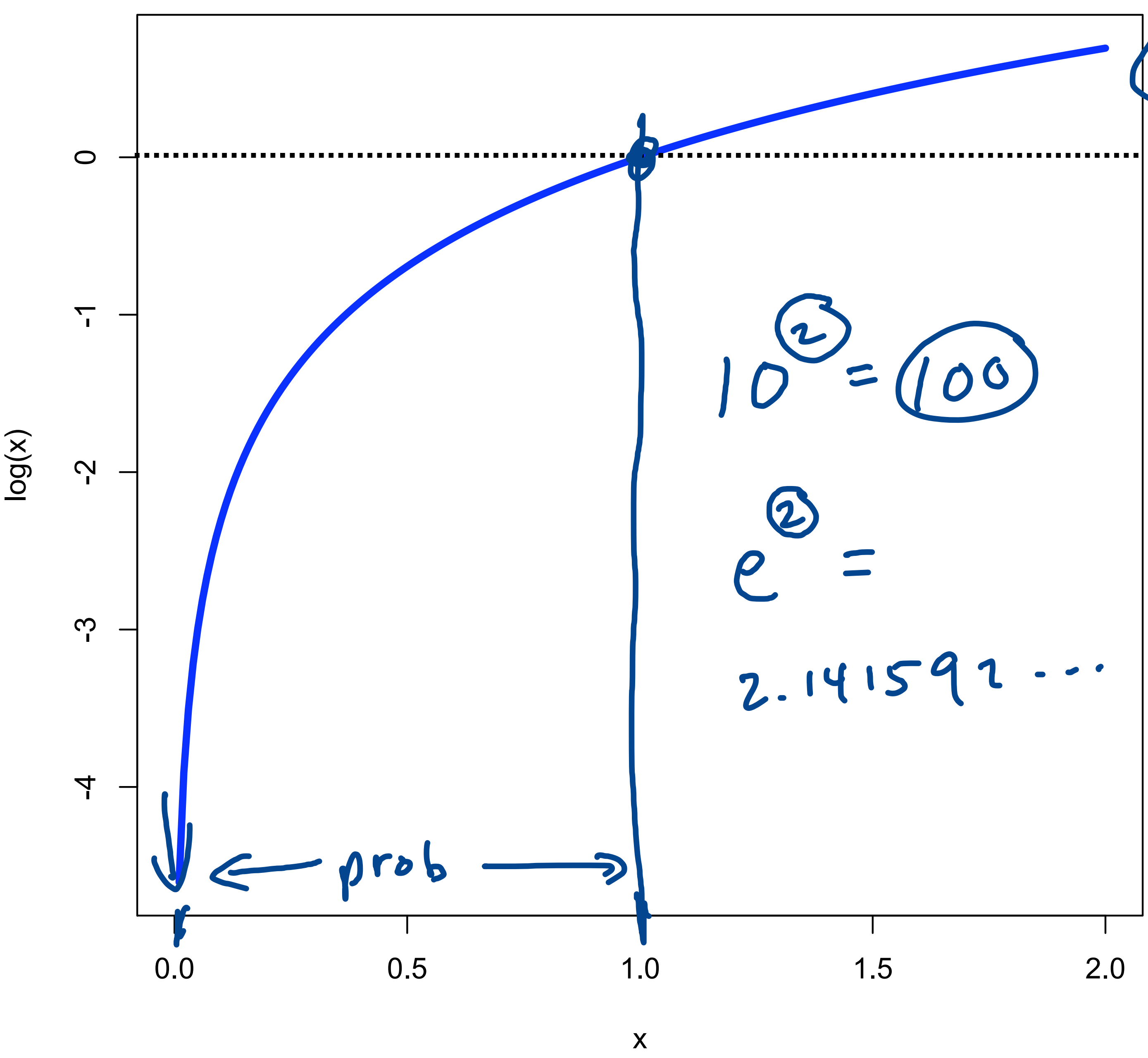
Data from 91st amino acid position in the large subunit of the RuBisCO enzyme

Likelihood Criterion

the tree that makes you least surprised at the observed data is **best**

least surprised = most probable

stopped here 2024-01-18



-lnL 3043.0123

lnL -3043.01

$10^{2} = 100$

$e^{2} =$

2.141592...

DISCRETE DATA

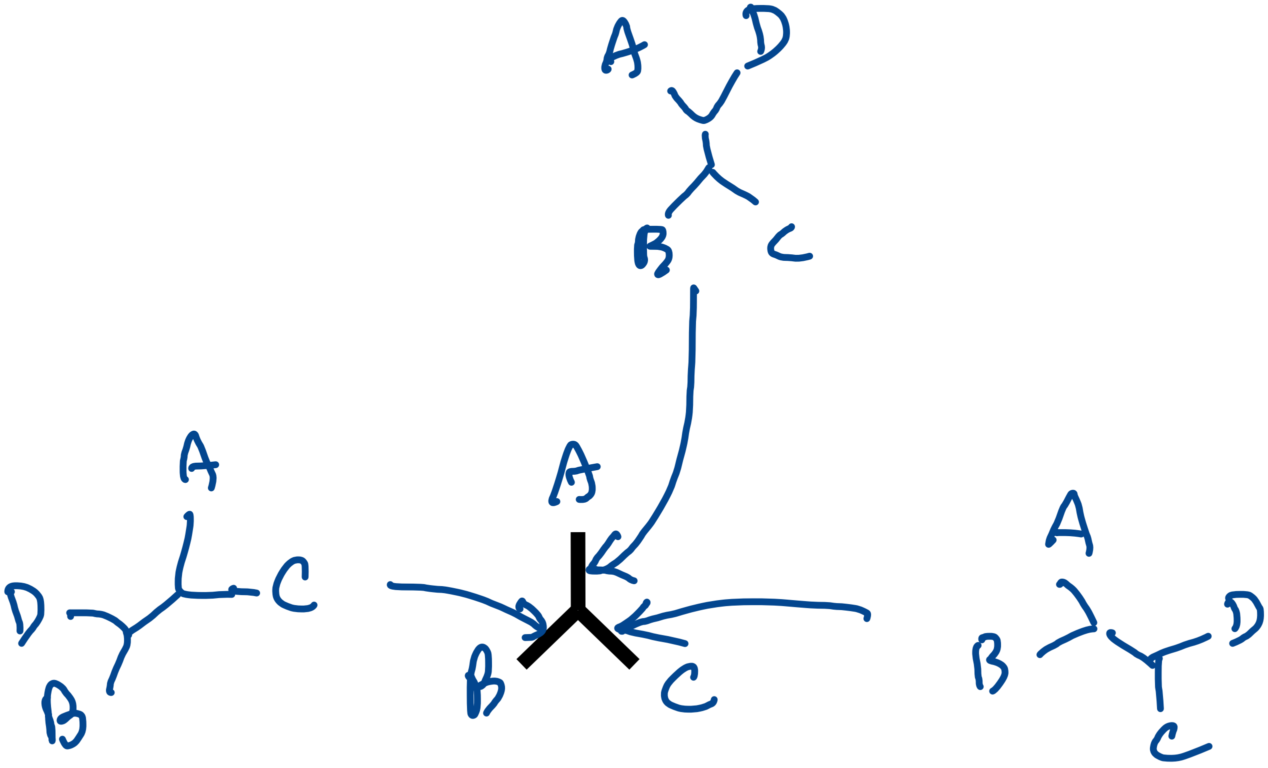
LIKELIHOOD IS A PROB.

prob 0 ⟷ 1

log prob $-\infty$ 0

Likelihoods vs. log-likelihoods

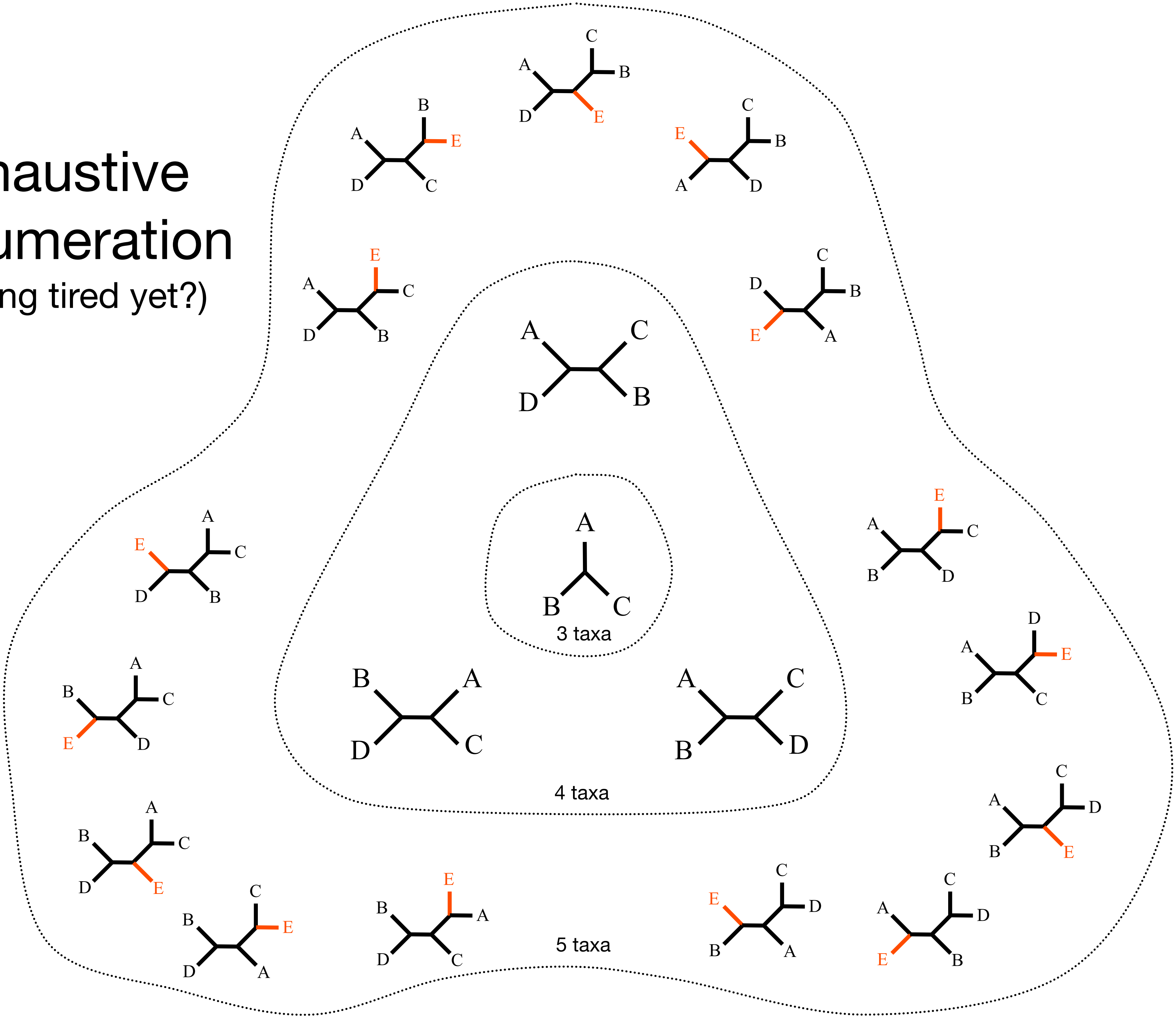
Exhaustive Enumeration



add 2 edges/taxon

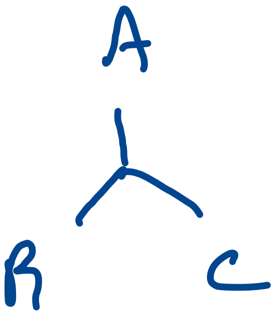
Exhaustive Enumeration

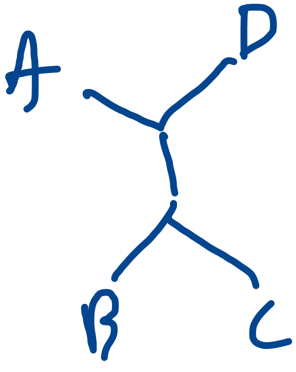
(getting tired yet?)



Note the pattern

Taxa	Unrooted Topologies	Edges
2	1	1
3	1	3
4	3	5
5	15	7
6	105	9





n taxa

$(2n-5)!!,$

$7 \cdot 5 \cdot 3 \cdot 1 = 105$

Why not enumerate?

Taxa	Number of unrooted trees
4	3
5	15
6	105
7	945
8	10,395
9	135,135
10	2,027,025
11	34,459,425
12	654,729,075
13	13,749,310,575
14	316,234,143,225
15	7,905,853,580,625
16	213,458,046,676,875
17	6,190,283,353,629,375
18	191,898,783,962,510,625
19	6,332,659,870,762,850,625
20	221,643,095,476,699,771,875
21	8,200,794,532,637,891,559,375
22	319,830,986,772,877,770,815,625

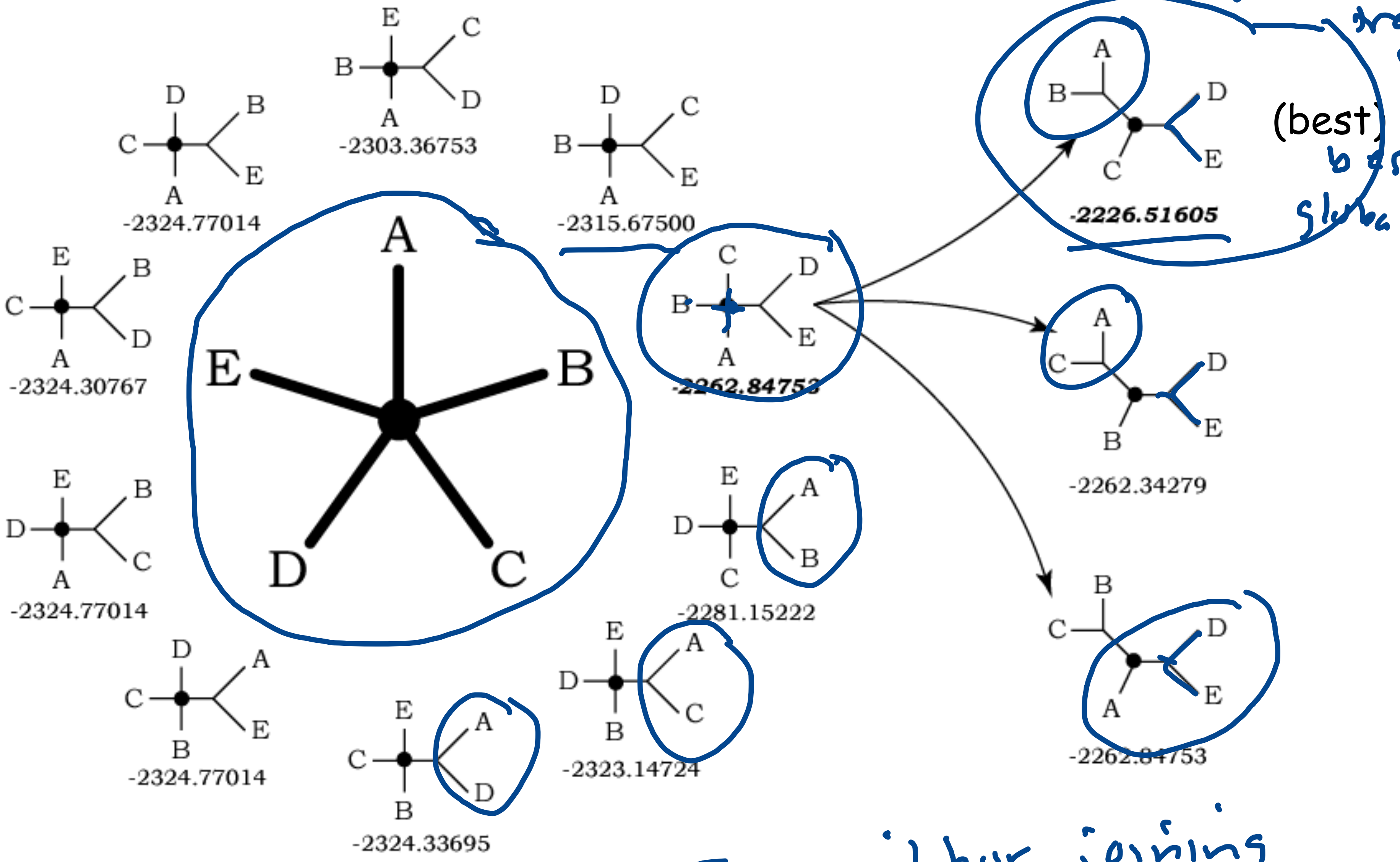
4.8 billion years

23

175

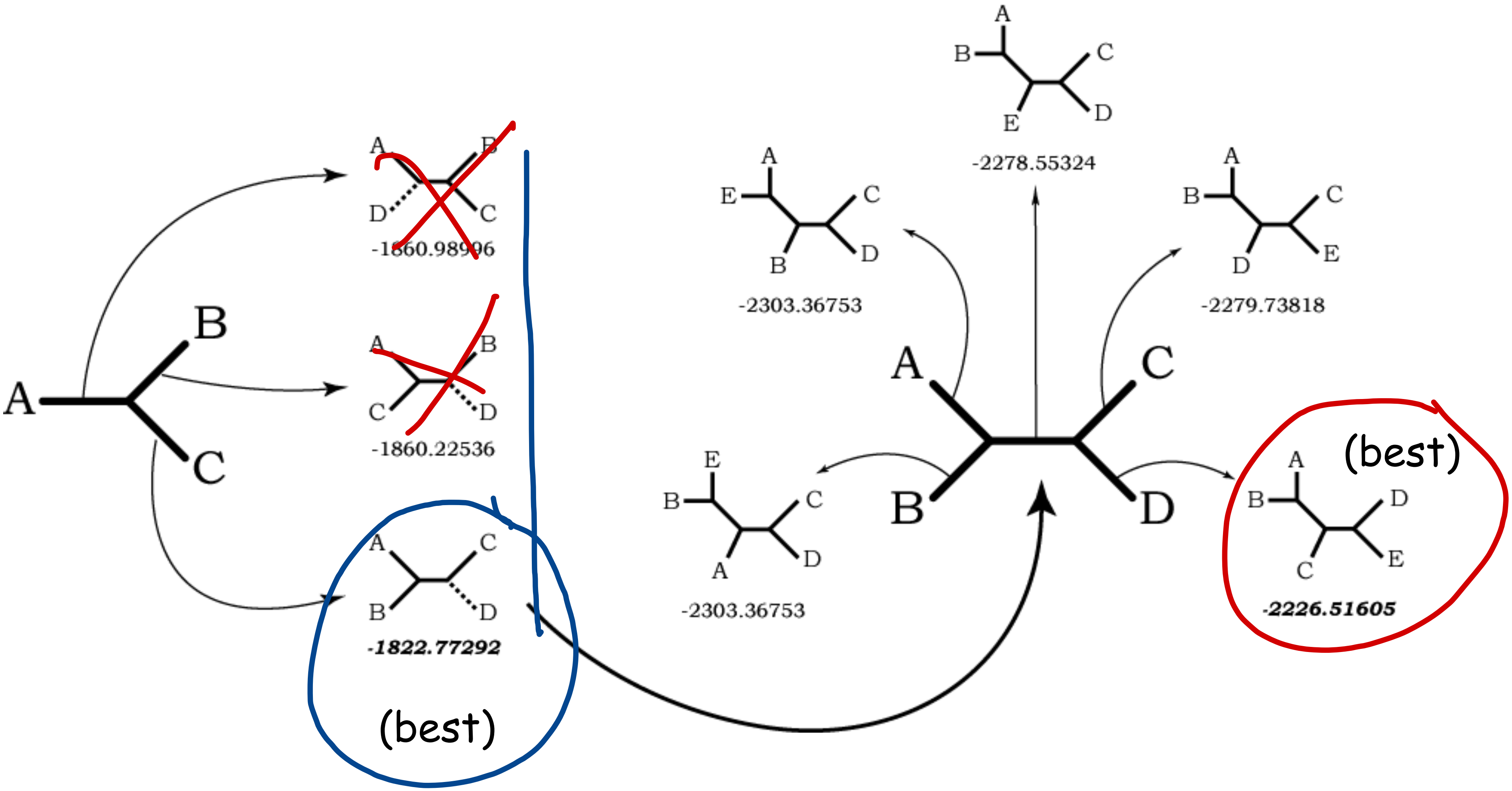
Star decomposition

no guarantee that this tree is best globally

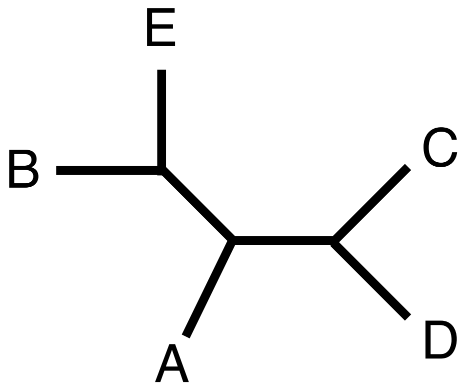


NJ neighbor joining

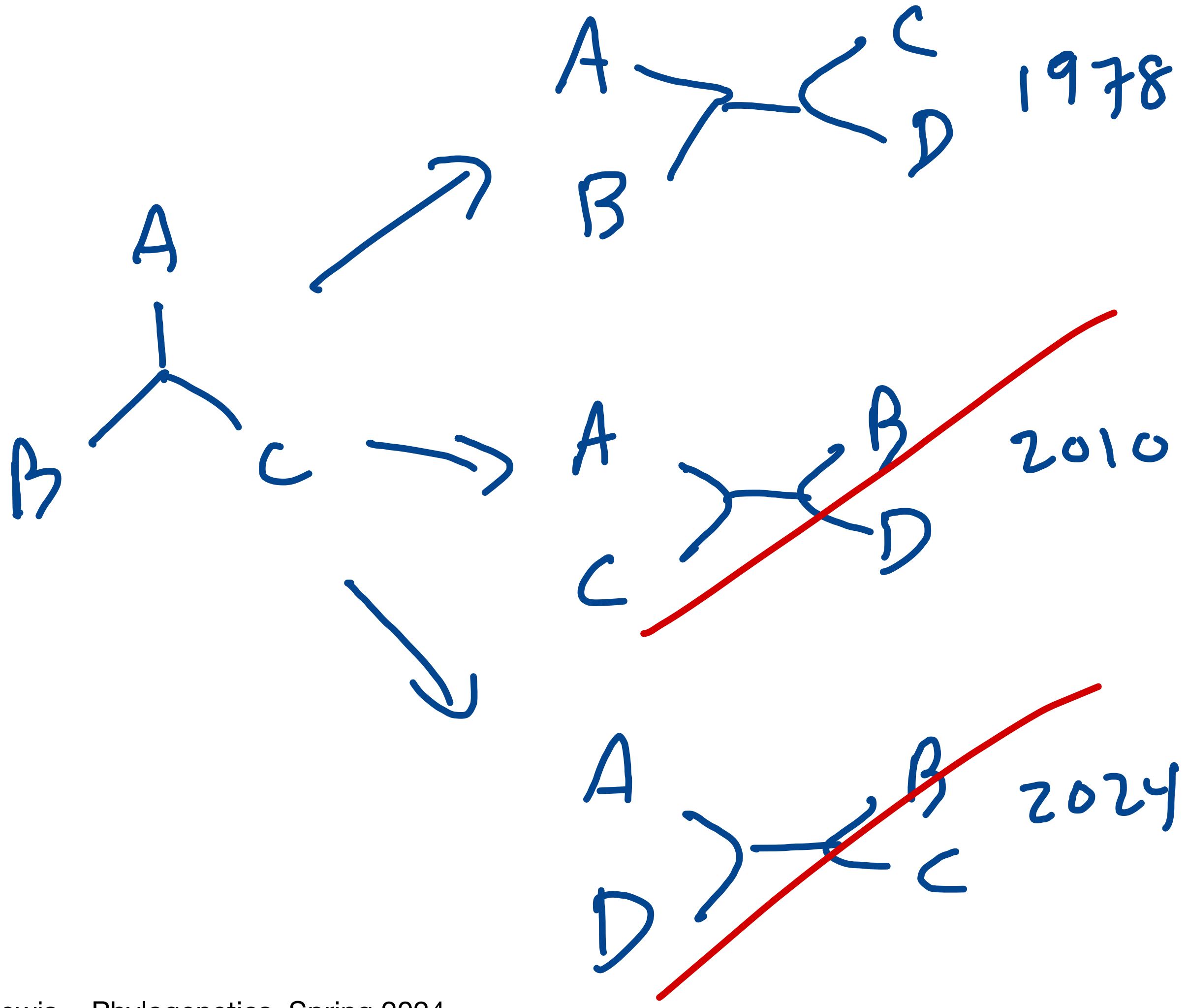
Stepwise Addition



Branch and bound

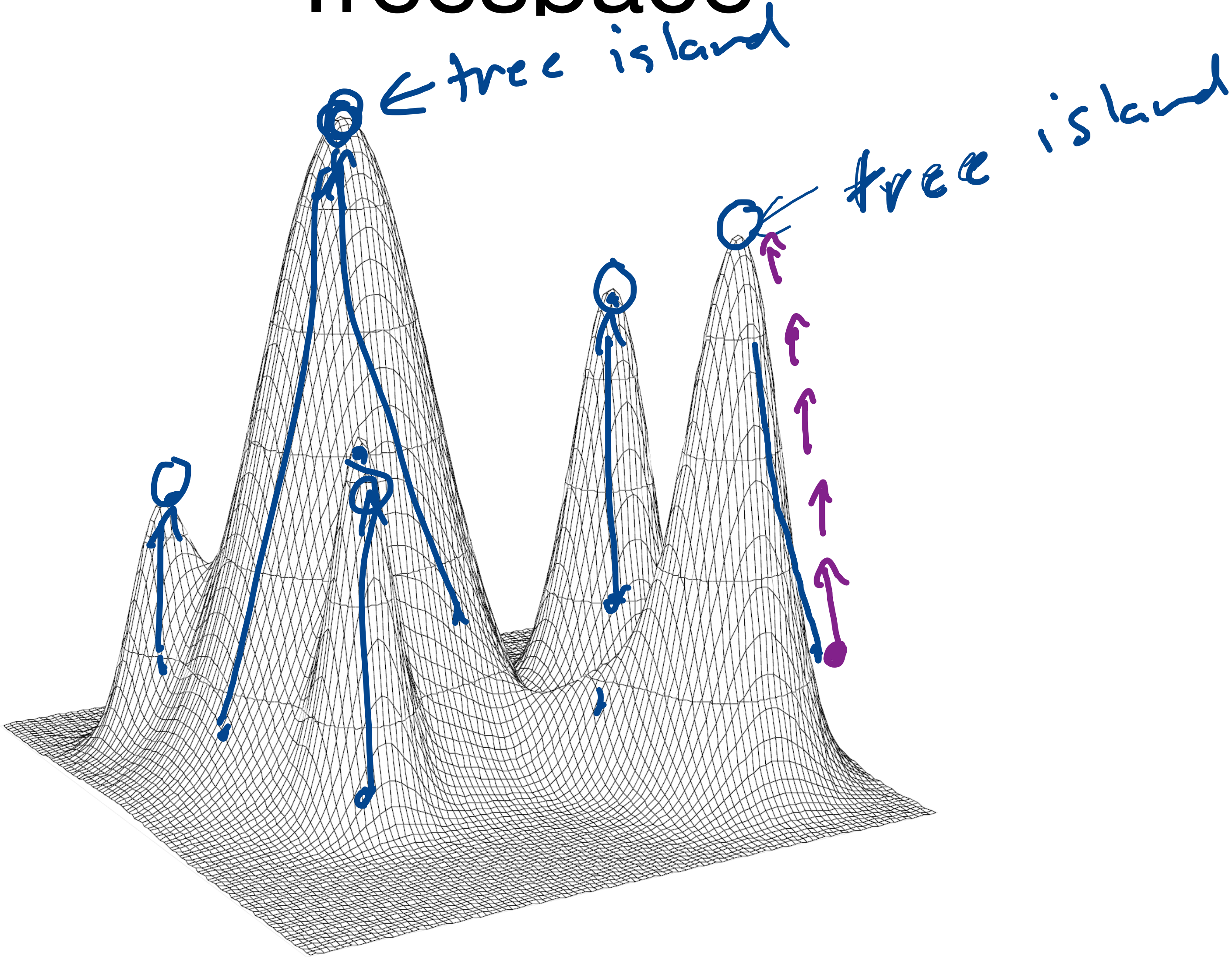


← At start, we know this tree has length 1982 steps



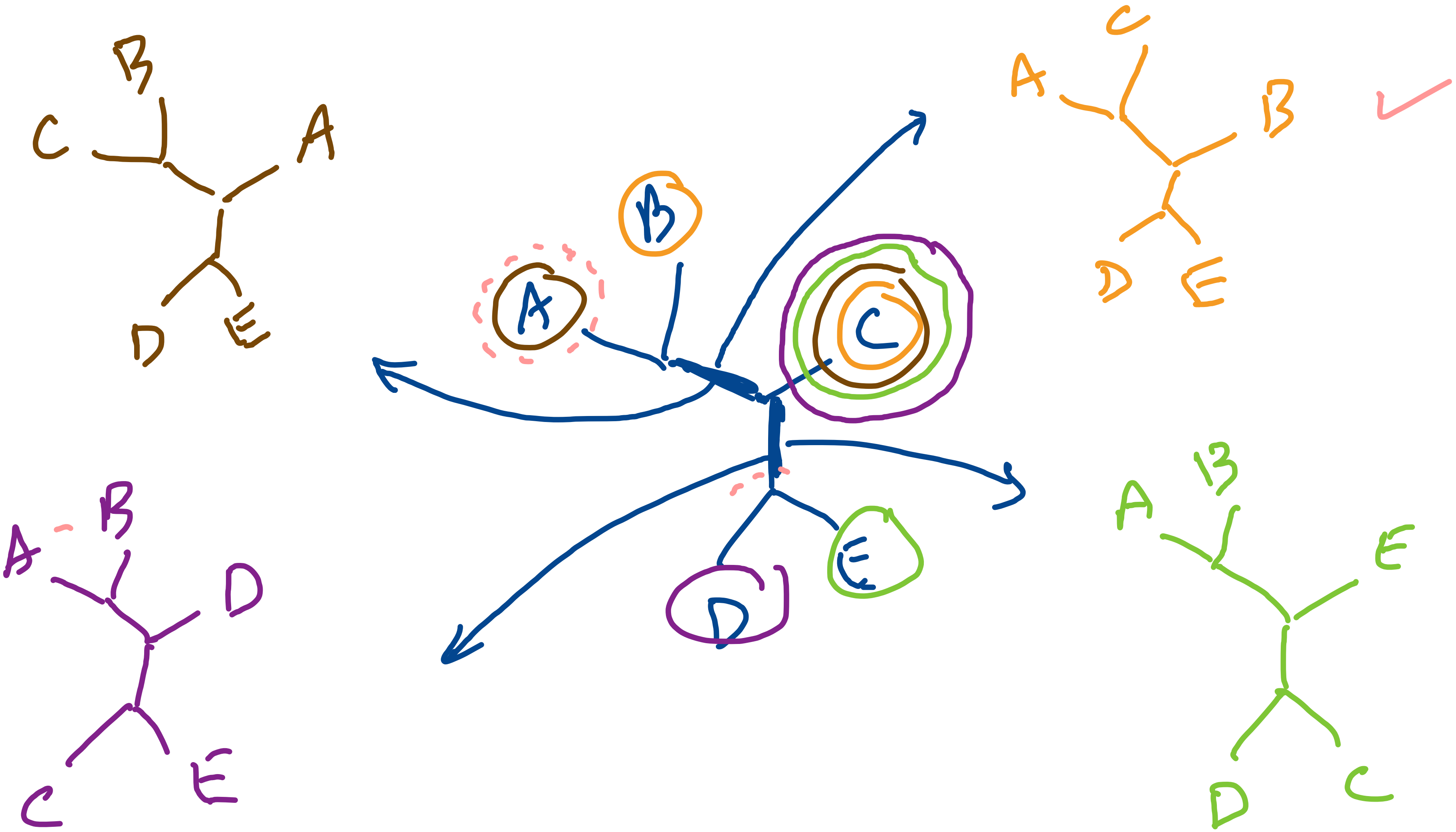
global optimum guaranteed

Treespace



STOPPED HERE 2024-01-23

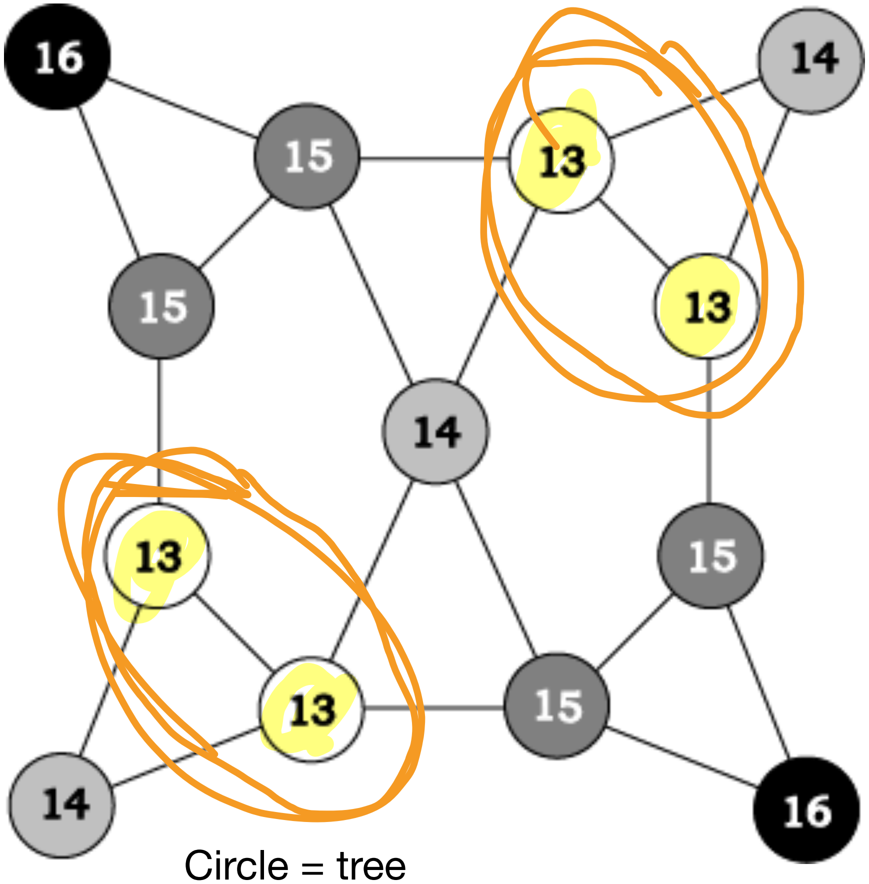
Heuristic search: NNI branch swapping



NNI = Nearest Neighbor Interchange

NNI islands

A line in this graph means that an NNI move between trees is possible



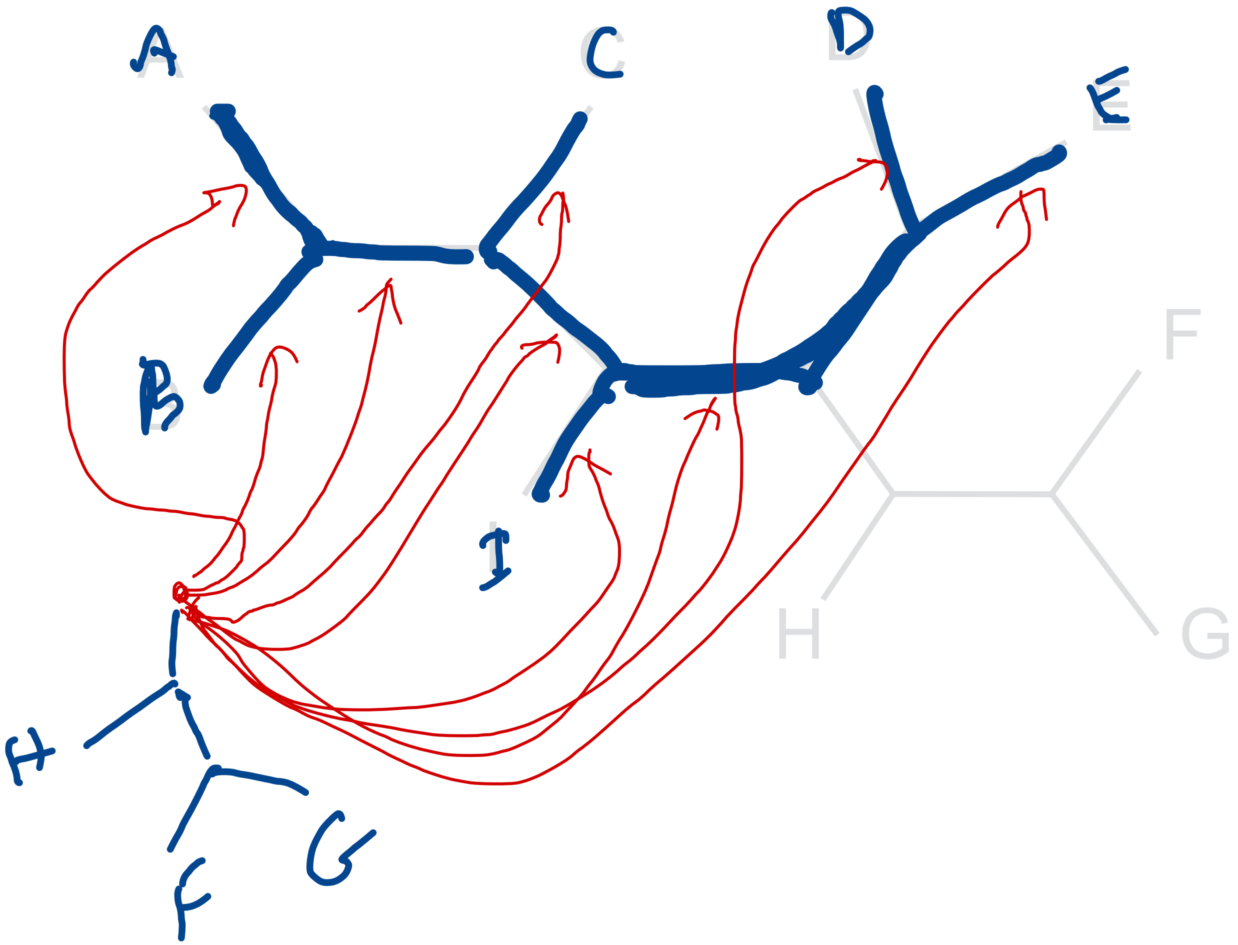
Circle = tree
Number = parsimony tree length
Note: 2 trees omitted for clarity

Sites

Taxa	1	2	3	4	5	6	7	8
A	**A**	**C**	**G**	**C**	**A**	**G**	**G**	**T**
B	**A**	**T**	**G**	**G**	**T**	**G**	**A**	**T**
C	**G**	**C**	**T**	**C**	**A**	**C**	**G**	**G**
D	**A**	**C**	**T**	**G**	**T**	**C**	**G**	**T**
E	**G**	**T**	**T**	**C**	**T**	**G**	**A**	**G**

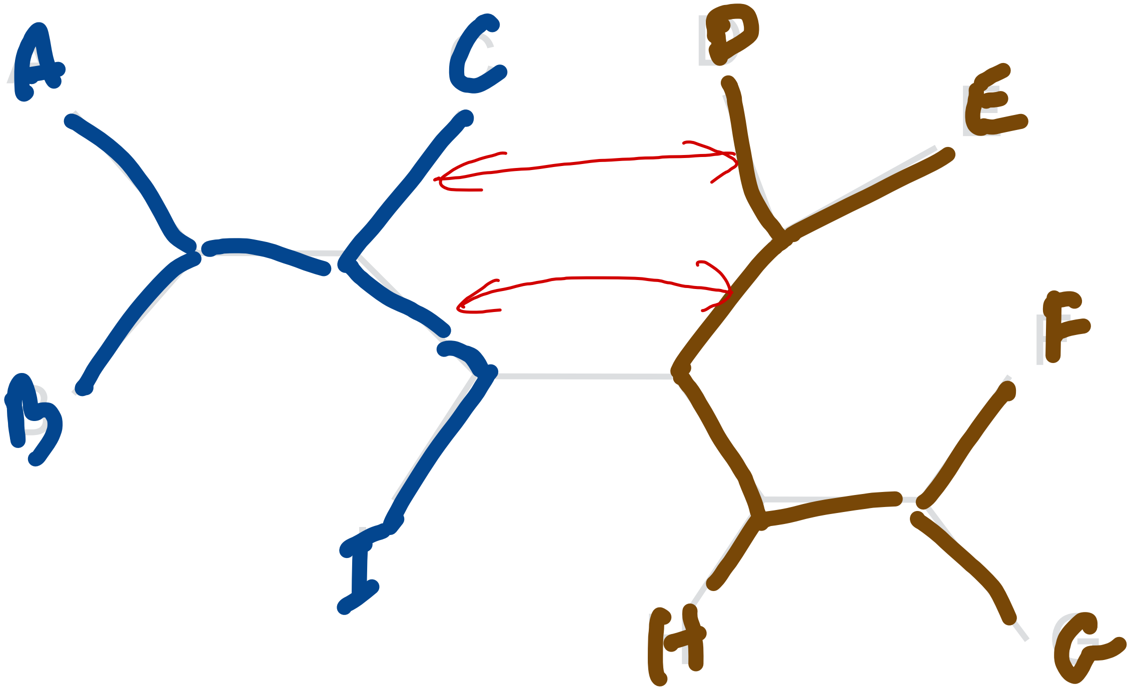
The (contrived) data above produces two NNI islands under parsimony.

Heuristic search: SPR branch swapping



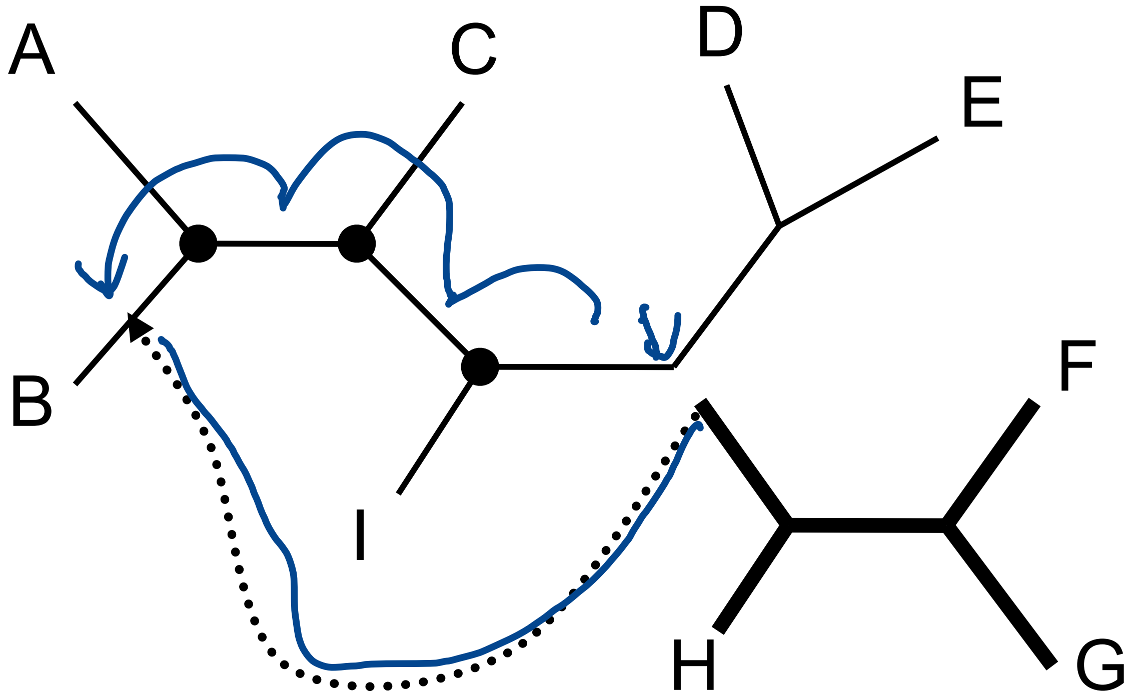
SPR = Subtree Pruning/Reconnection

Heuristic search: TBR branch swappng

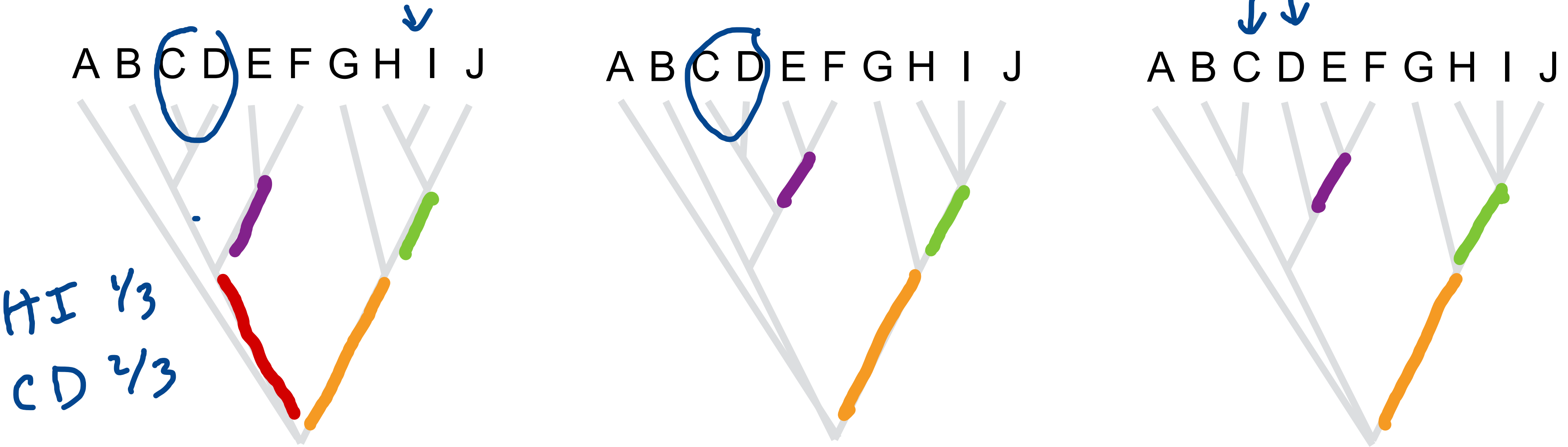


TBR = Tree Bisection/Reconnection

Reconnection Limit

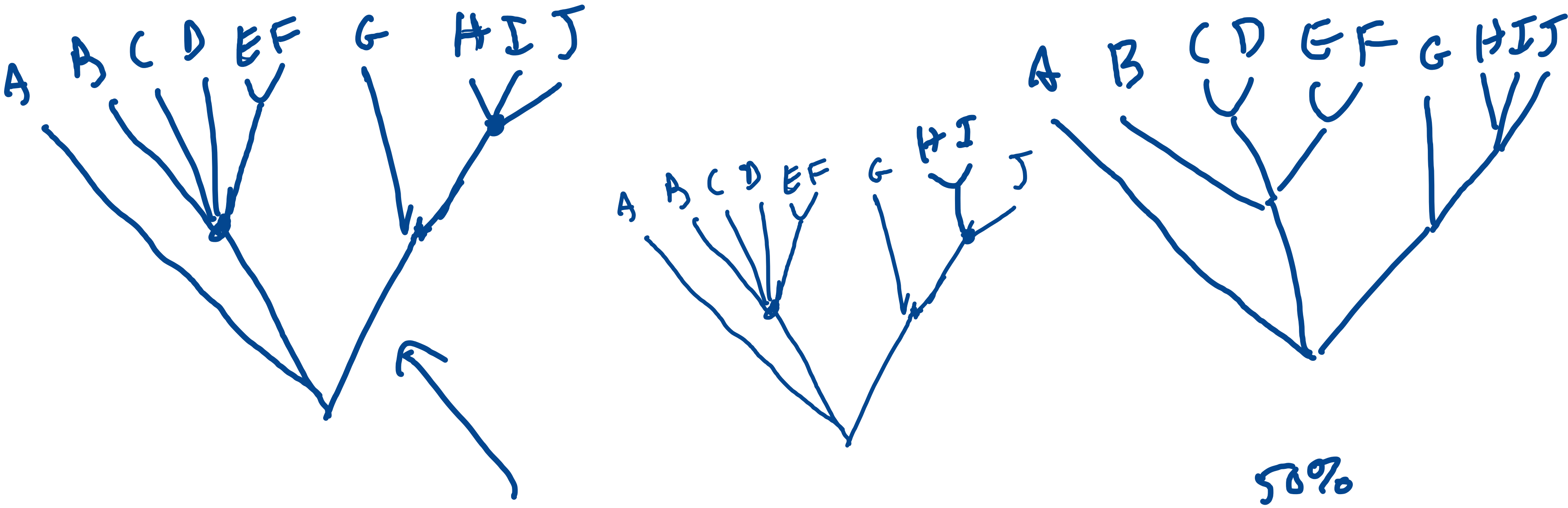


Consensus Trees



HI 1/3

CD 2/3



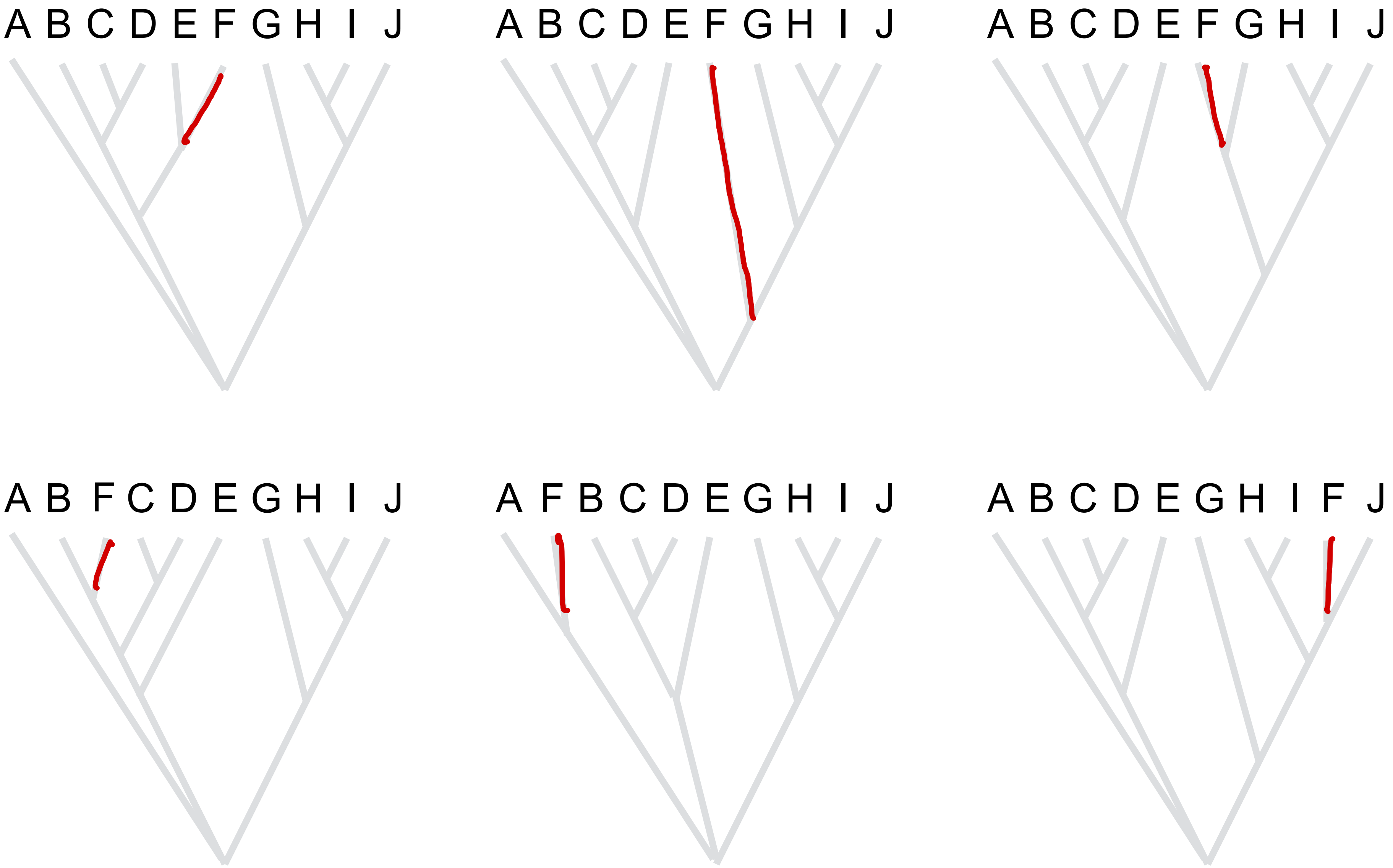
STRICT

SEMISTRICT

50%
MAJORITY
RULE

Maximum Agreement Subtree

F IS A "ROGUE" TAXON



PAUP* commands

If you want this...	then this is the command in PAUP*
Exhaustive enumeration	alltrees
Stepwise addition	hsearch swap=none start=stepwise addseq=random
Star decomposition	stardecomp
Neighbor-joining	nj
Branch-and-bound	bandb
NNI heuristic search	hsearch swap=nni
SPR heuristic search	hsearch swap=spr
TBR heuristic search	hsearch swap=tbr reconlimit=infinity
Semistrict consensus tree	contree all / strict=no semistrict
Majority-rule consensus tree	contree all / nostrict majrule percent=50
Maximum agreement subtree	agree all