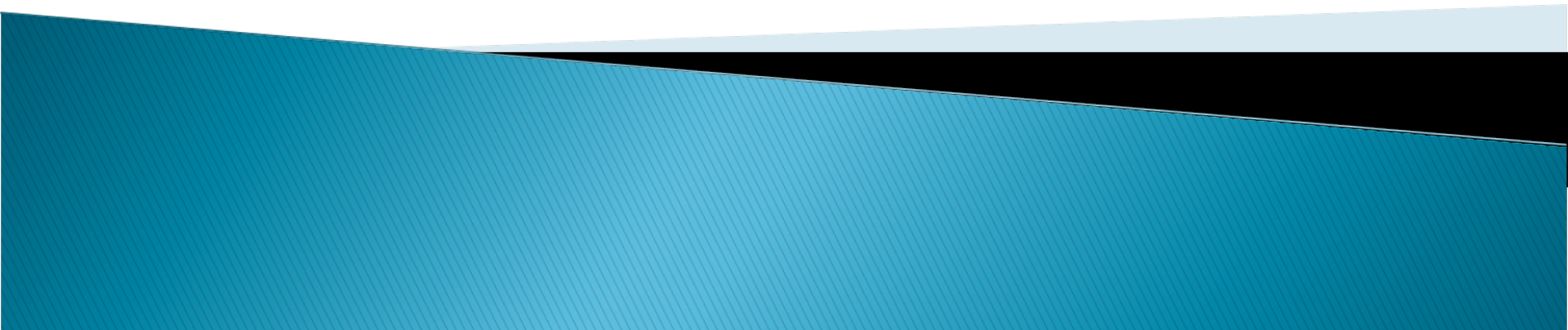


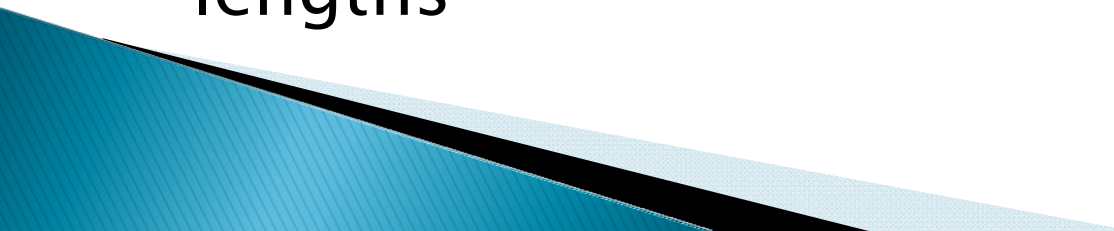
Neighbor Joining Method

Karthik Pasupathy R

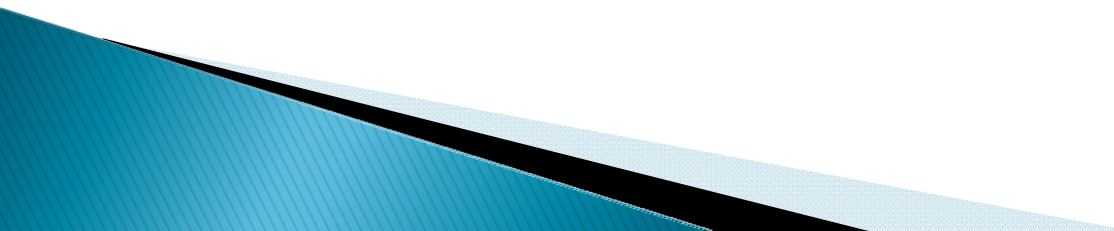
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What is NJ method?

- ▶ Nj method is a clustering approach for the reconstruction of phylogenetic trees
 - ▶ It is based on the ST method (Sattath and Tversky) method of tree construction
 - ▶ The input is the 'n' number of taxa
 - ▶ The output is an unrooted tree with branched lengths
- 

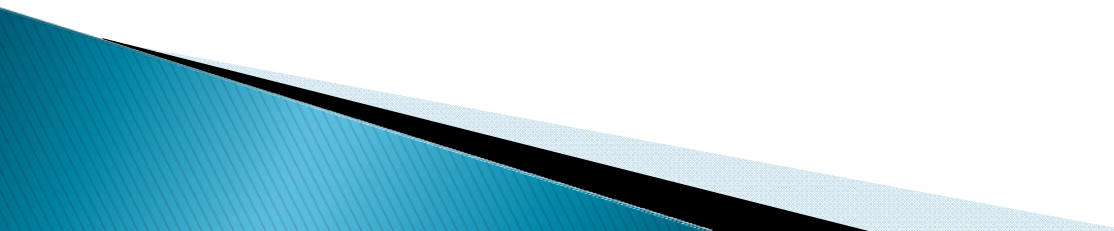
Other algorithms

- ▶ Distance Wagner method
 - ▶ Modified Farris method (FM)
 - ▶ Sattath and Tversky method (ST)
 - ▶ Fitch method
- 

ST method vs NJ method

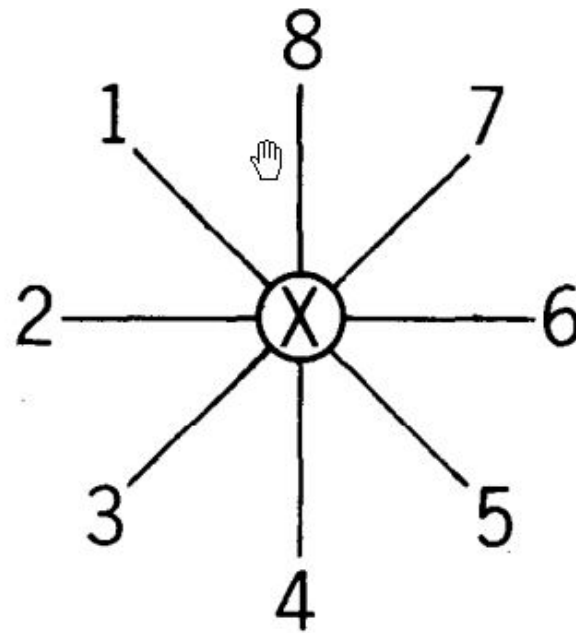
- ▶ In ST method , the objective of the algorithm is to construct the topology of a phylogenetic tree.
- ▶ NJ method not only provides topology but also provides final tree with branched lengths

Algorithm

- ▶ Construct a unresolved tree with star topology
 - ▶ Construct a Distance matrix and calculate the value of S_a , S_b , S_c S_n
 - ▶ Group neighbors based on distance
 - ▶ Repeat the steps until you get the final tree
- 

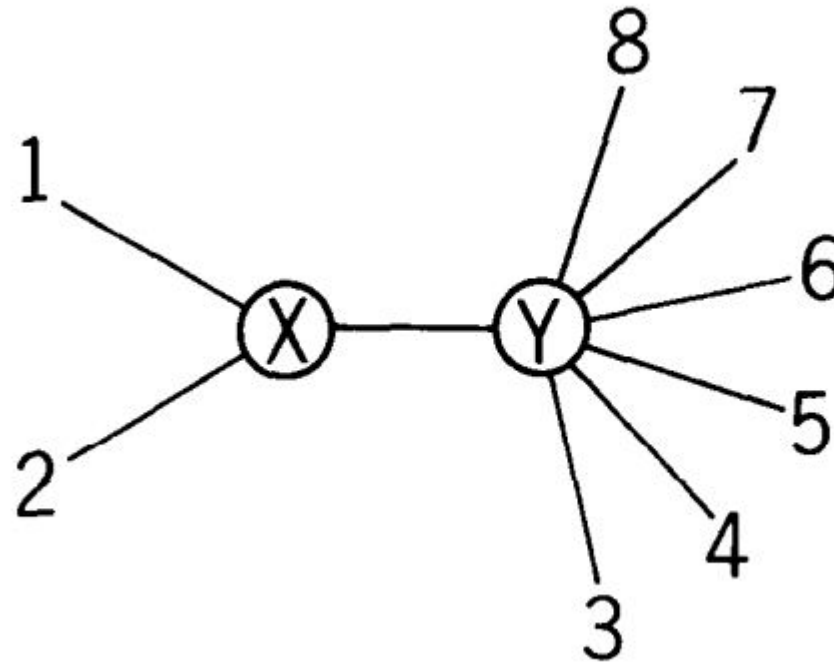
Algorithm

- ▶ construct an unresolved tree with star topology



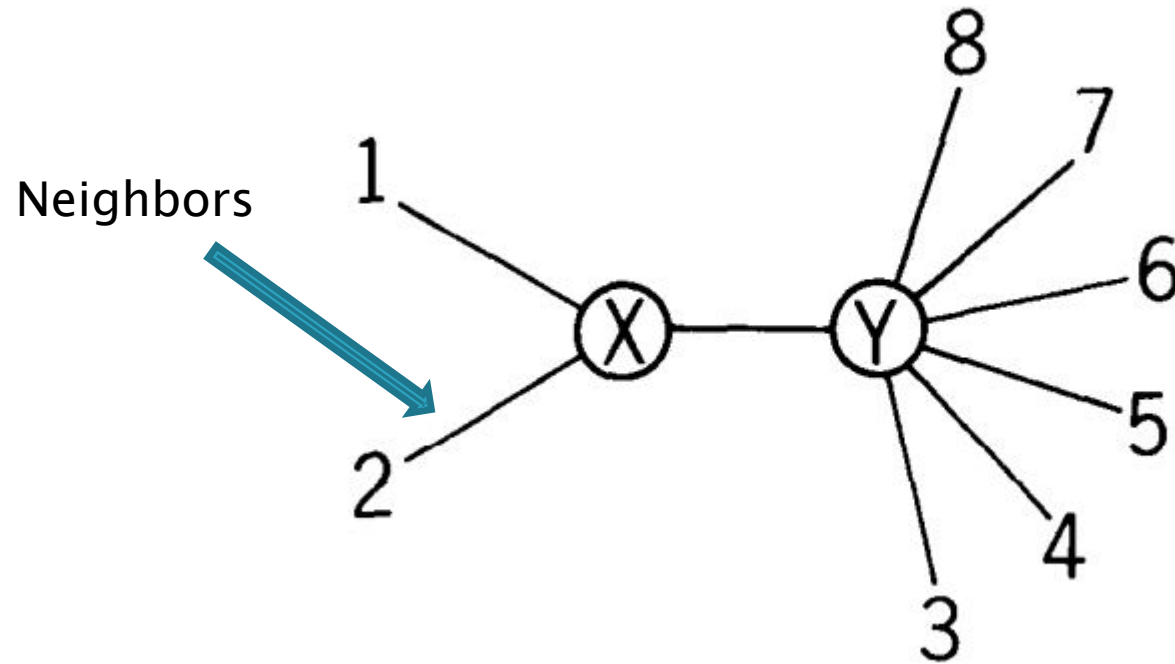
Algorithm

- ▶ Join the closest neighbors (OTUs with similar characters)



Algorithm

- ▶ Join the closest neighbors (OTUs with similar characters)



Distance matrix

| | A | B | C | D | E |
|---|---|----|---|---|---|
| B | 5 | | | | |
| C | 4 | 7 | | | |
| D | 7 | 10 | 7 | | |
| E | 6 | 9 | 6 | 5 | |
| F | 8 | 11 | 8 | 9 | 8 |

| | U ₁ | C | D | E |
|---|----------------|---|---|---|
| C | 3 | | | |
| D | 6 | 7 | | |
| E | 5 | 6 | 5 | |
| F | 7 | 8 | 9 | 8 |

| | U ₁ | C | U ₂ |
|----------------|----------------|---|----------------|
| C | 3 | | |
| U ₂ | 3 | 4 | |
| F | 7 | 8 | 6 |

| | U ₂ | U ₃ |
|----------------|----------------|----------------|
| U ₃ | 2 | |
| F | 6 | 6 |

| | U ₄ |
|---|----------------|
| F | 5 |

Step 1

S calculations

$$S_A = (5+4+7+6+8)/4 = 7.5$$

$$S_B = (5+7+10+9+11)/4 = 10.5$$

$$S_C = (4+7+7+6+8)/4 = 8$$

$$S_D = (7+10+7+5+9)/4 = 9.5$$

$$S_E = (6+9+6+5+8)/4 = 8.5$$

$$S_F = (8+11+8+9+8)/4 = 11$$

$$S_{U_1} = (3+6+5+7)/3 = 7$$

$$S_C = (3+7+6+8)/3 = 8$$

$$S_D = (6+7+5+9)/3 = 9$$

$$S_E = (5+6+5+8)/3 = 8$$

$$S_F = (7+8+9+8)/3 = 10.6$$

$$S_{U_1} = (3+3+7)/2 = 6.5$$

$$S_C = (3+4+8)/2 = 7.5$$

$$S_{U_2} = (3+4+6)/2 = 6.5$$

$$S_F = (7+8+6)/2 = 10.5$$

$$S_{U_2} = (2+6)/1 = 8$$

$$S_{U_3} = (2+6)/1 = 8$$

$$S_F = (6+6)/1 = 12$$

Because $N - 2 = 0$,
we cannot do this
calculation.

$S_x = (\text{sum all } D_{ix})/(N - 2)$,
where N is the # of
OTUs in the set.

Step 2

Calculate pair with
smallest (M), where
 $M_{ij} = D_{ij} - S_i - S_j$.

Smallest are

$$M_{AB} = 5 - 7.5 - 10.5 = -13$$

$$M_{DE} = 5 - 9.5 - 8.5 = -13$$

Choose one of these (AB here).

Smallest is

$$M_{CU_1} = 3 - 7 - 8 = -12$$

$$M_{DE} = 5 - 9 - 8 = -12$$

Choose one of these (DE here).

Smallest is

$$M_{CU_1} = 3 - 6.5 - 7.5 = -11$$

Smallest is

$$M_{U_2F} = 6 - 8 - 12 = -14$$

$$M_{U_3F} = 6 - 8 - 12 = -14$$

$$M_{U_2U_3} = 2 - 8 - 8 = -14$$

Choose one of these ($M_{U_2U_3}$ here).

Step 3

Create a node (U) that
joins pair with lowest
 M_{ij} such that
 $S_U = D_{ij}/2 + (S_i - S_j)/2$.

U_1 joins A and B:

$$S_{AU_1} = D_{AB}/2 + (S_A - S_B)/2 = 1$$

$$S_{BU_1} = D_{AB}/2 + (S_B - S_A)/2 = 4$$

U_2 joins D and E:

$$S_{DU_2} = D_{DE}/2 + (S_D - S_E)/2 = 3$$

$$S_{EU_2} = D_{DE}/2 + (S_E - S_D)/2 = 2$$

U_3 joins C and U_1 :

$$S_{CU_3} = D_{CU_1}/2 + (S_C - S_{U_1})/2 = 2$$

$$S_{U_1U_3} = D_{CU_1}/2 + (S_{U_1} - S_C)/2 = 1$$

U_4 joins U_2 and U_3 :

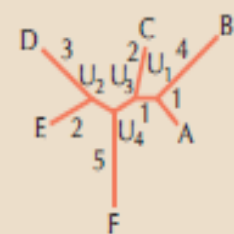
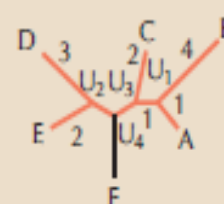
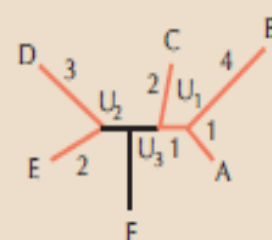
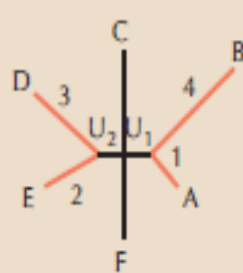
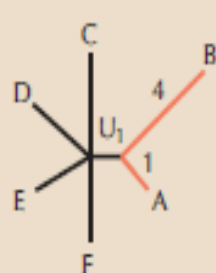
$$S_{U_2U_4} = D_{U_2U_3}/2 + (S_{U_2} - S_{U_3})/2 = 1$$

$$S_{U_3U_4} = D_{U_2U_3}/2 + (S_{U_3} - S_{U_2})/2 = 1$$

For last pair, connect
 U_4 and F with branch
length = 5.

Step 4

Join i and j according to S
above and make all
other taxa in form of
a star. Branches in black
are of unknown length.
Branches in red are of
known length.



Step 5

Calculate new distance
matrix of all other taxa
to U with

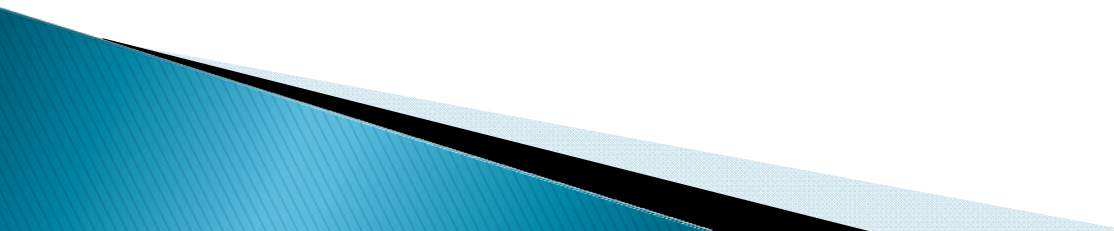
$$D_{xU} = D_{ix} + D_{jx} - D_{ij}$$

where i and j are those


Comments

Note this is the same
tree we started with
(drawn in unrooted
form here).

Advantages

- ▶ Provides sub-optimal solution that is close to the optimal tree
 - ▶ Faster tree Building method
 - ▶ It is a polynomial – time algorithm. So it can also be used for large data sets
 - ▶ Statistically consistent
- 

Disadvantages

- ▶ Cannot find common ancestor as the final output is an unrooted tree
 - ▶ Tests only a single tree
 - ▶ May not find true topology since it is a greedy algorithm
 - ▶ Intermediate ancestors can be ignored (as it does not follow step by step approach)
- 

References

- ▶ The Neighbor-joining Method: A New Method for Reconstructing Phylogenetic Tree
Naruya Saitou² and Masatoshi Nei ; Mol. Biol. Evol. 4(4):406–425.1987.
- ▶ <http://mbe.oxfordjournals.org/content/4/4/406.long>
- ▶ http://en.wikipedia.org/wiki/Neighbor_joining
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- ▶ http://www.megasoftware.net/mega3/WebHelp/phylogenetictrees_rh/rh_neighbor_joining_method.htm

THANK YOU