Quiz Section Week 5
April 26, 2018

Review

Topics (not guaranteed to be comprehensive!)

- Alignments
  - Reasons to align sequences
  - Needleman-Wunsch algorithm
  - Smith-Waterman algorithm
  - Effects of parameter variation (including gap penalties)
  - Testing for statistical significance of an alignment
- Phylogenetic trees
  - Rooted and unrooted topologies
  - Defining the best tree with UPGMA and Neighbor Joining
  - Concept of parsimony
  - Fitch algorithm: quantifying how parsimonious a tree is, assigning internal states
  - Finding the most parsimonious tree: Hill climbing w/ Nearest-Neighbor interchanges
  - Bootstrapping to quantify confidence in tree partitions
- Clustering
  - Defining a clustering problem
  - Hierarchical clustering
    - Impact of using single/complete/average linkage
  - K-means: Objective and algorithm
- Networks
  - Reasons to make and analyze networks
  - Basic network definitions
  - Dijkstra's Algorithm
  - Network motifs and their uses

Topics (not guaranteed to be comprehensive!)

- Programming
  - Variables and types
  - String methods
  - List methods
  - Conditionals
  - Loops
  - Functions

Phylogenetic trees

UPGMA/Neighbor Joining

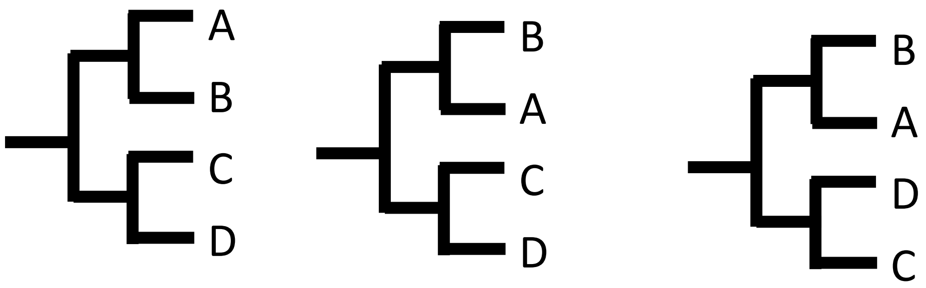
- Define the best tree: based on distance between leaves
- Find the best tree using: polynomial time algorithm to construct the best tree from a distance matrix

Parsimony approach

- Define the best tree: Minimum # of mutations required to traverse tree
- Find the best tree: by enumerating all trees (exhaustive search), or by heuristic approach like Nearest-Neighbor Interchange Hill-Climbing

Tree topologies

Are these the same tree?



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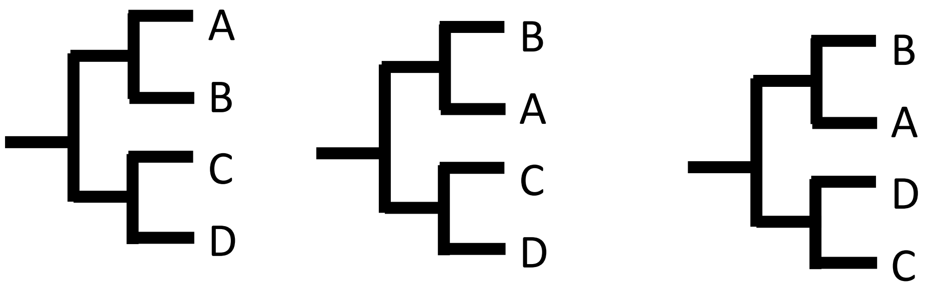
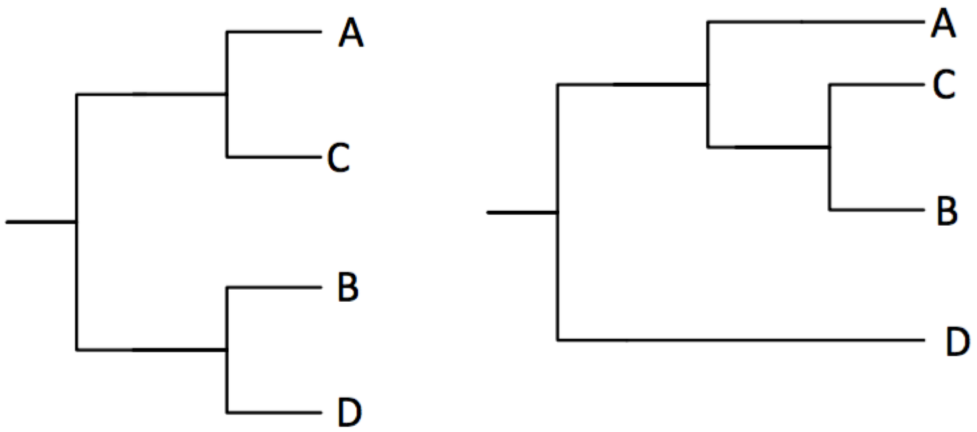


How about these?

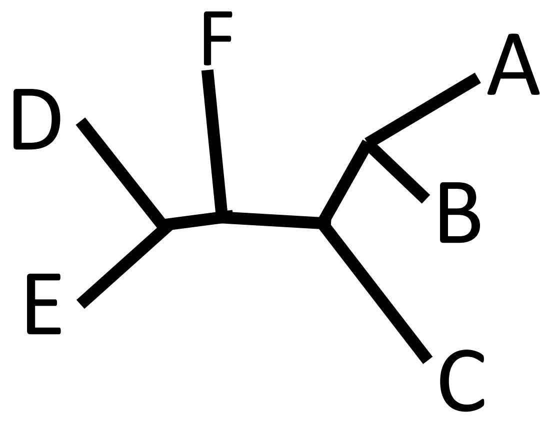


Counting tree topologies

For N leaves

# of unrooted topologies = 3*5*7*…*(2N-5)
# of branches = 2N-3

E.g. an unrooted tree with 6 nodes



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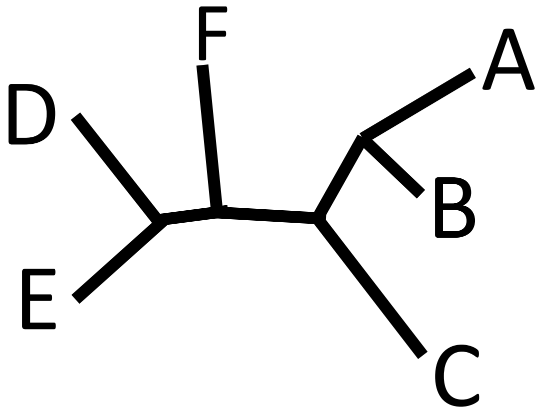

How many different topologies?
3*5*7 = **105**

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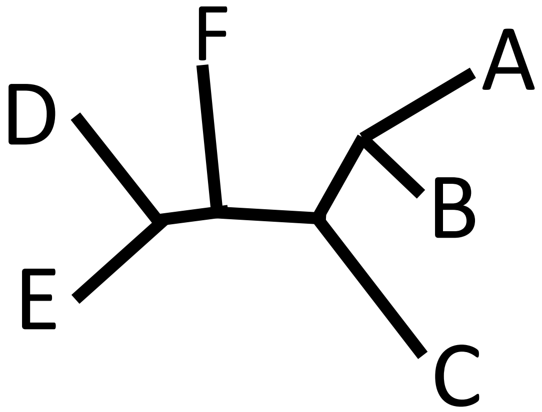

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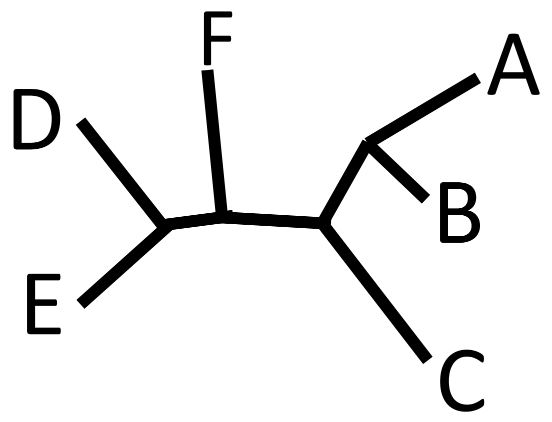

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How many branches?
2N-3 = **9**

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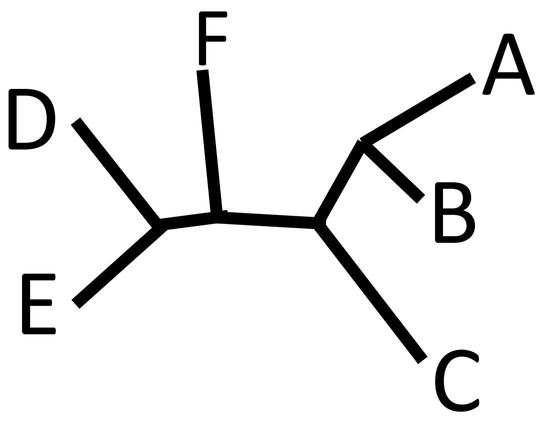

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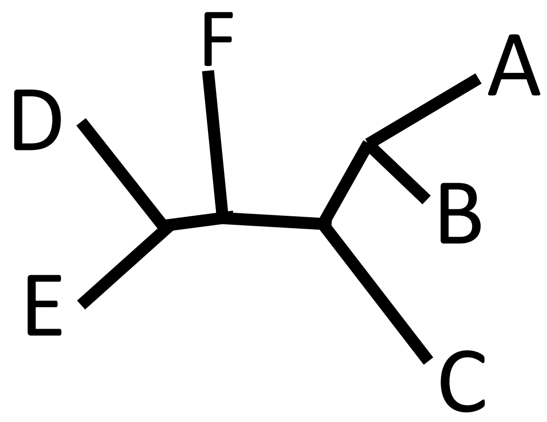

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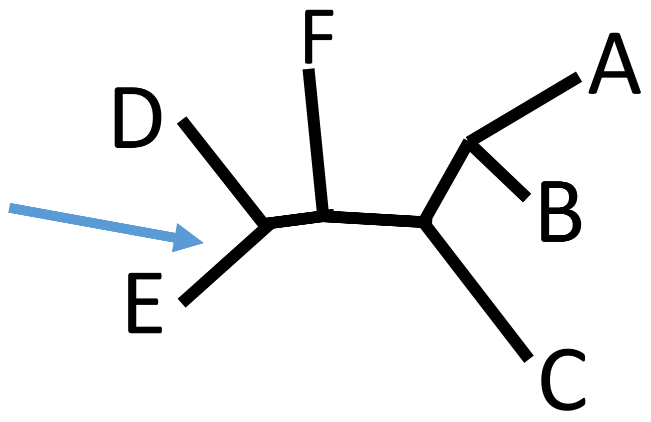

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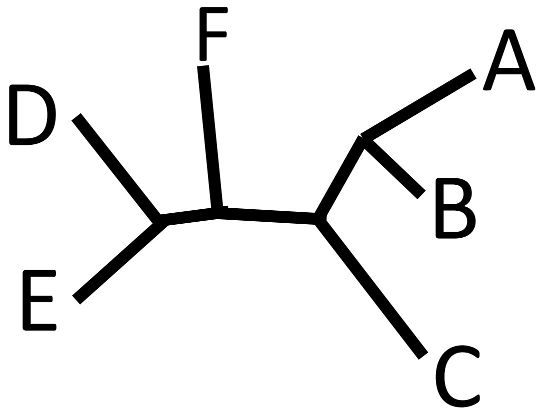

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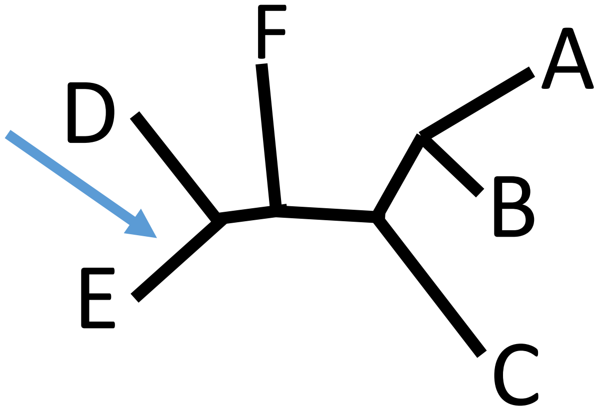
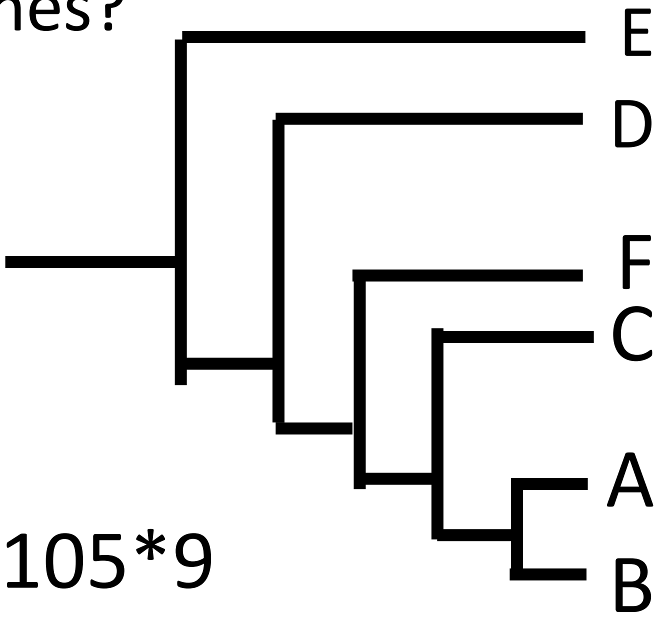
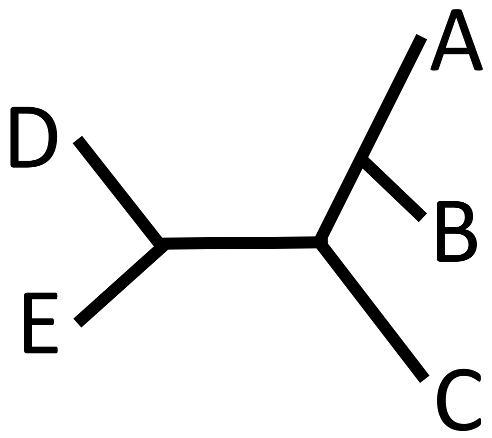




Total options = 105*9
= 945

Nearest Neighbor Interchange trees

For each internal branch generate two variant trees that swap the relationships of the four outside branches



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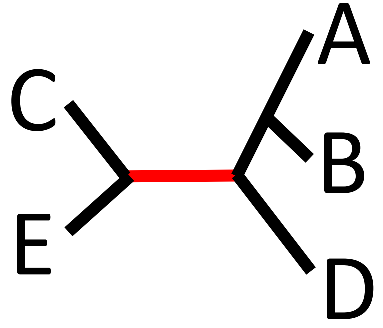

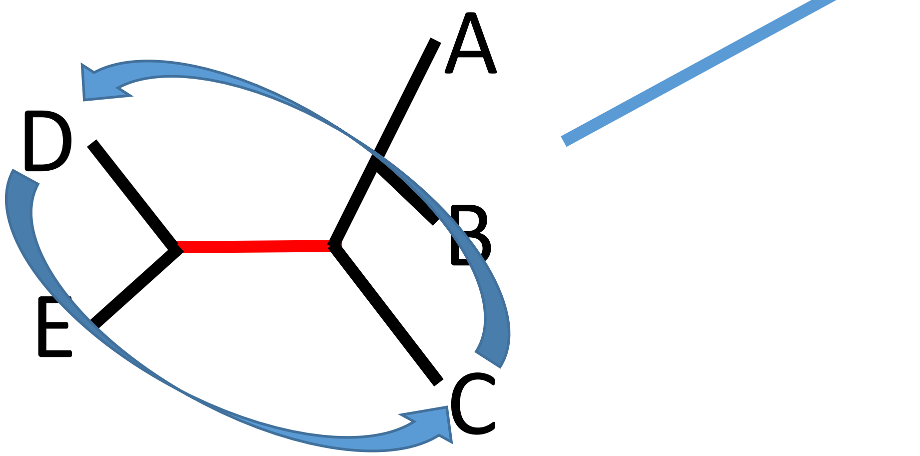

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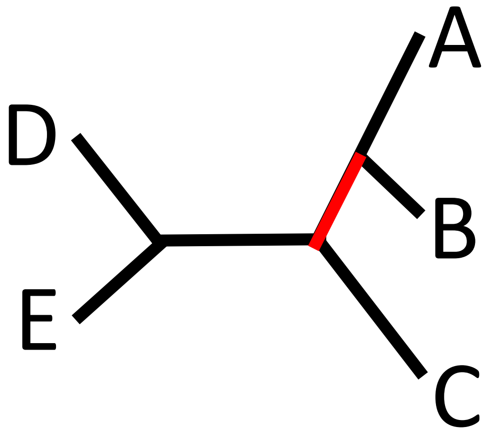

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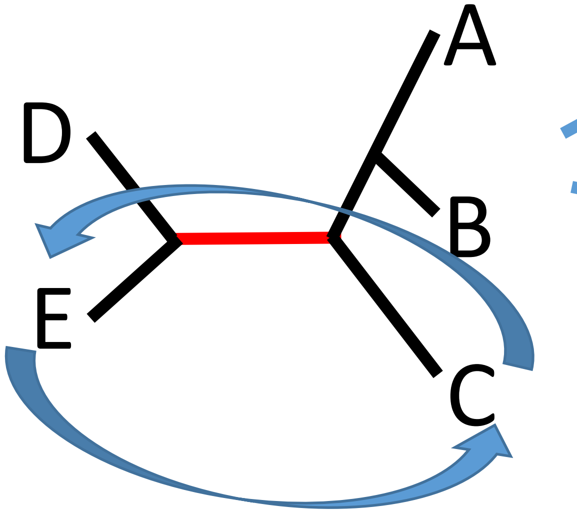

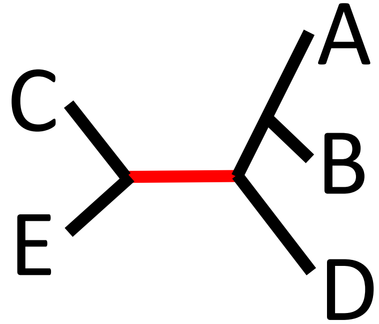

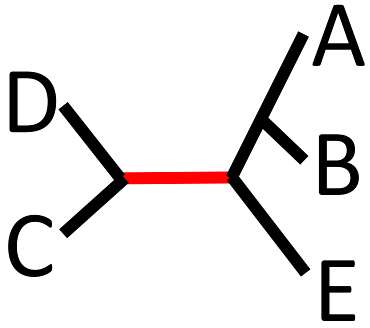

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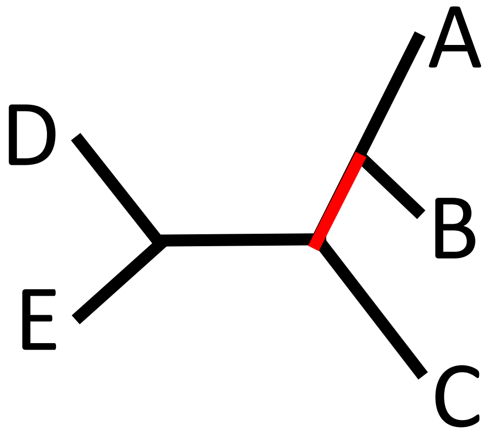

Nearest Neighbor Interchange trees

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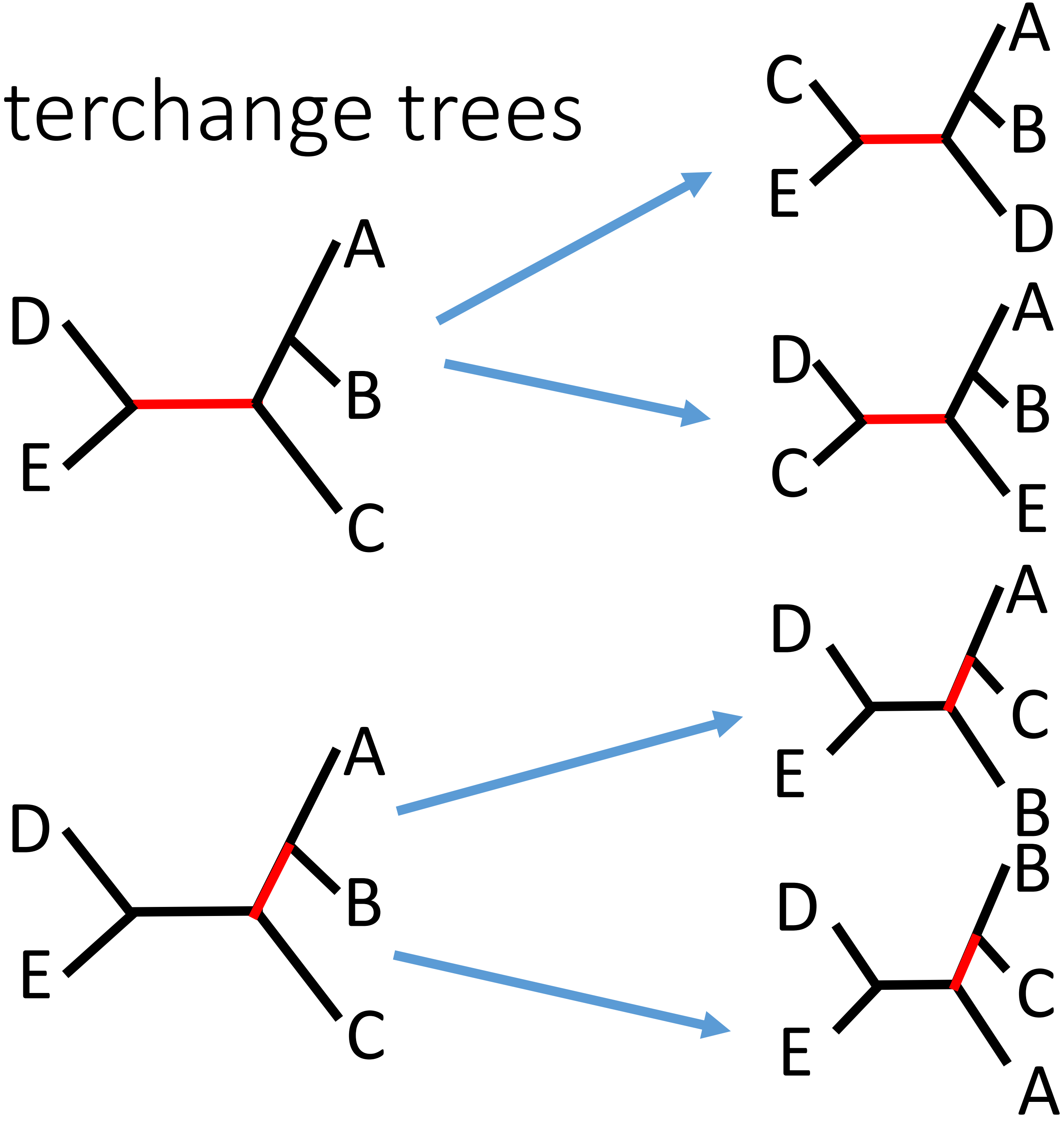
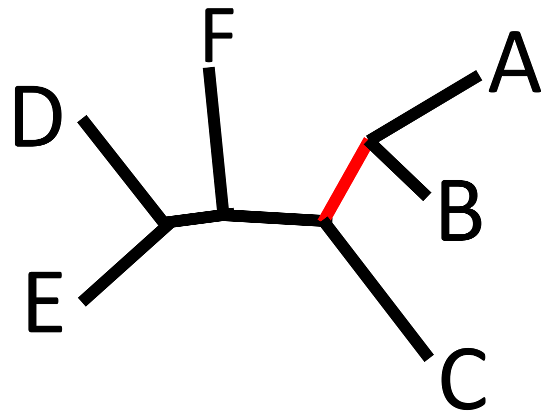


NN Practice: Draw both interchanges from swapping this branch



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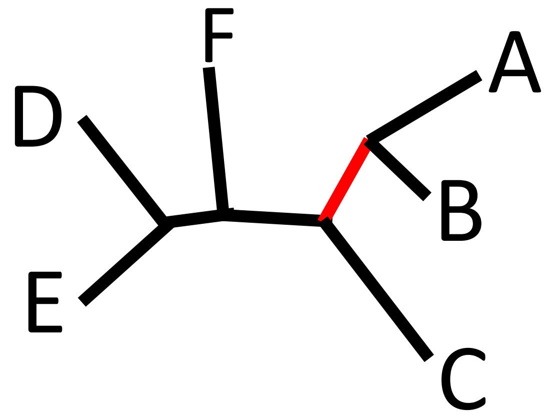
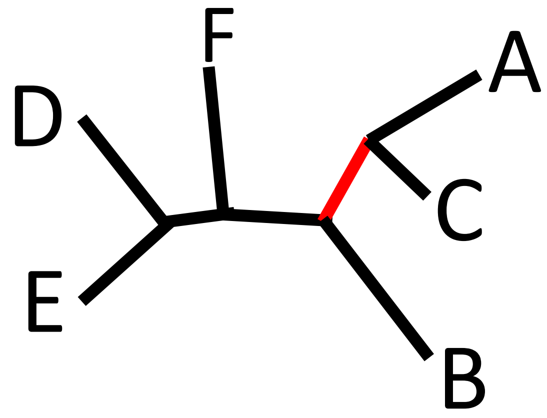
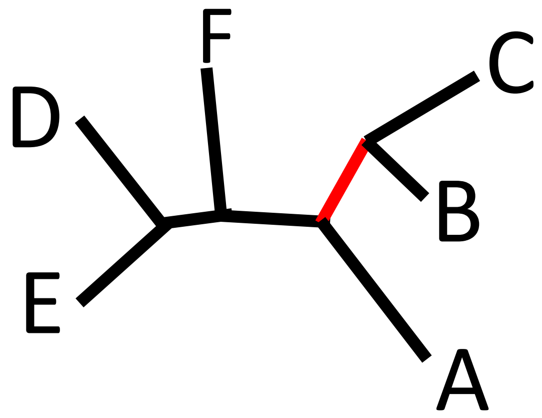
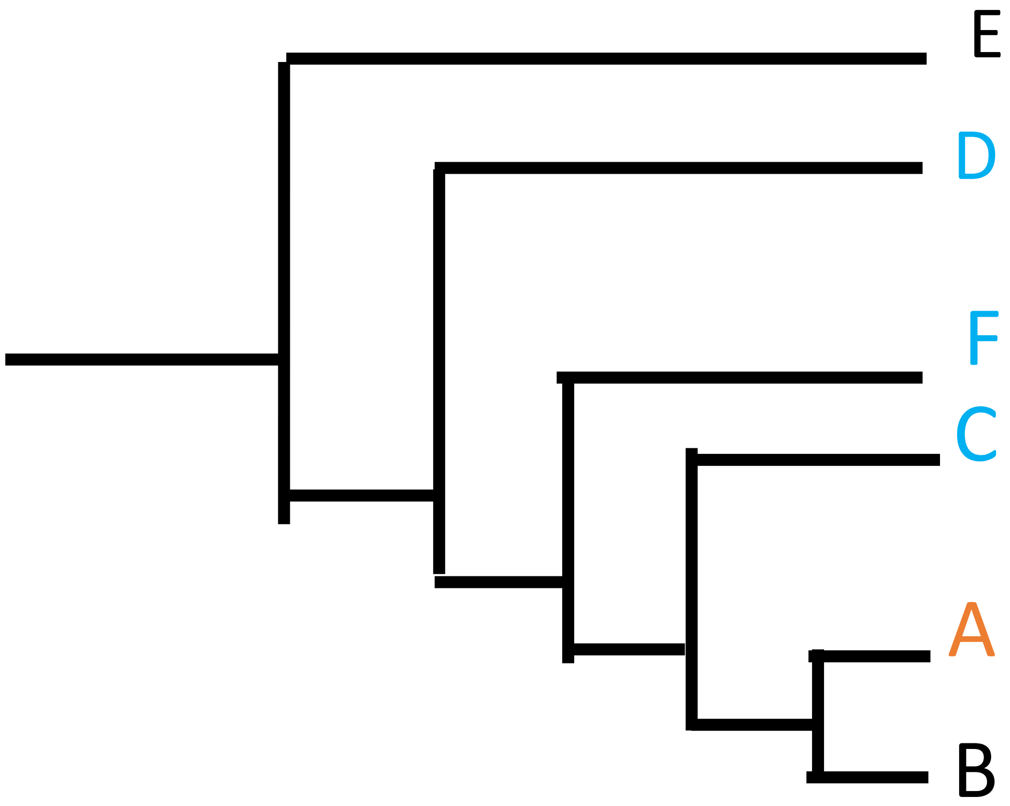


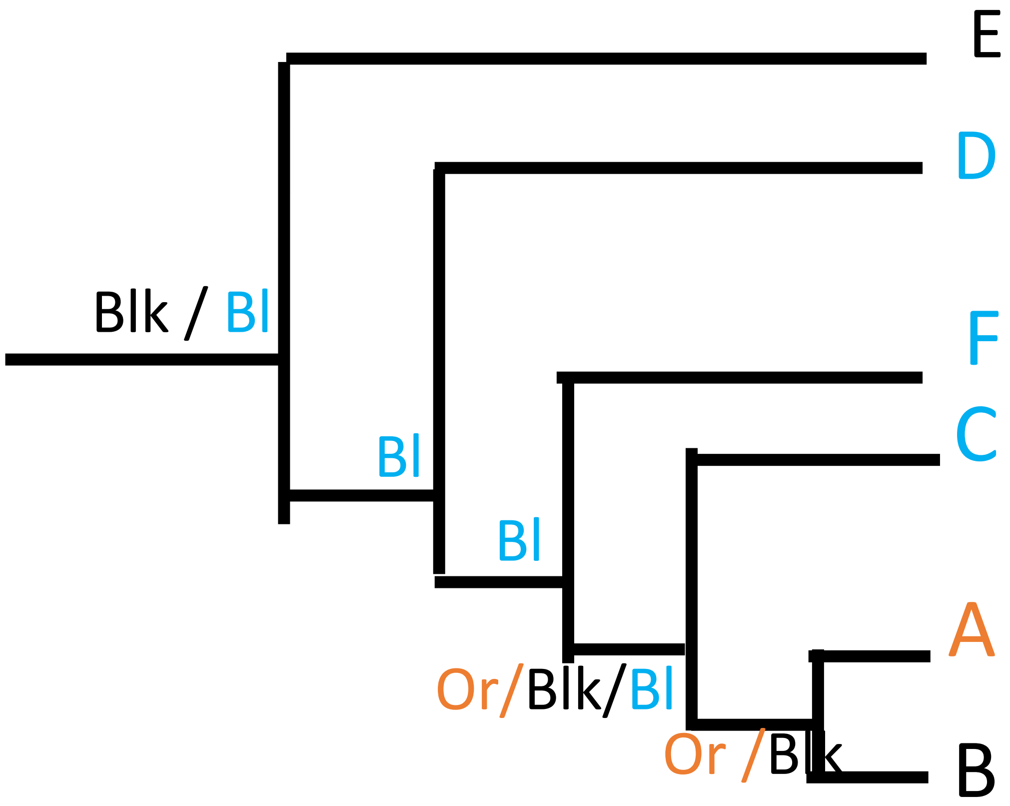




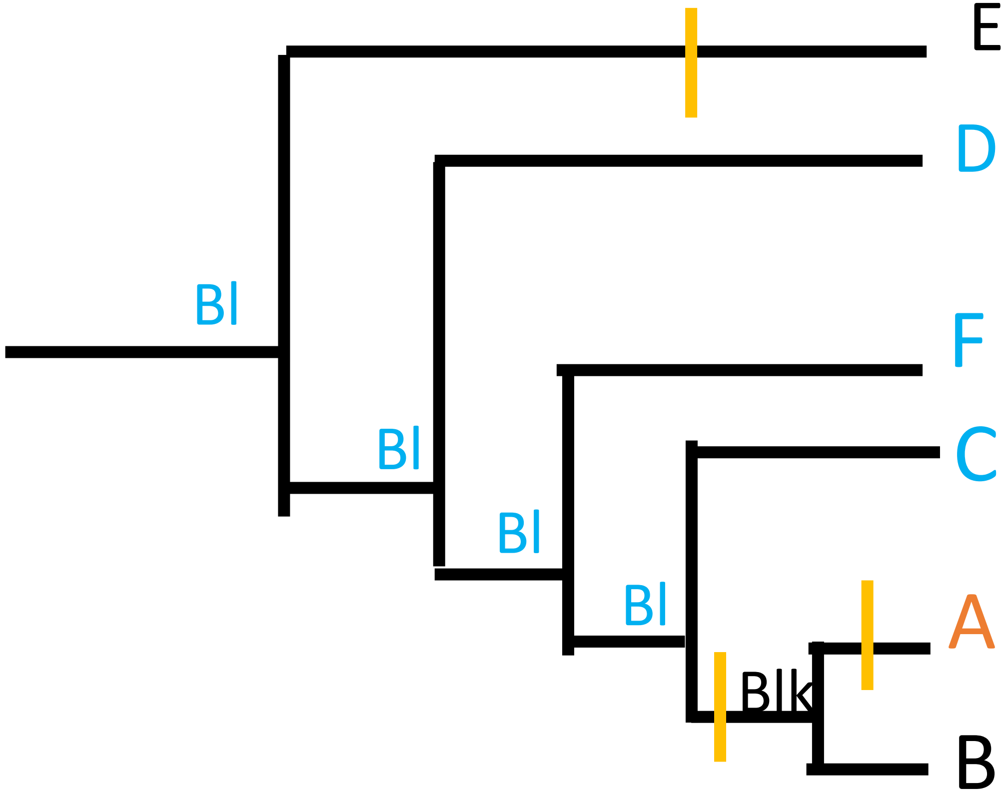
Fitch algorithm practice



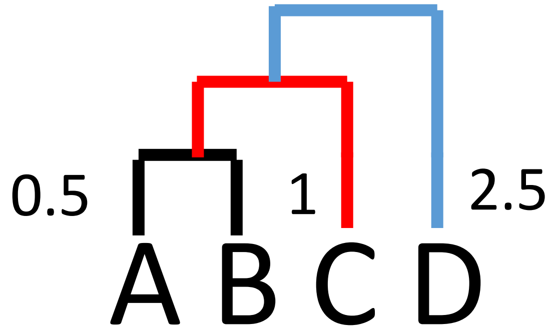
Fitch algorithm practice: bottom-up



Fitch algorithm practice: top-down



Hierarchical clustering with complete linkage example

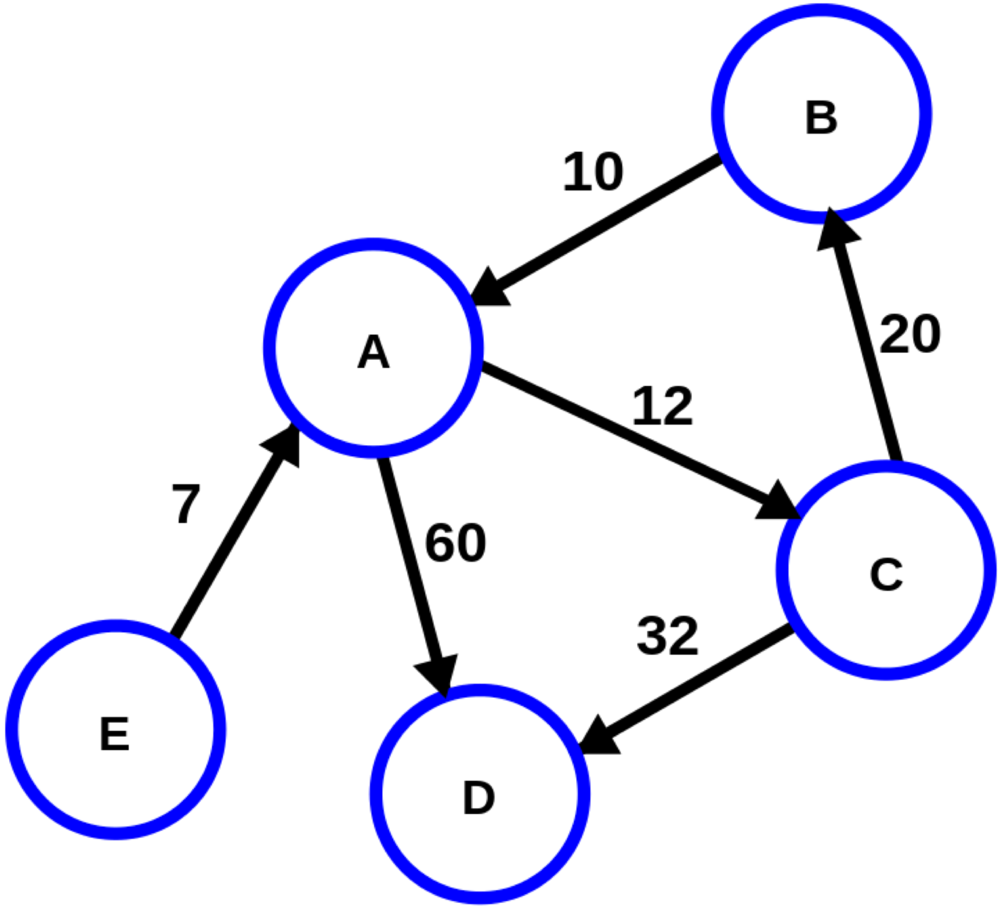


	A	B	C	D
A	0	1	2	4
B	1	0	2	5
C	2	2	0	5
D	4	5	5	0

	A,B	C	D
A,B	0	2	5
C	2	0	5
D	5	5	0

	A,B,C	D
A,B,C	0	5
D	5	0

Dijkstra’s Algorithm



Another data type: Dictionaries

- a data structure that consists of an unordered set of *key: value* pairs
  - think of as *word: definition* pairs!

Q: How could we encode the entire genetic code?

https://docs.python.org/3/tutorial/datastructures.html

Dictionaries: How could we encode the entire genetic code?

```
>>> genetic_code = {"ATG": "Start", "TGA": "Stop", "TAG":
"Stop"}
>>> genetic_code["TAA"] = "Stop"
>>> genetic_code.get("TGA")
'Stop'
>>> genetic_code["TGA"]
'Stop'
>>> genetic_code.get("sss") #nothing or 'None' if not defined
>>> genetic_code["sss"]
KeyError: 'ttt'
```

https://docs.python.org/3/tutorial/datastructures.html

Creating a dictionary

```
#create an empty dictionary
myDict = {}

#create a dictionary with three entries
myDict = {"Curly":4123, "Larry":2057, "Moe":1122}

#add another entry
myDict["Shemp"] = 2232

#change Moe's phone number
myDict["Moe"] = 4040

#delete Moe from dictionary
del myDict["Moe"]
```

Rules for dictionaries

- The first item is a key.

- Each key can appear only once in a dict.

- A key must be an immutable object: number, string, or tuple.

- Lists cannot be keys (they are mutable).

- The key is the item you'll use to do look-ups.

- Each key is paired with a value.

Some useful dictionary methods

```
>>> genetic_code.items()
[('TAA', 'Stop'), ('TGA', 'Stop'), ('TAG', 'Stop'),
('ATG', 'Start')]
>>> genetic_code.keys()
['TAA', 'TGA', 'TAG', 'ATG']
>>> genetic_code.values()
['Stop', 'Stop', 'Stop', 'Start']
```

Another use of dictionaries: store counts of named elements

Example: Calculate # of each nucleotide in a sequence

```
sequence = "GACCCT"
nuc_counts = {'A': 0, 'C': 0, 'T':0, 'G': 0}
for nuc in sequence:
     #Add to the count for the given nucleotide
```

Another common use of dictionaries: store counts of named elements

Calculate # of each nucleotide in a sequence

```
sequence = "GACCCT"
nuc_counts = {'A': 0, 'C': 0, 'T':0, 'G': 0}
for nuc in sequence:
    nuc_counts[nuc] = nuc_counts[nuc] + 1
```

Traversing a dictionary by key

```
# birthdays is a dictionary with names as keys
# and birth dates as values


for person in birthdays.keys():
    print "Send", person, "a card on", birthdays[person]
```

dictionary basics

```
D = {'dna':'T','rna':'U'}    # dictionary literal assignment
D = {}                       # make an empty dictionary
D.keys()                     # get the keys as a list
D.values()                   # get the values as a list
D['dna']                     # get a value based on key
D['dna'] = 'T'               # set a key:value pair
del D['dna']                 # delete a key:value pair
'dna' in D                   # True if key 'dna' is found in D, else False
```

The keys must be immutable objects (e.g. string, int, tuple).

The values can be anything (including a list or another dictionary).

The order of elements in the list returned by **D.keys()** or **D.values()** is arbitrary (effectively random).

Each key can be stored only once in the dictionary, so if you set the value for a key for a second time it OVERWRITES the old value!