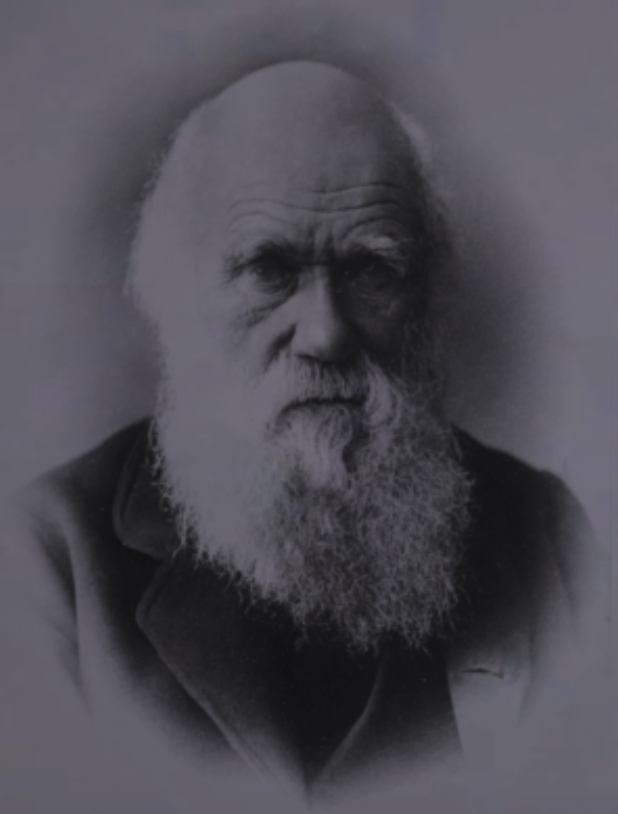
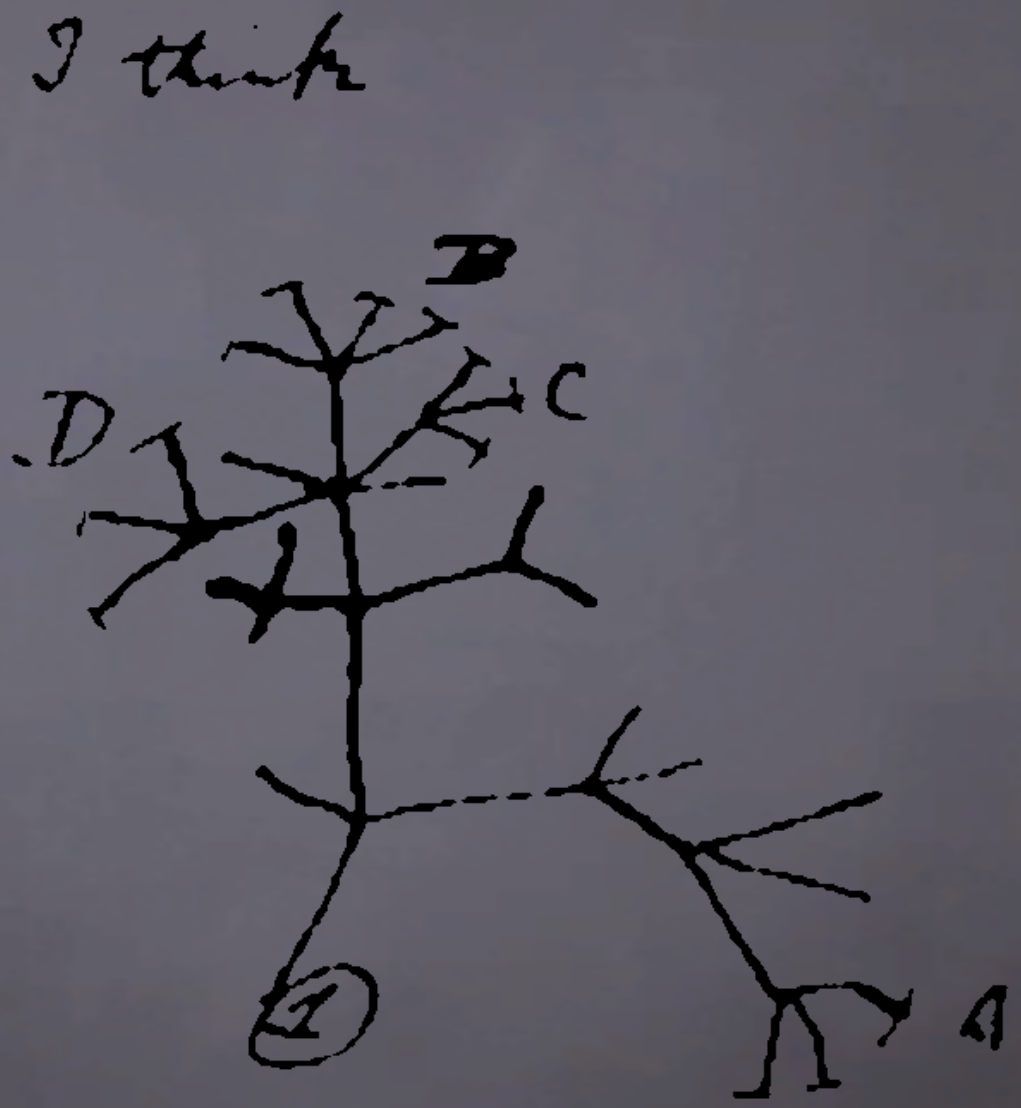
Lecture: Algorithmic Bioinformatics

Doctoral School, Université Dauphine, 2022

Some slides graciously provided by Daniel Huson & Celine Scornavacca

Phylogenetic Trees - Motivation





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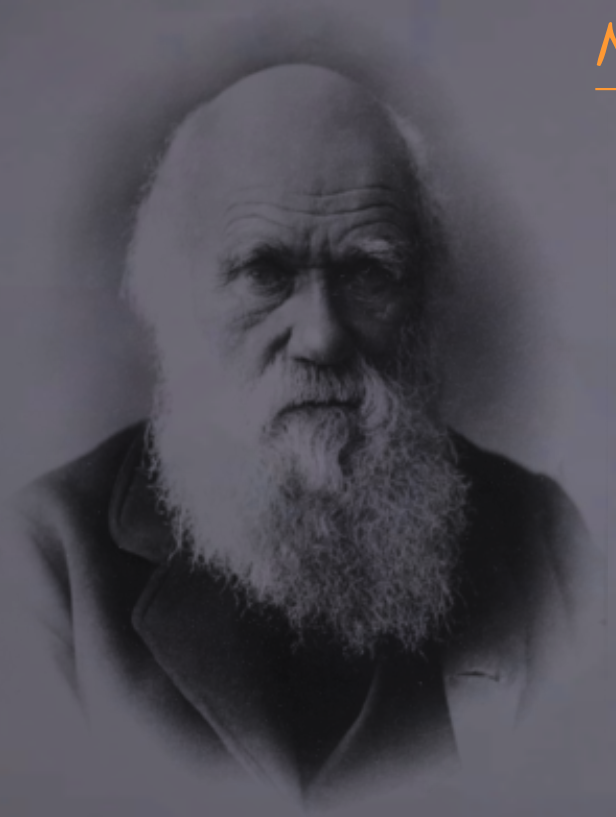

Motivation

- study relation between species
- evolution of characteristics
- co-evolution (host-parasite)
- geological migration
- genetic development of viruses/diseases

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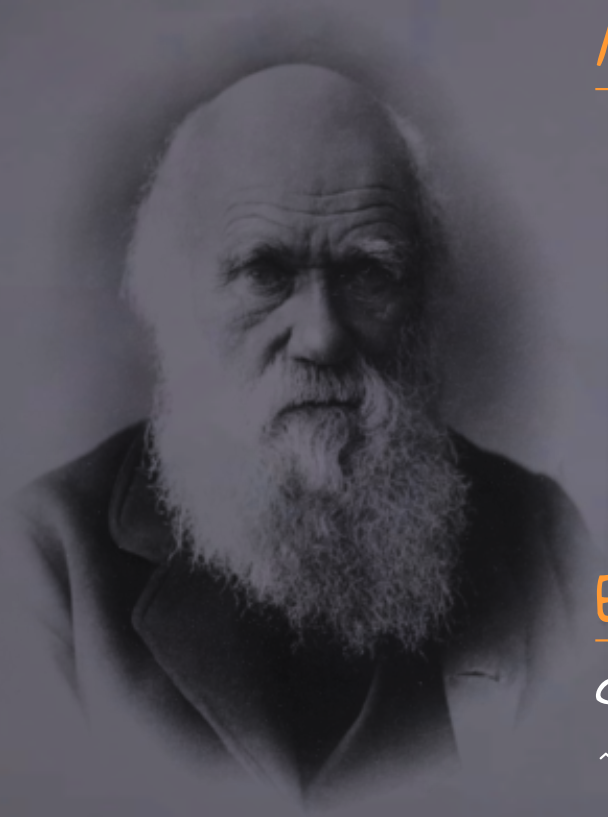

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- study relation between species
- evolution of characteristics
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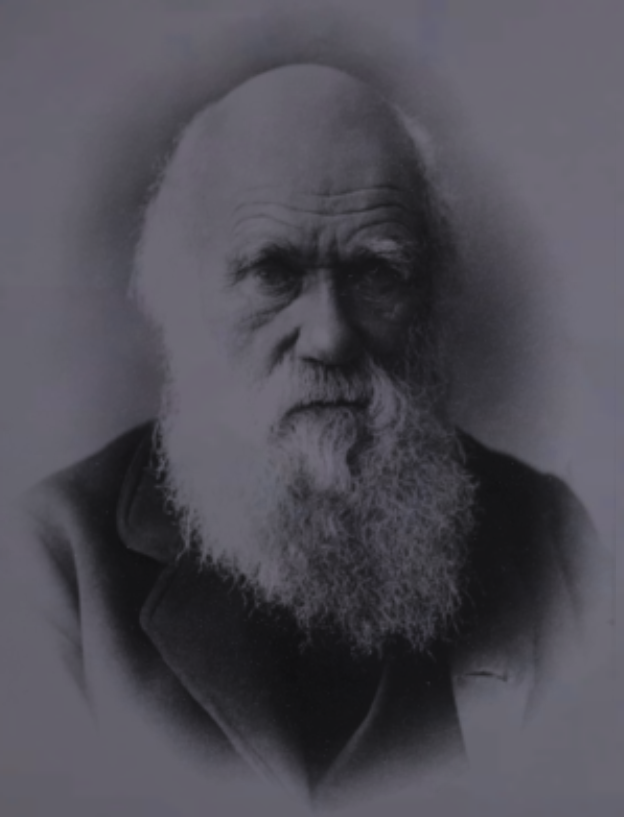
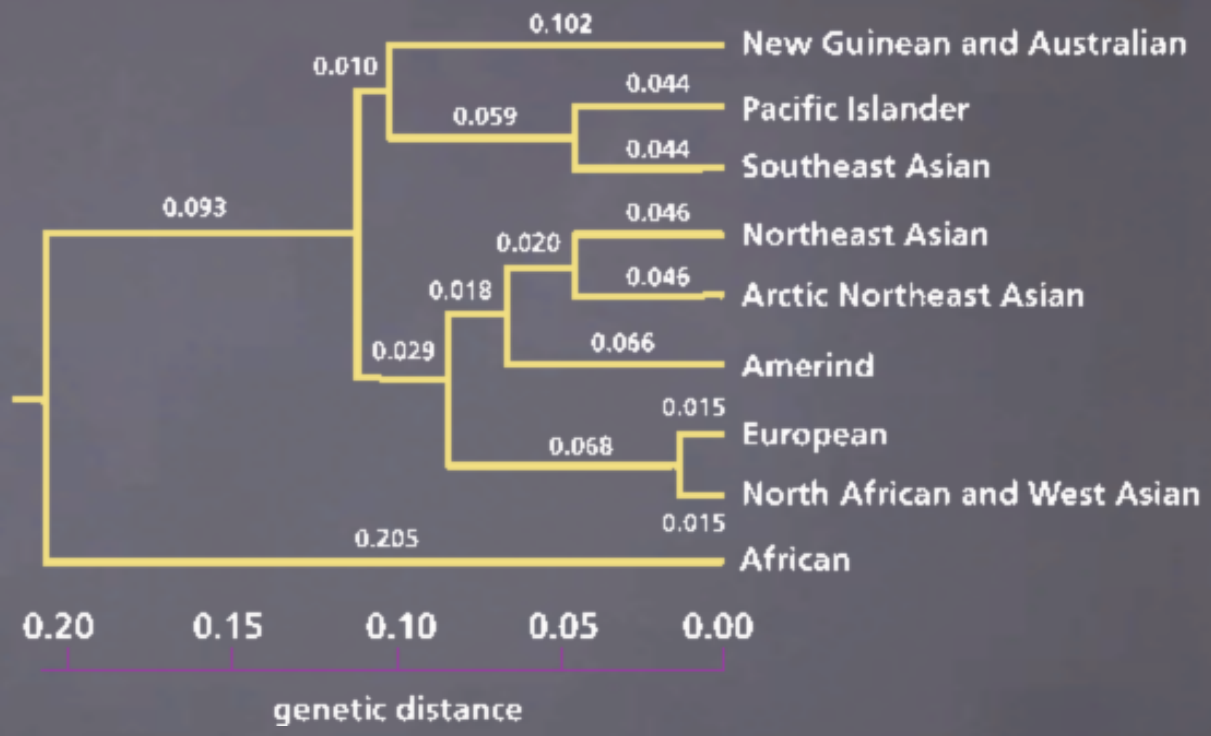
Evolution

genetic material changes over time
$\rightsquigarrow$ new species "branch off"
$\rightsquigarrow$ "tree of life"

Phylogenetic Trees - Motivation





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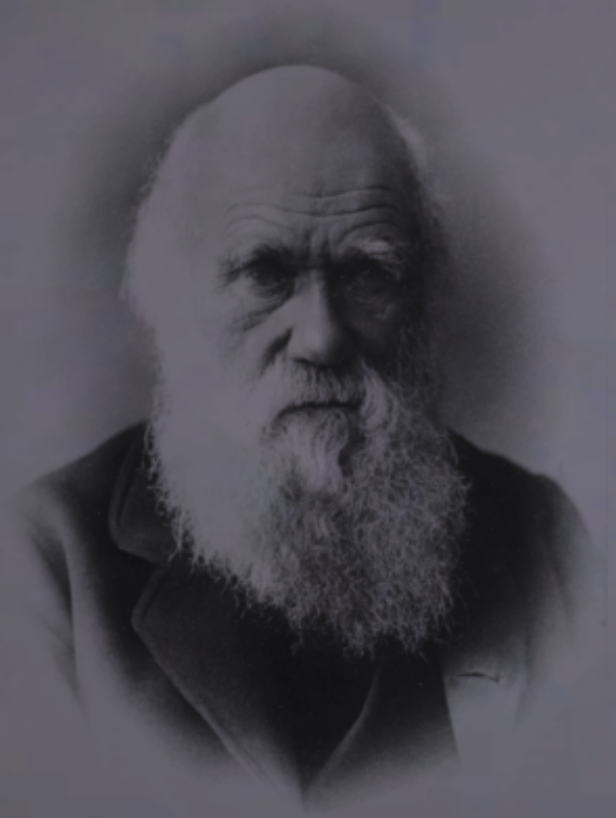
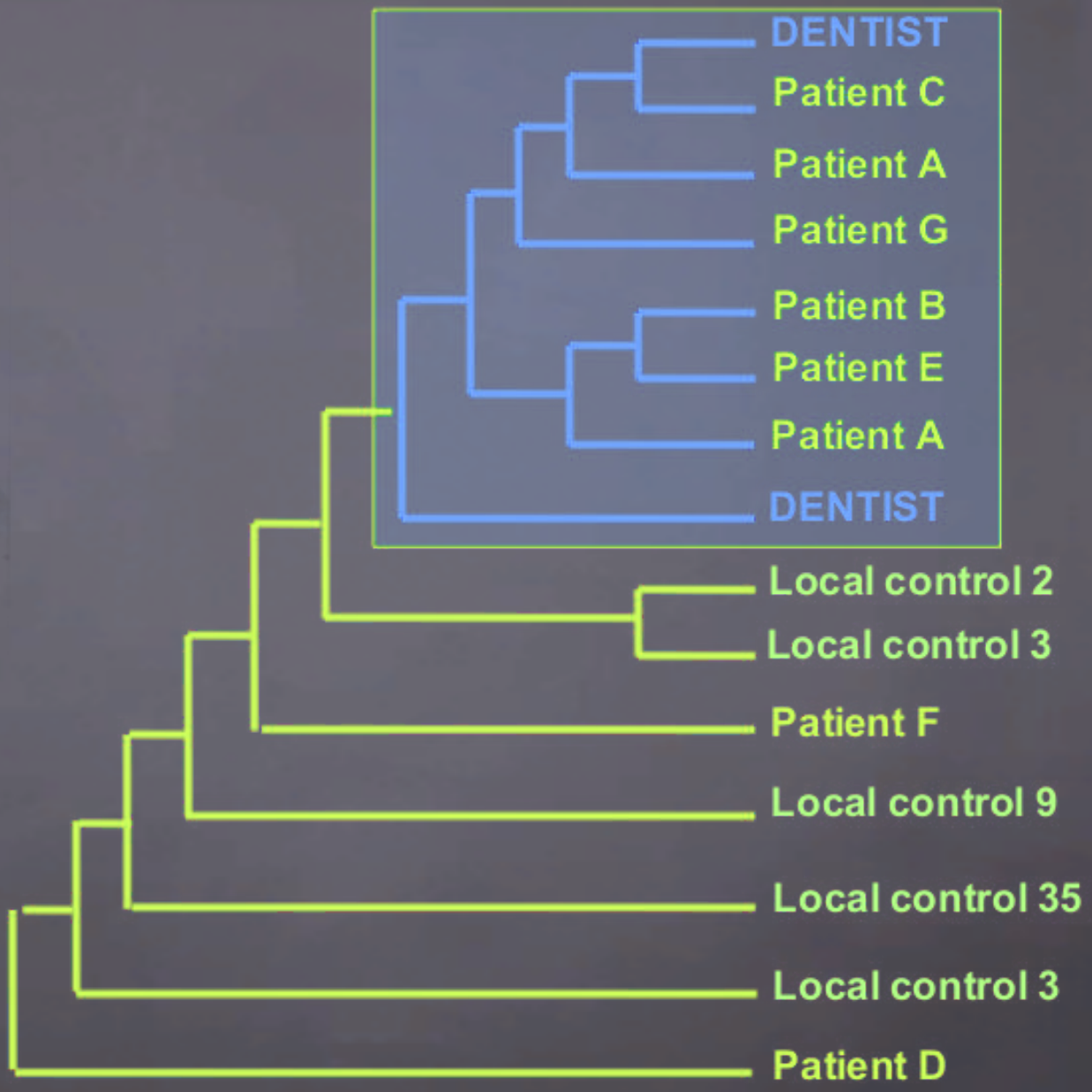
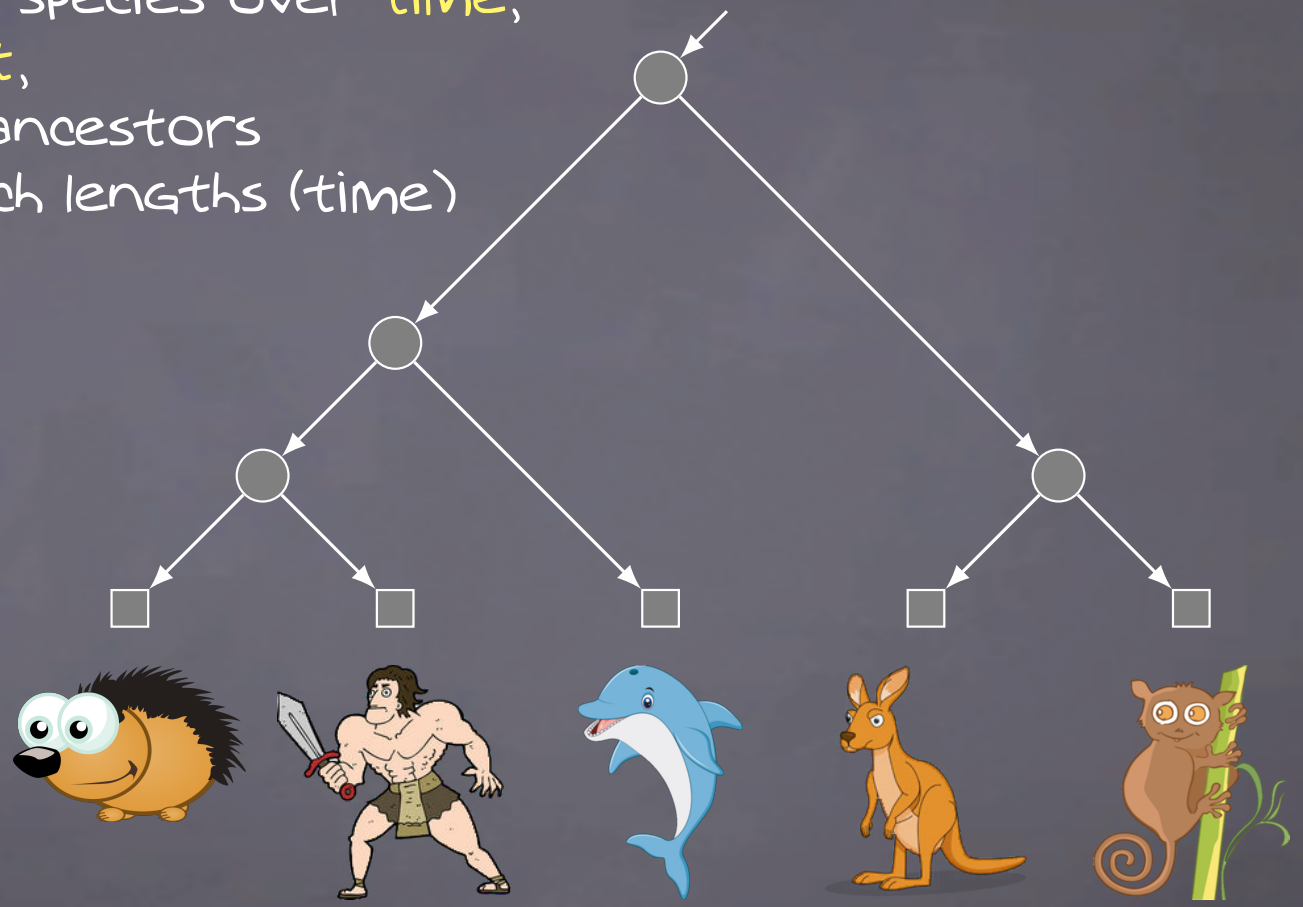




Ou et al. (1992), Page et Holmes (1998)

Rooted Phylogenetic Trees

evolution of species over time,
leaves extant,
hypothetical ancestors
possibly branch lengths (time)



Notation

taxon, cluster, triplet

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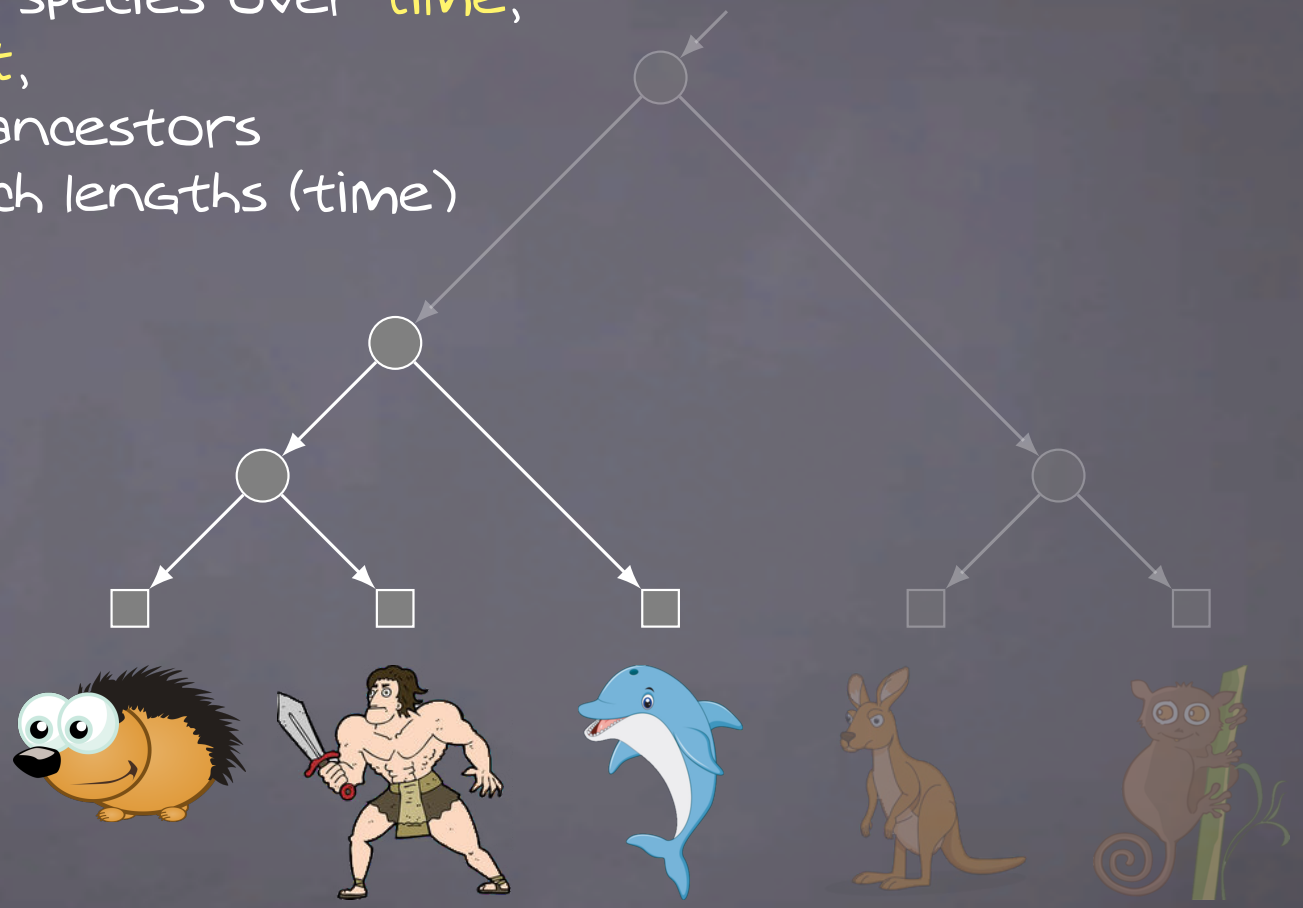

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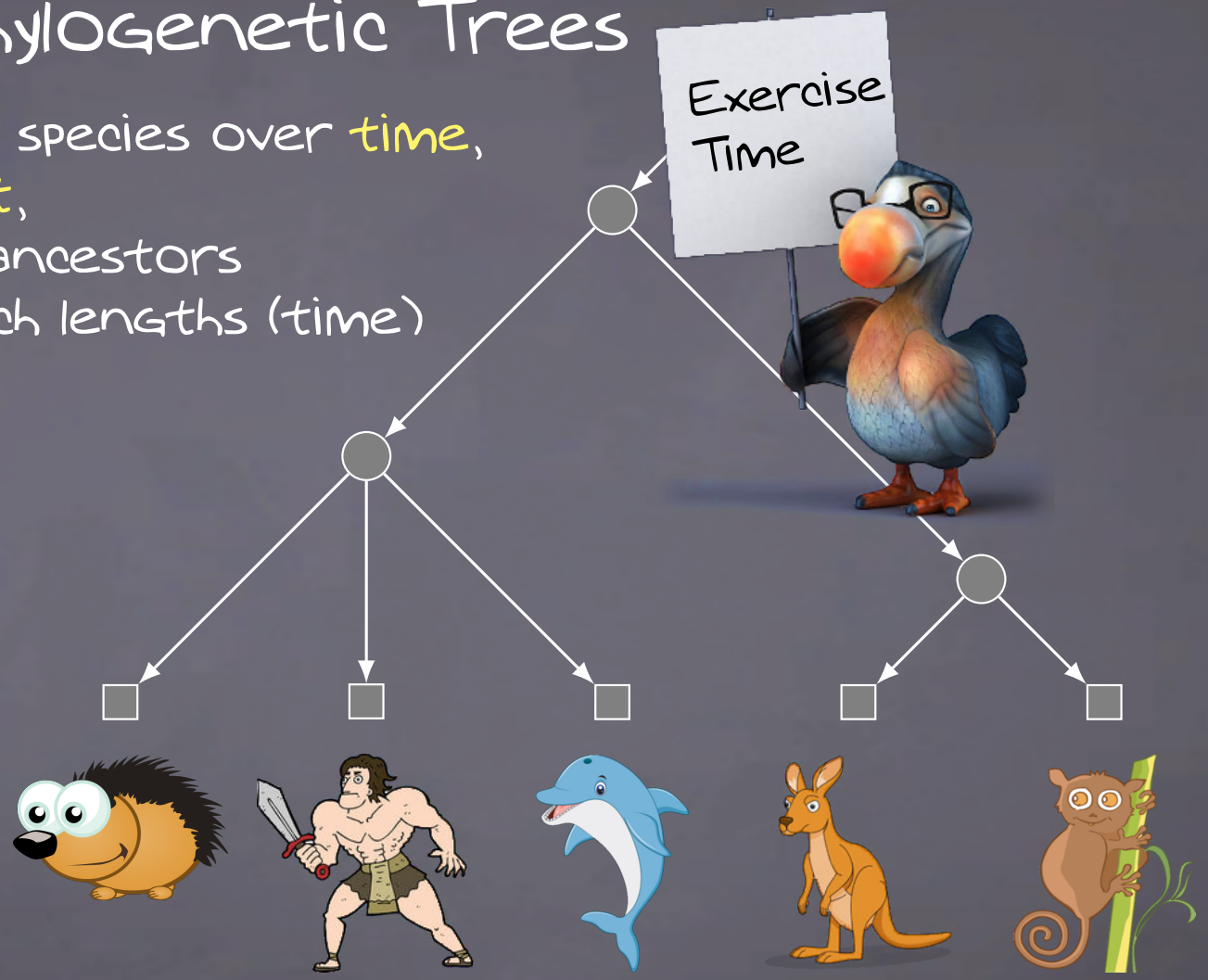


Notation

taxon, cluster, triplet

"Polytomies"

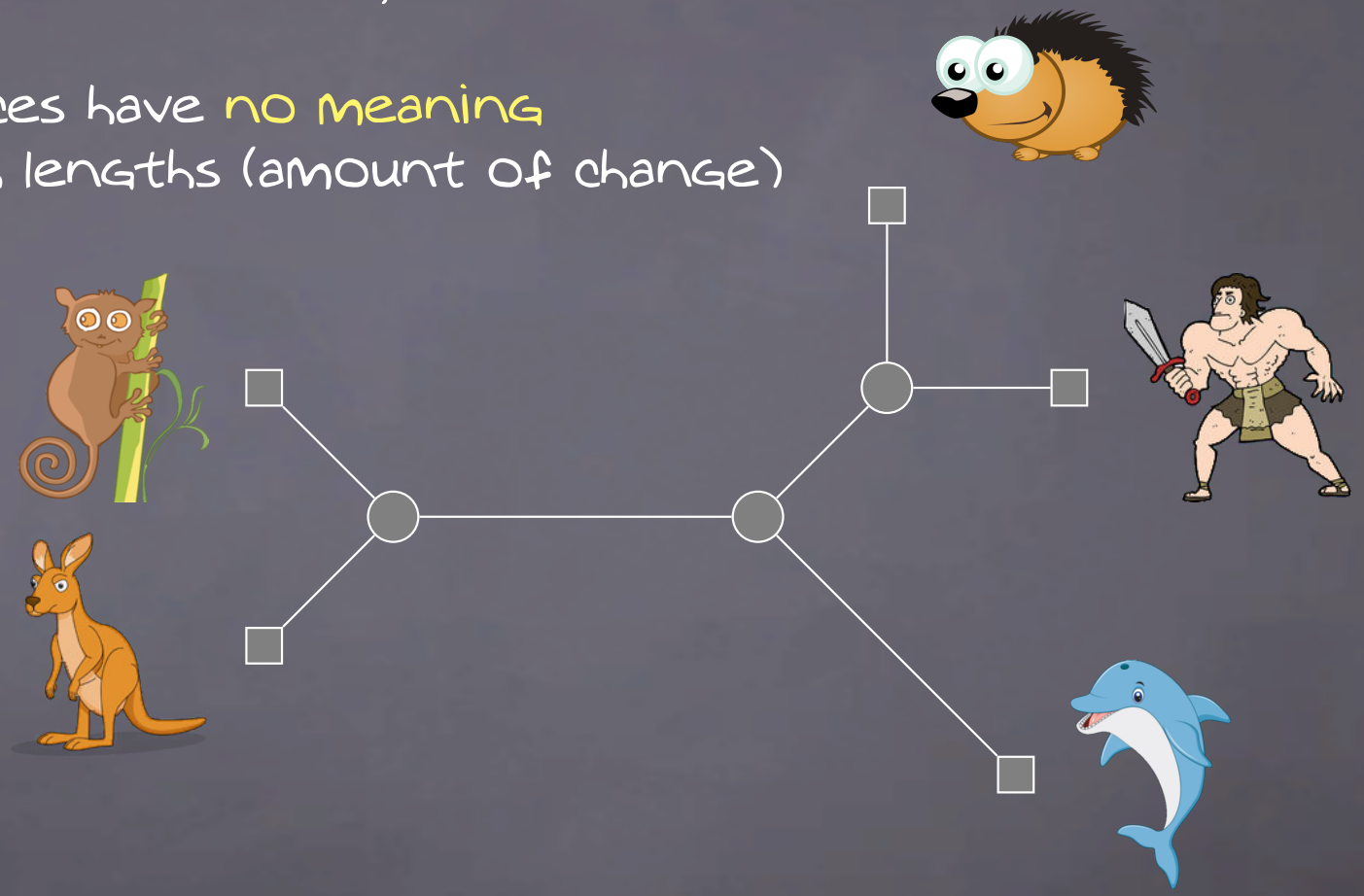
history not clear ⇝ "soft"
known "fan out" ⇝ "hard"

Exercise:

use $xy|z \leftrightarrow LCA(xy)<LCA(xz)=LCA(xyz)$ to prove $ab|c + bc|d \rightarrow ac|d$

Unrooted Phylogenetic Trees

similarity between genomes,
leaves extant,
internal vertices have no meaning
possibly branch lengths (amount of change)



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taxon, split, quartet

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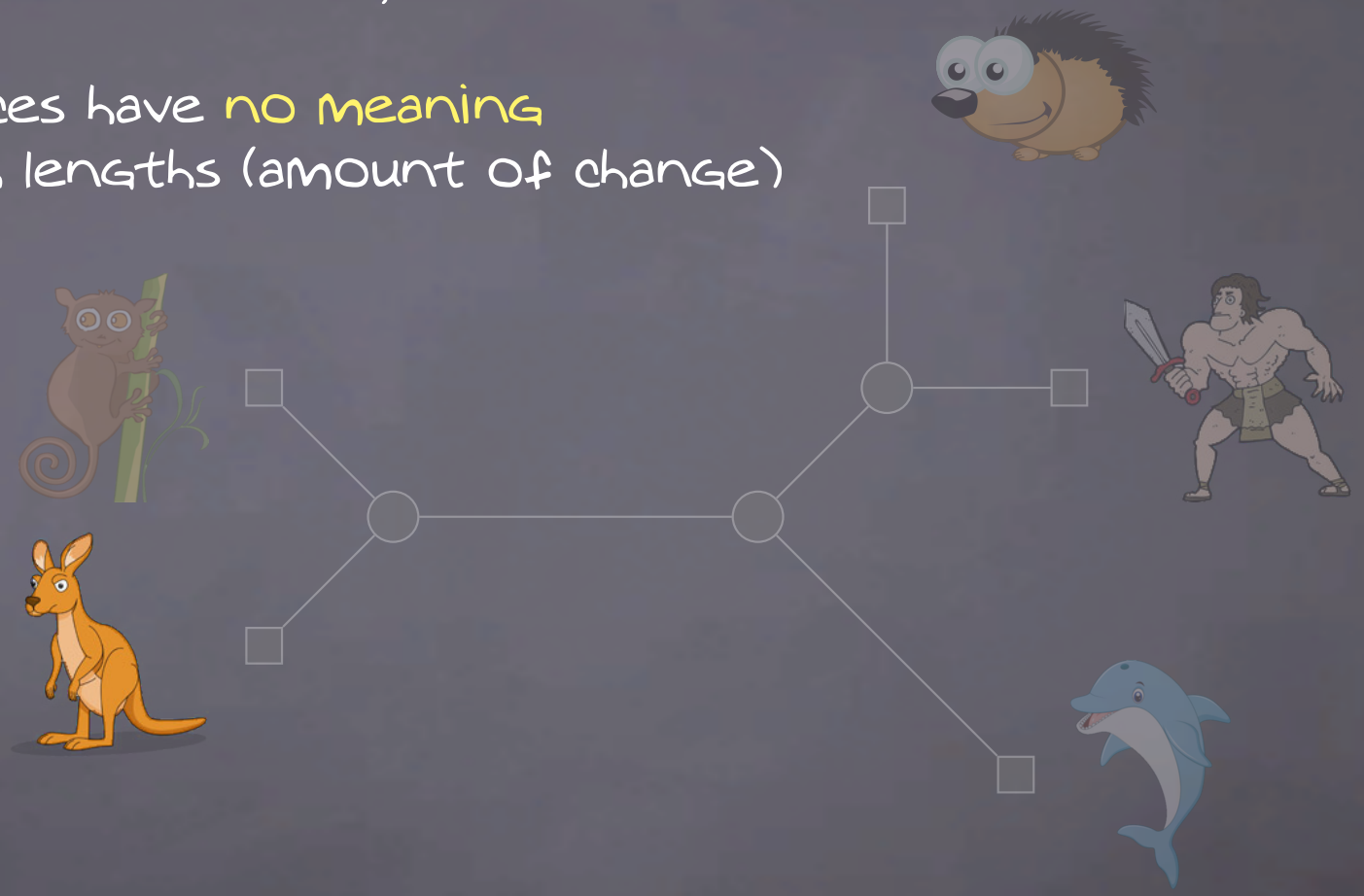

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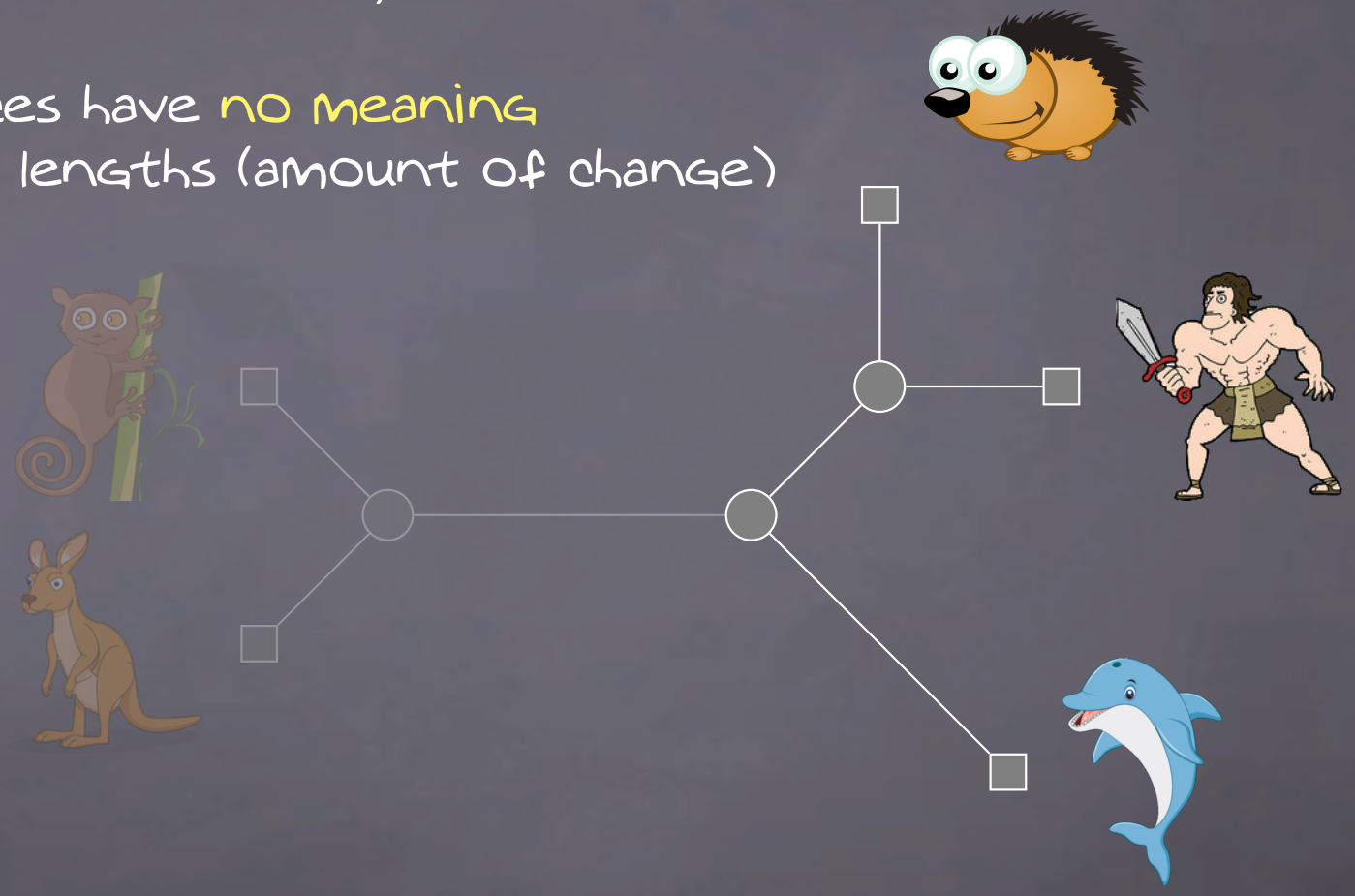

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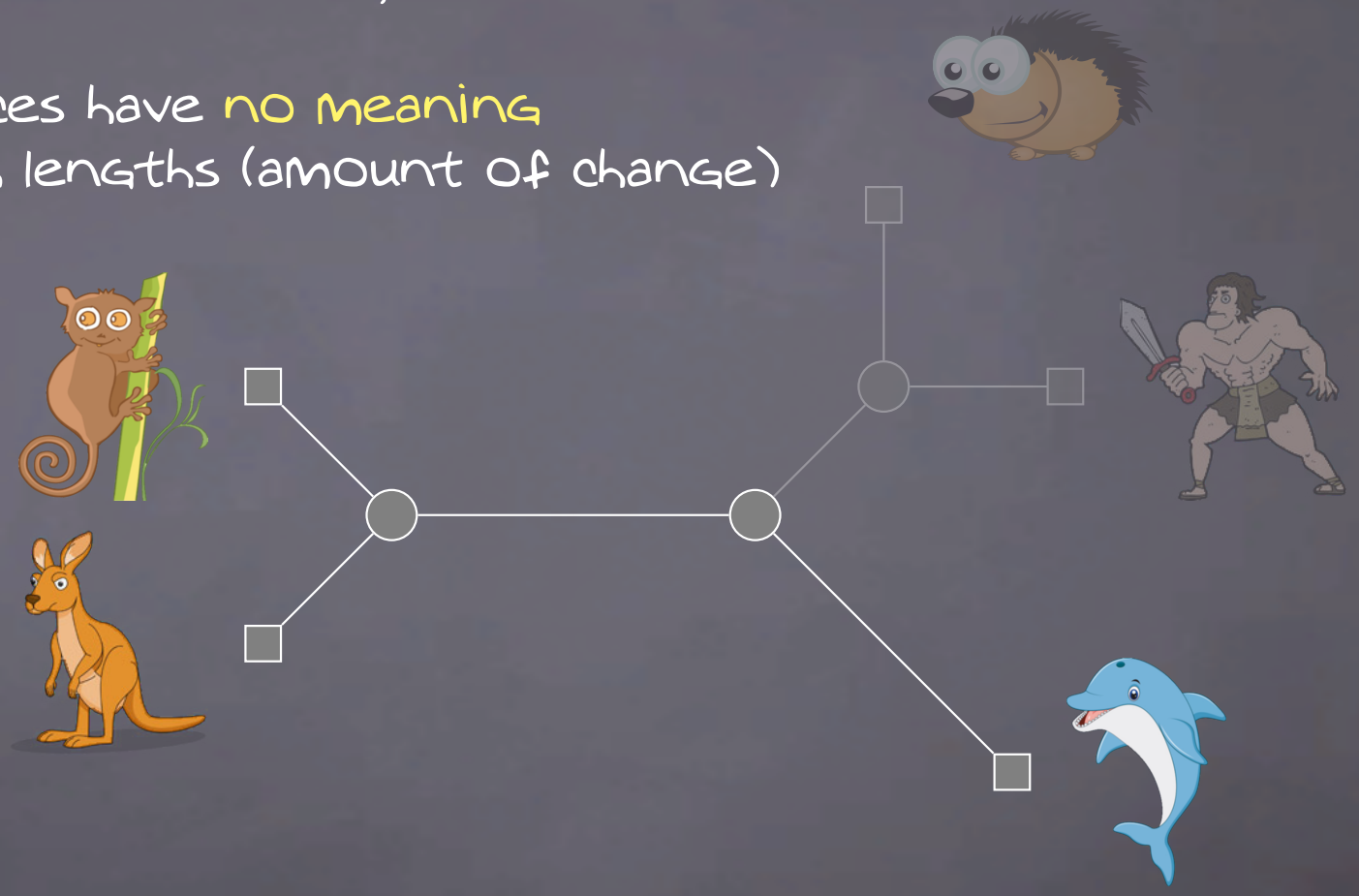

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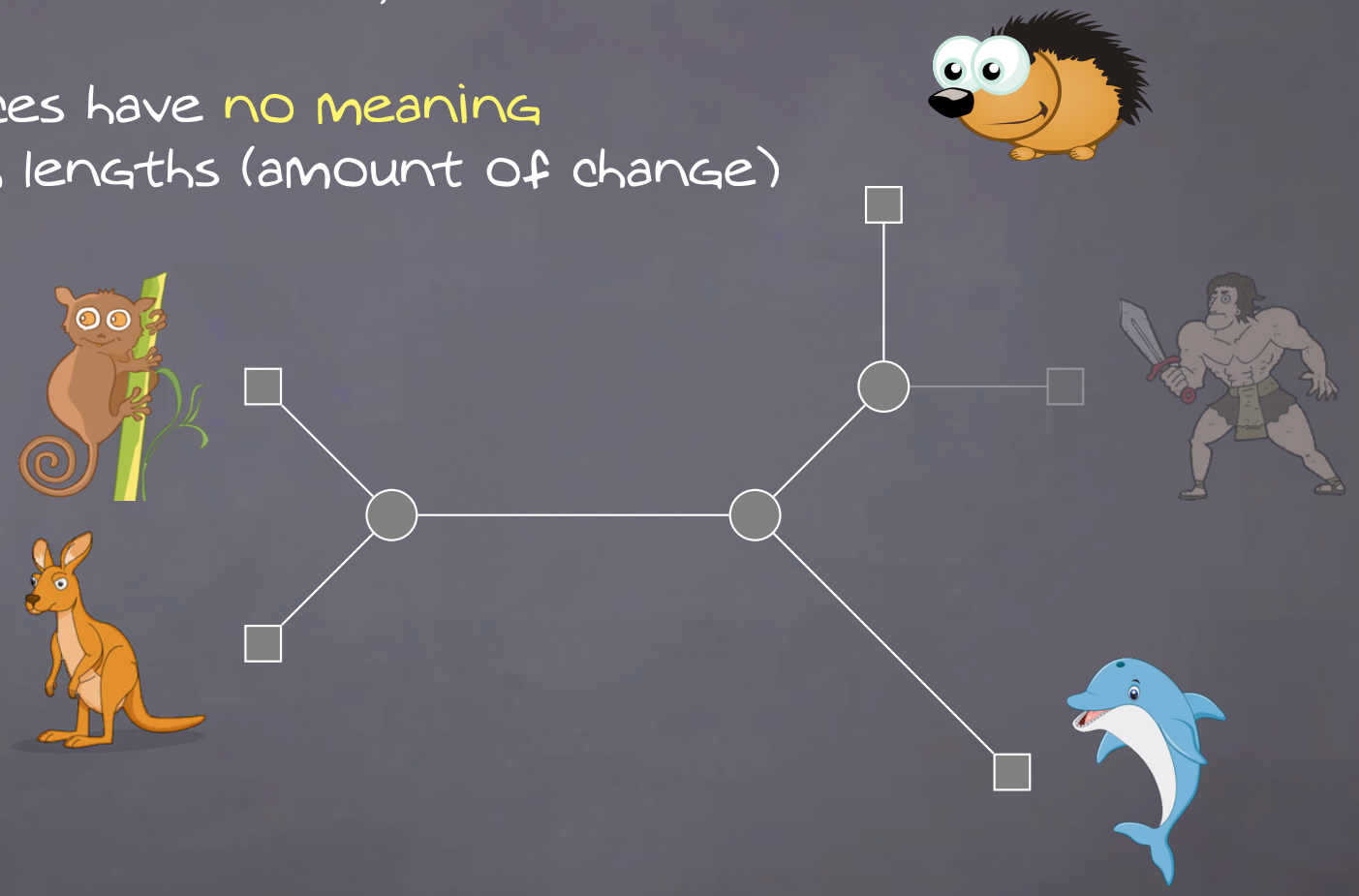

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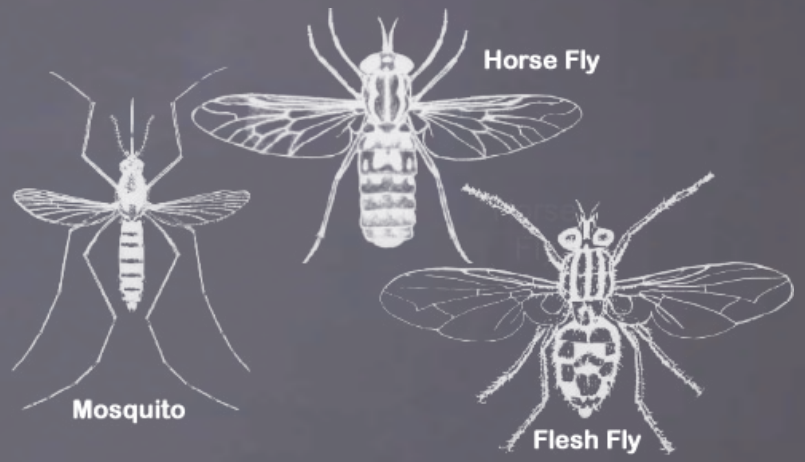
taxon, split, quartet

Reconstructing Phylogenetic Trees

Group Species By...

- morphology
- behavior
- geography

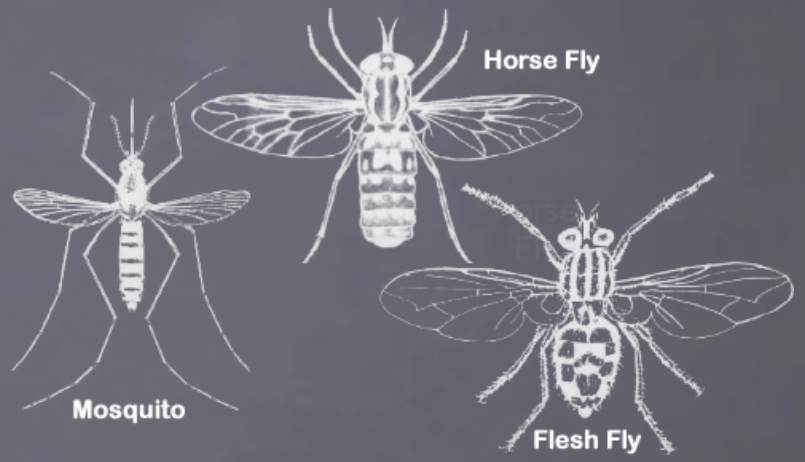


Diptera = two wings

Reconstructing Phylogenetic Trees

Group Species By...

- morphology
- behavior
- geography
- distance of sequences
- "genetic distance"
- etc.



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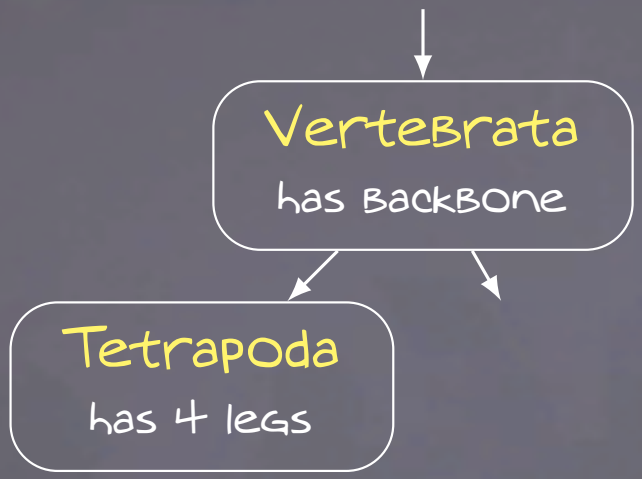

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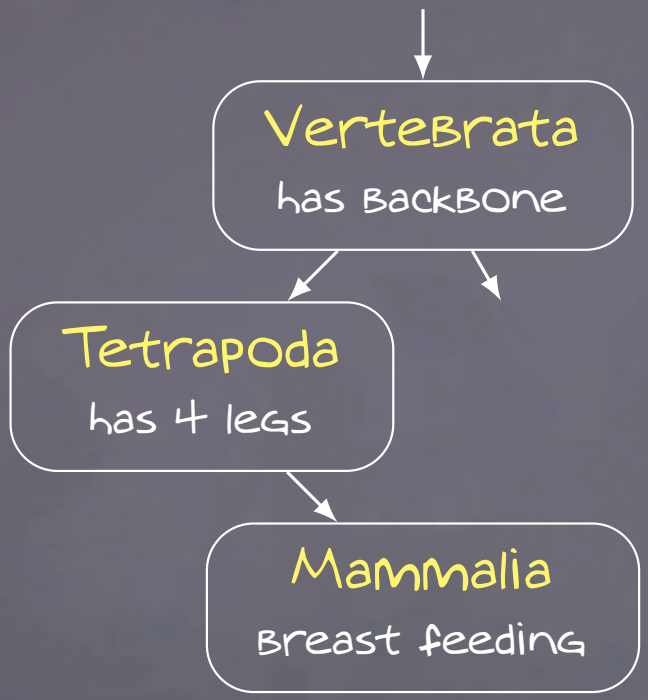

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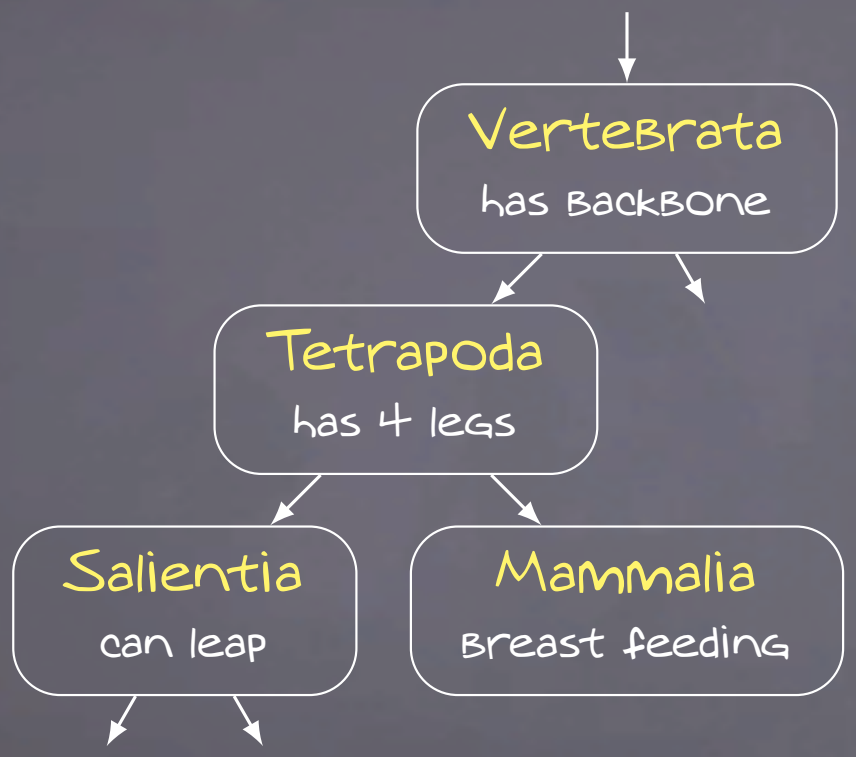

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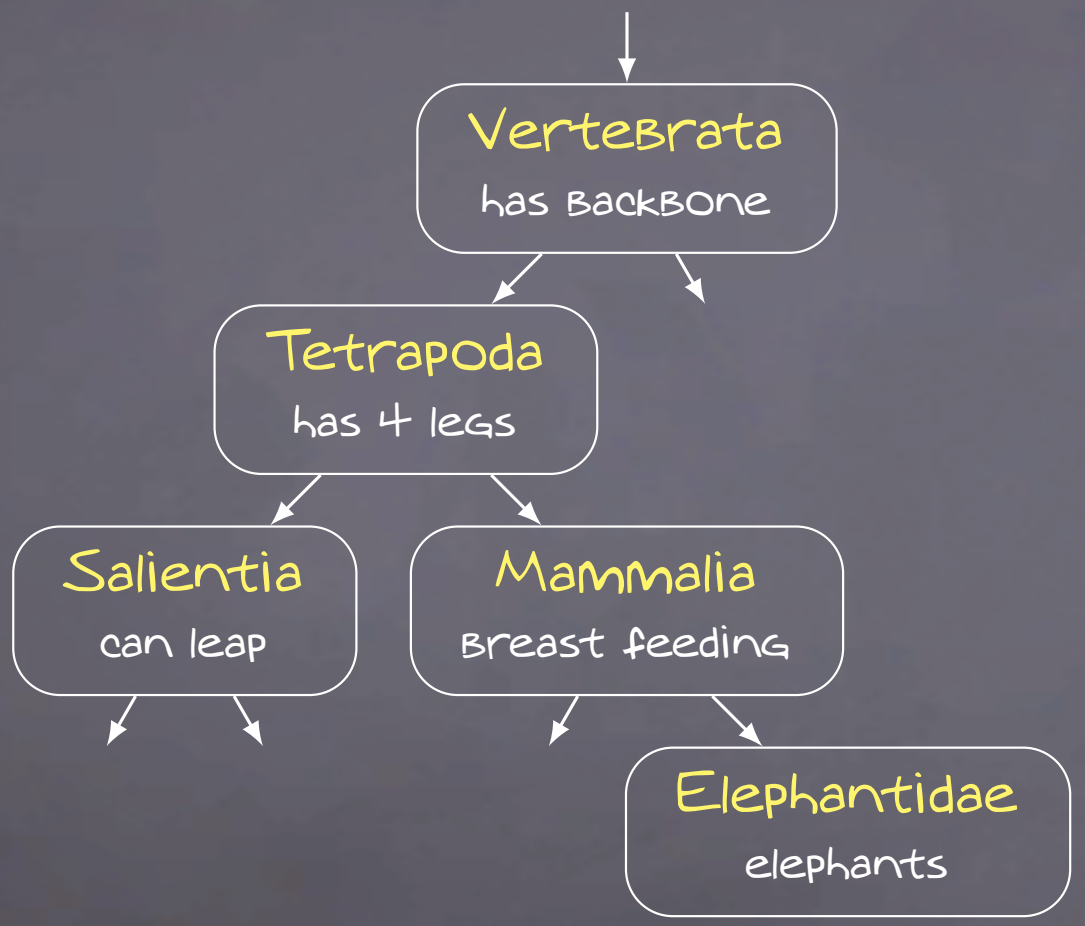

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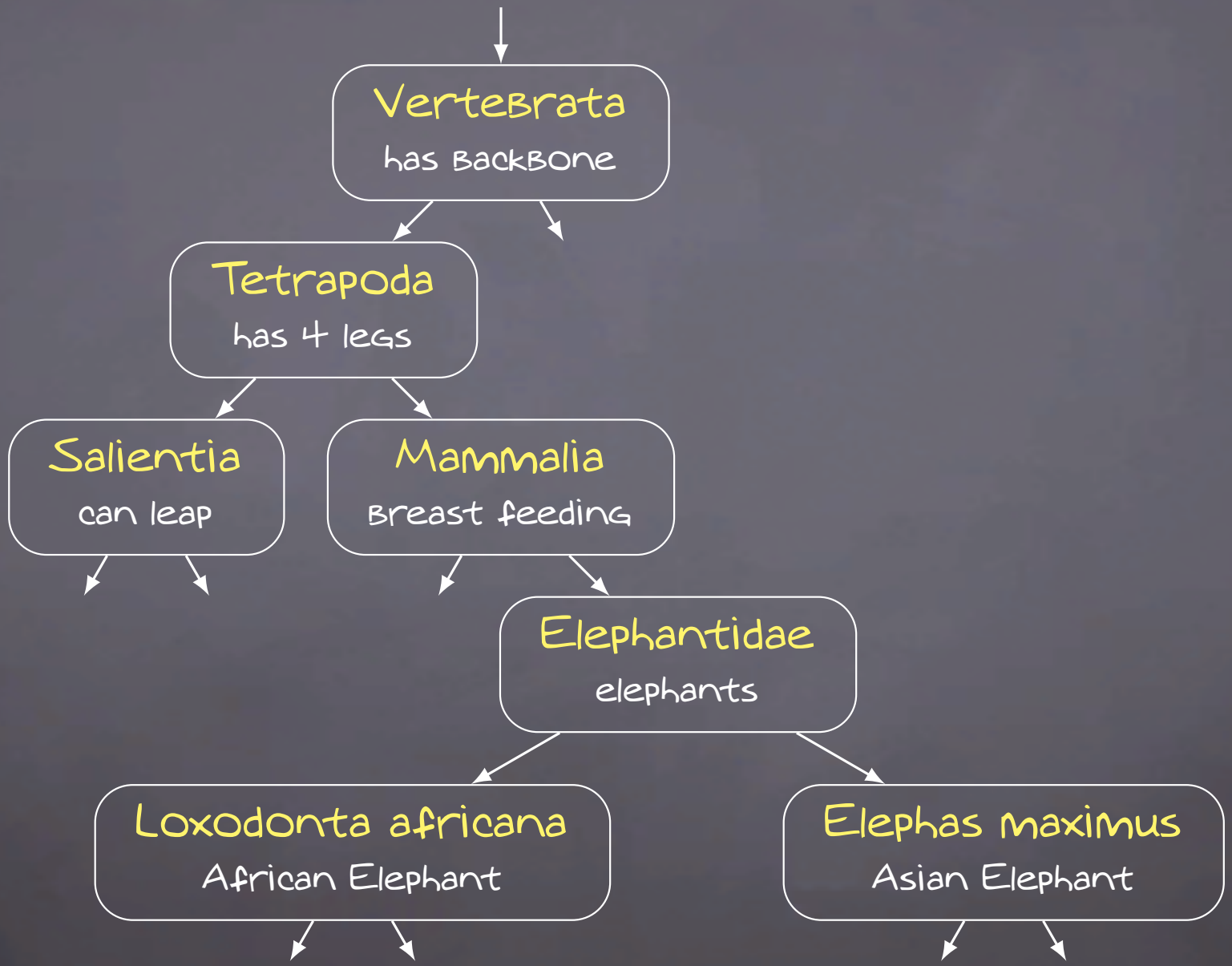

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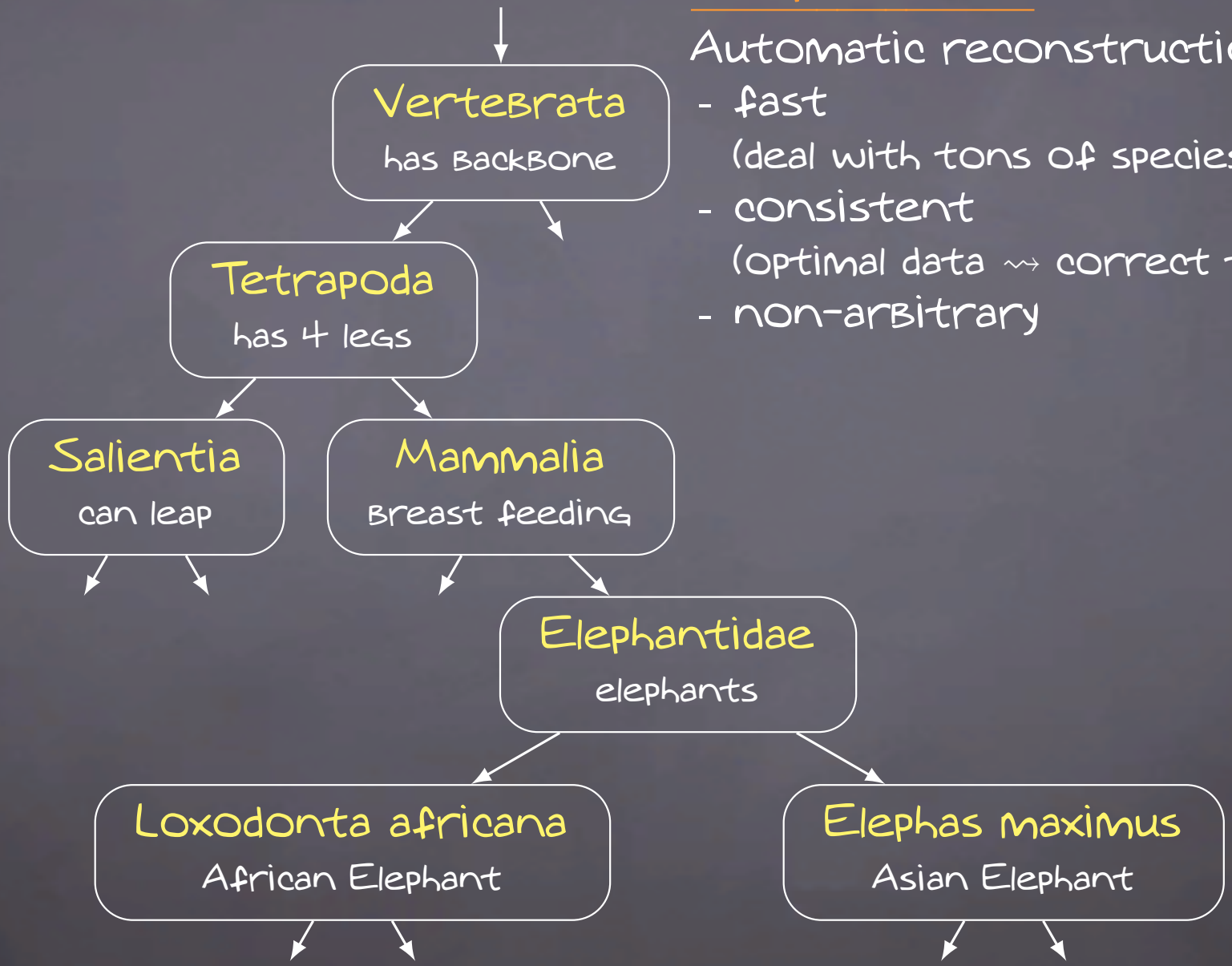

Keep in Mind

Automatic reconstruction should be

- fast
  (deal with tons of species & genes)
- consistent
  (optimal data $\rightsquigarrow$ correct tree)
- non-arbitrary

Distance-Based Reconstruction

Idea: cluster hierarchically

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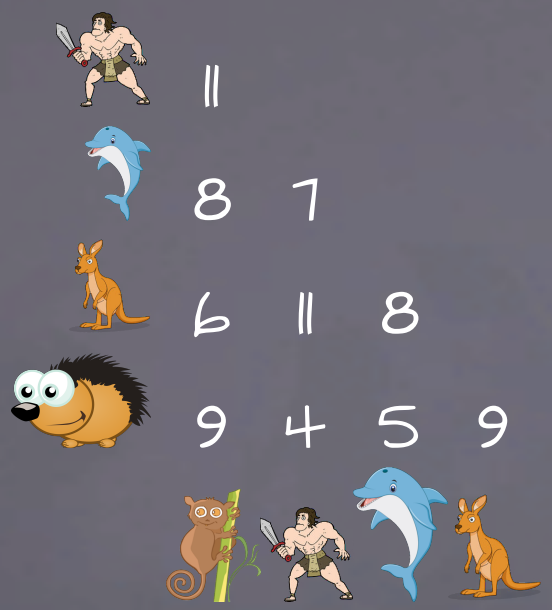

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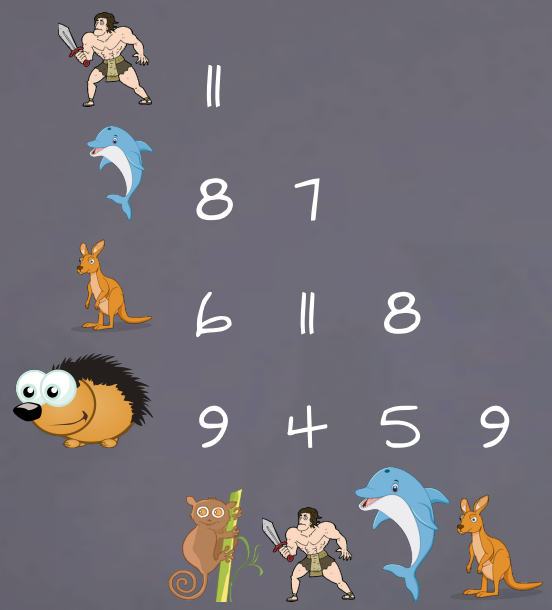

Idea: merge closest clusters

Branch lengths ??

assume molecular clock

⇝ ultrametric

Distance-Based Reconstruction

Idea: cluster hierarchically

Idea: merge closest clusters

update matrix

$$d_{X \cup Y, Z} = \frac{|X| d_{X,Z} + |Y| d_{Y,Z}}{|X| + |Y|}$$

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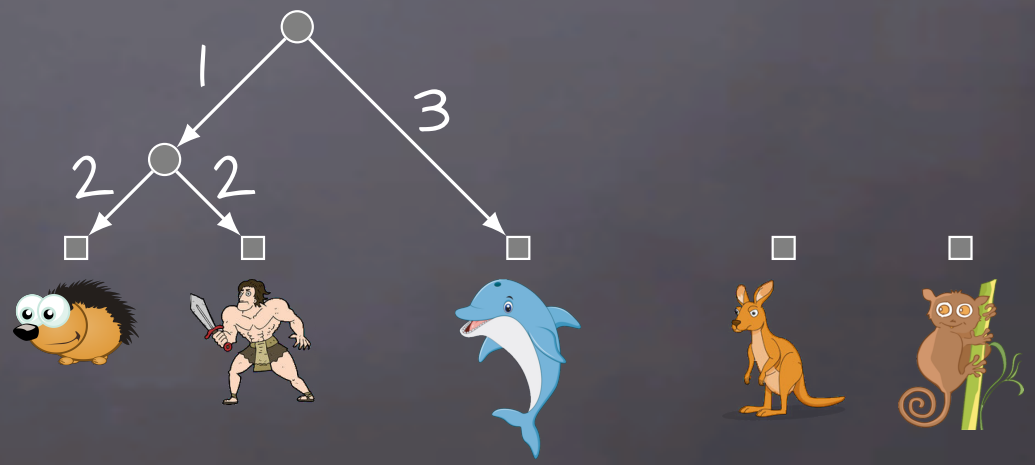

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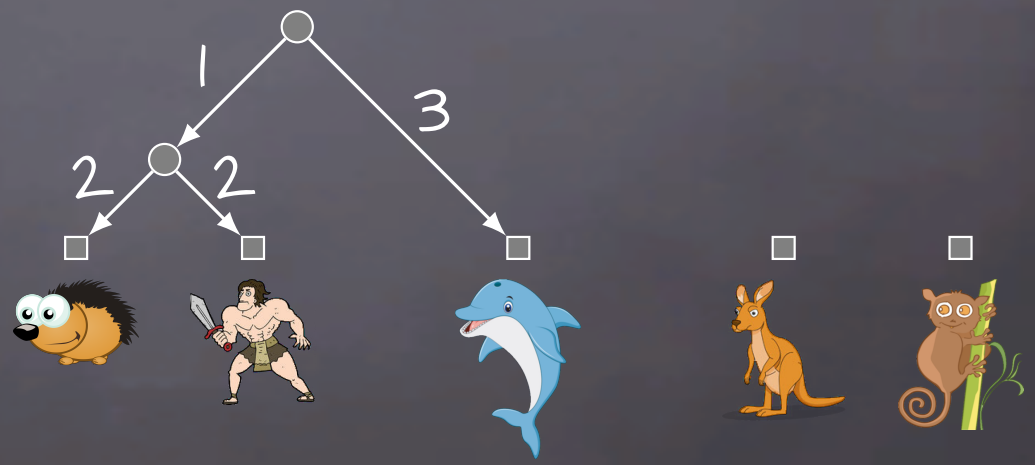

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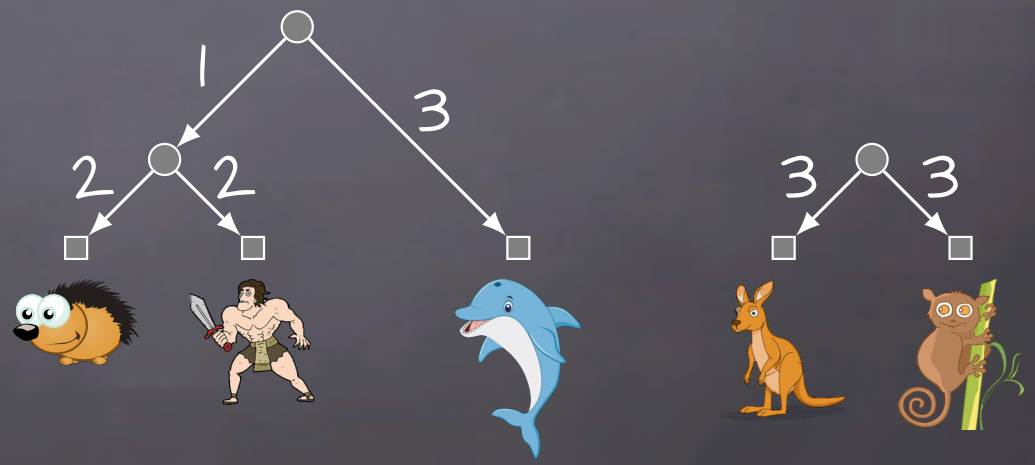

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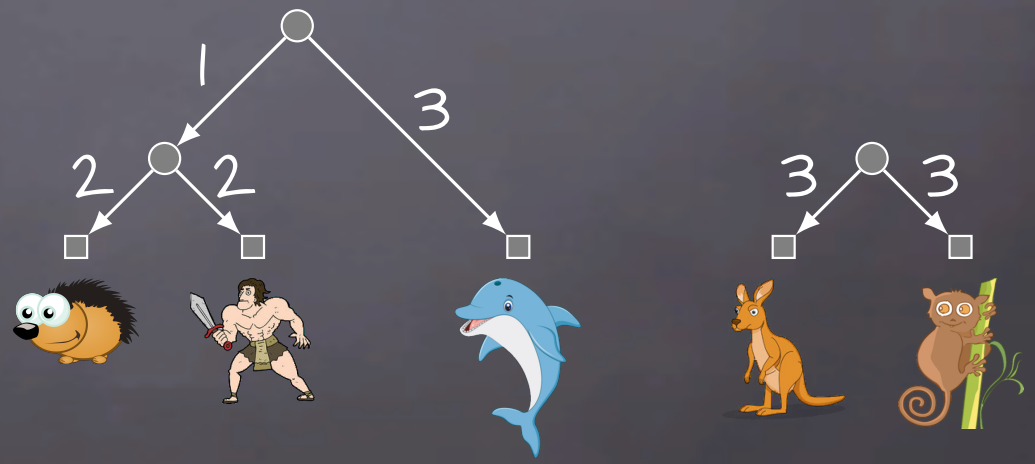

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28/3

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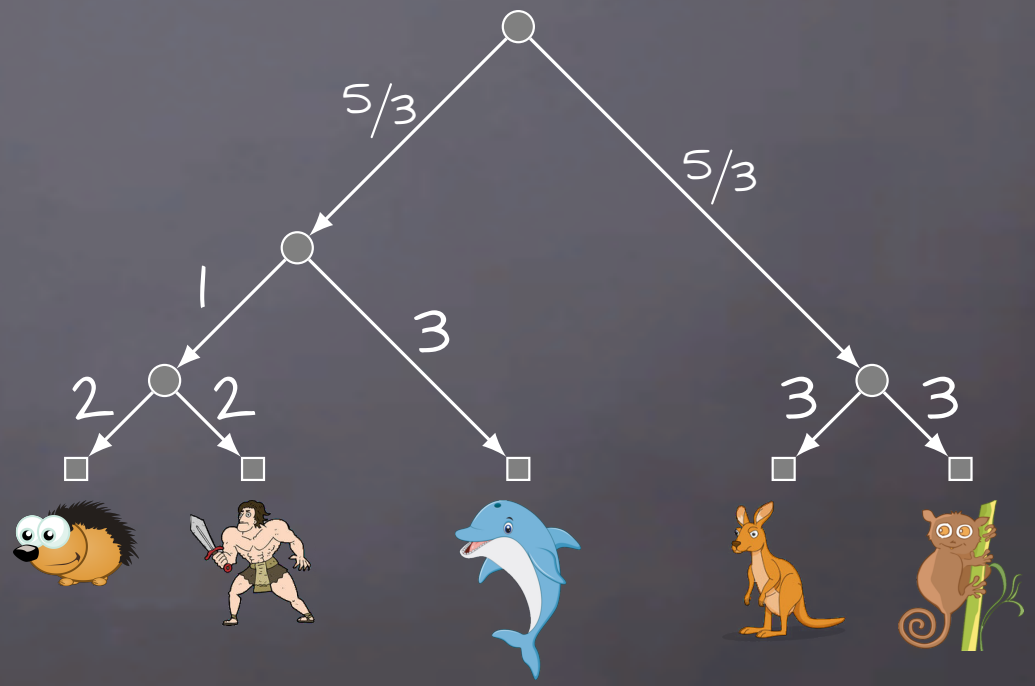

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Idea: cluster hierarchically

Unweighted Pair Group Method w/ Avg.

- find "closest pair"
- "join" them
- update distances & recurse

28/3

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Branch lengths ??

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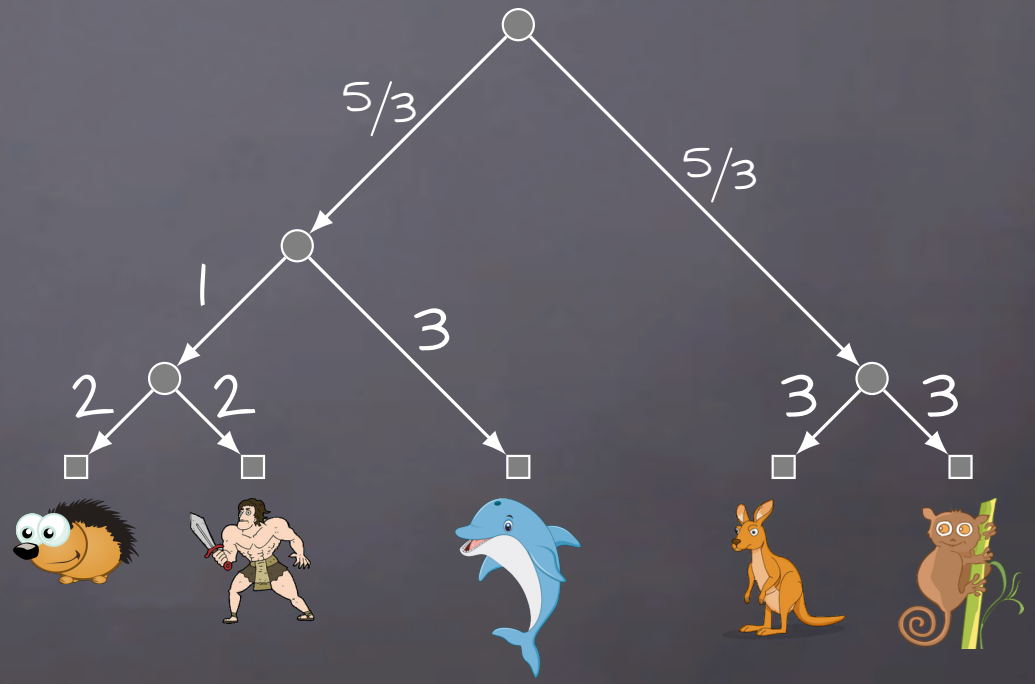

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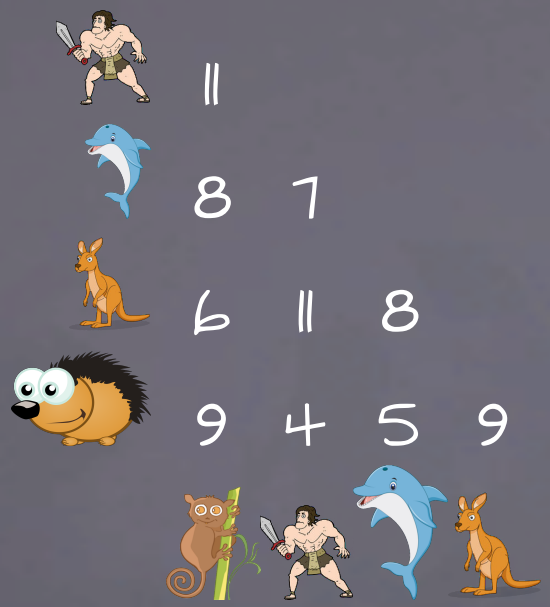

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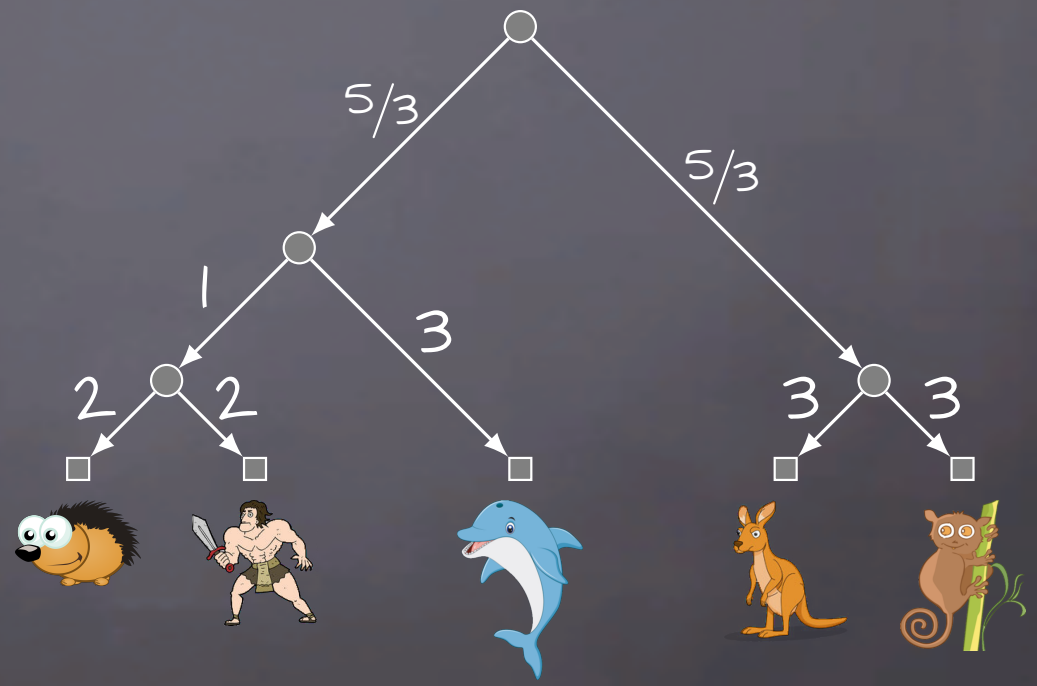

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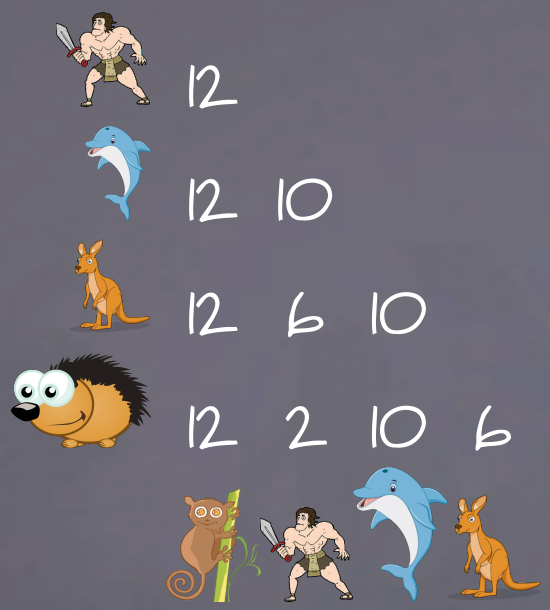

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Idea: merge closest clusters

update matrix

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Branch lengths ??

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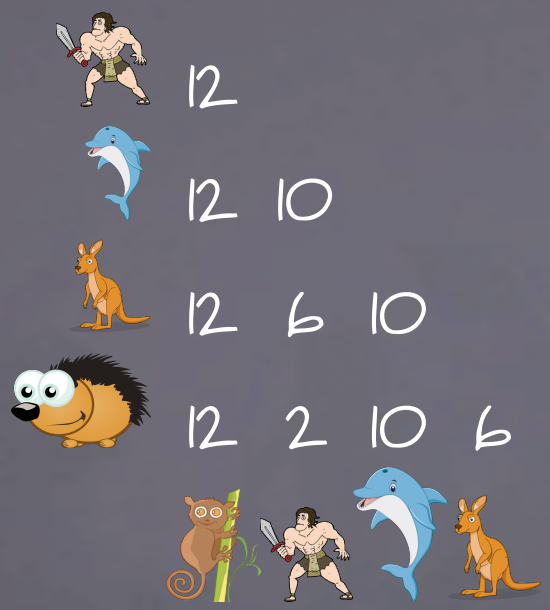

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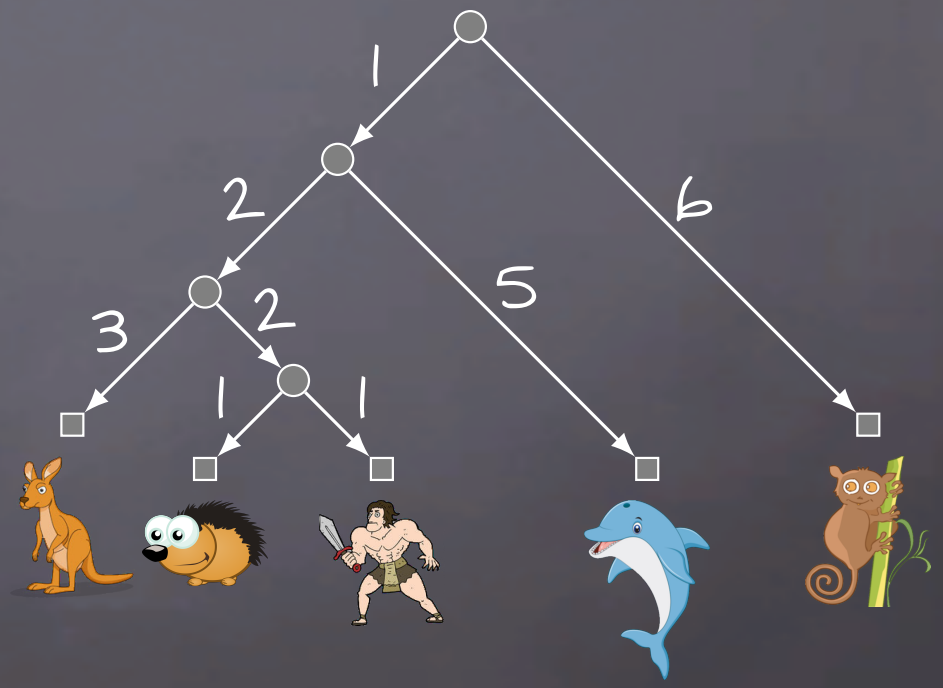

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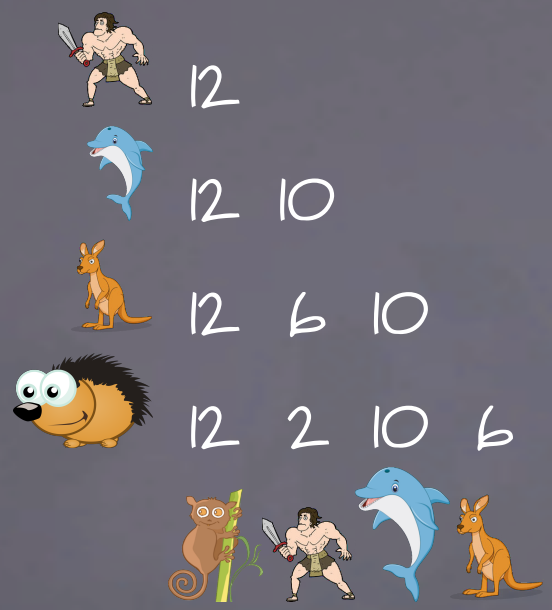

Unweighted Pair Group Method w/ Avg.

- find "closest pair"
- "join" them
- update distances & recurse
- only accurate if ultrametric

Idea: merge closest clusters

update matrix

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Branch lengths ??

assume molecular clock

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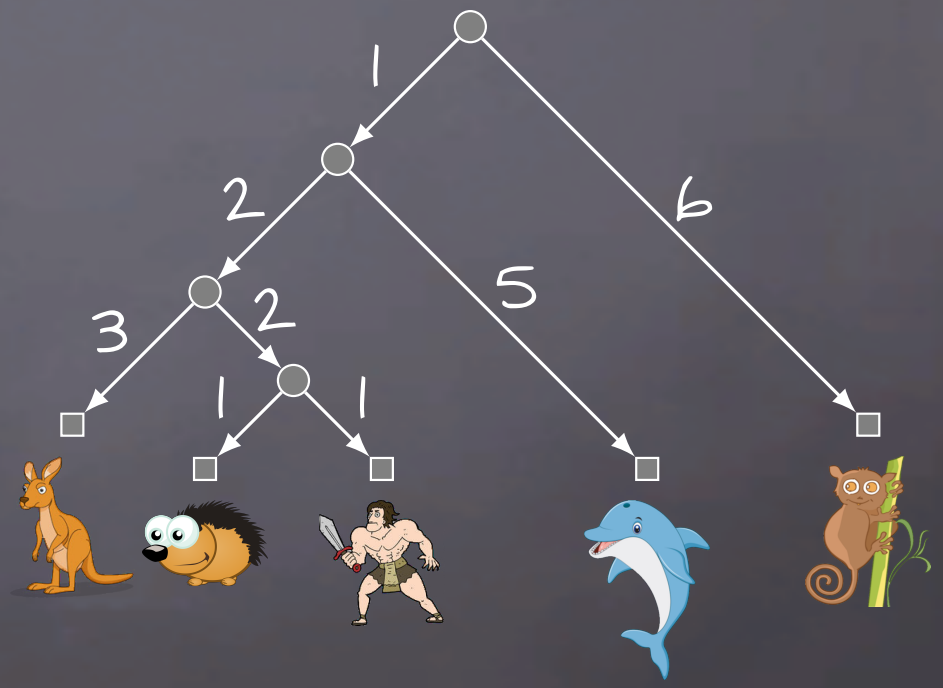

Distance-Based Reconstruction

What about unrooted trees? No root $\rightsquigarrow$ no molecular clock...

Distance-Based Reconstruction

B	9		
C	11	8	
D	9	12	10
	A	B	C

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Distance-Based Reconstruction

Problem: correct pairs may not be closest

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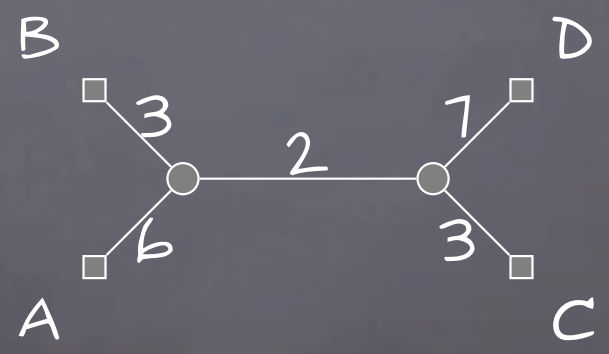

Distance-Based Reconstruction

Problem: correct pairs may not be closest

Neighbor Joining (unrooted)

- build eccentricity matrix:
  $Q_{X,Y} = \sum_Z (d_{X,Z} + d_{Y,Z} - d_{X,Y}) + 2d_{X,Y}$
- find max in Q
- join them
- update distances & recurse

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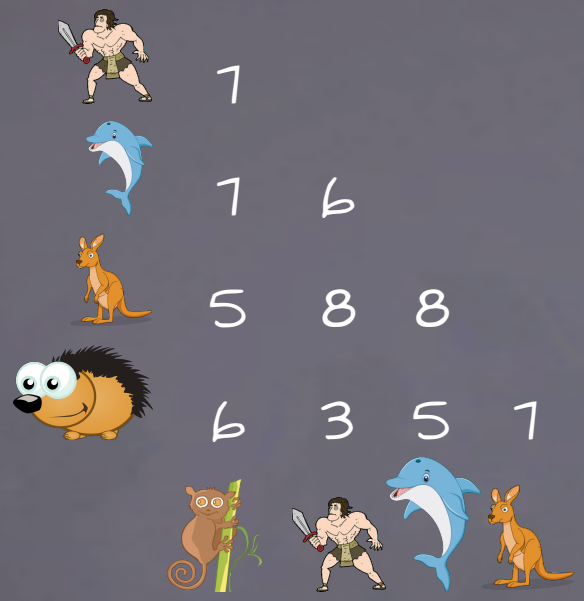

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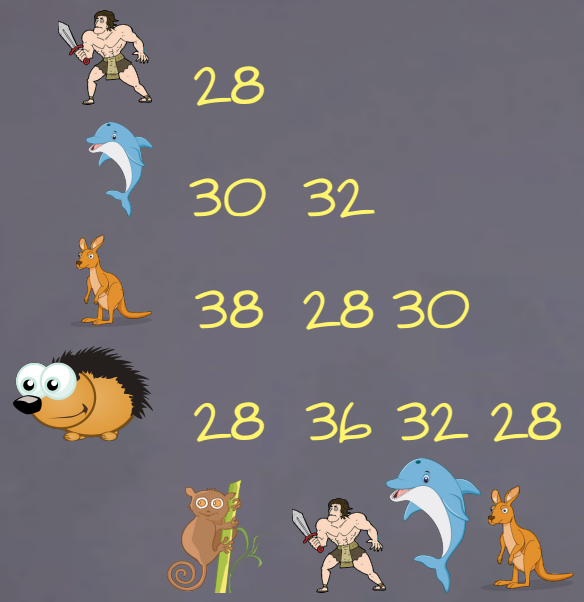
Distance-Based Reconstruction

Problem: correct pairs may not be closest

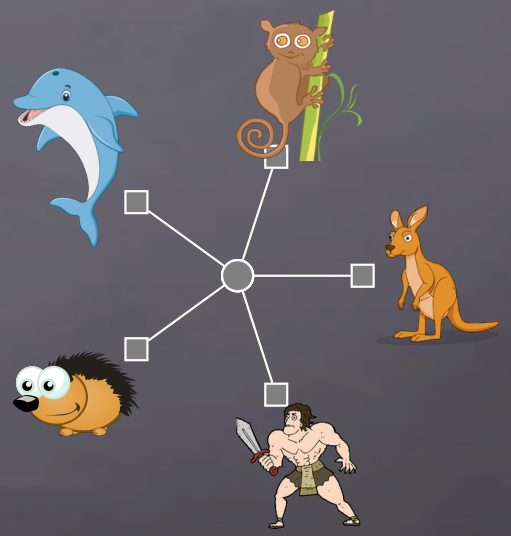


Neighbor Joining (unrooted)

- Build eccentricity matrix:
  $Q_{X,Y} = \sum_Z (d_{X,Z} + d_{Y,Z} - d_{X,Y}) + 2d_{X,Y}$
- find max in Q
- join them
- update distances & recurse

Theorem

$Q_{X,Y}$ max $\Leftrightarrow$ any tree T yielding Q has "cherry" (X, Y)



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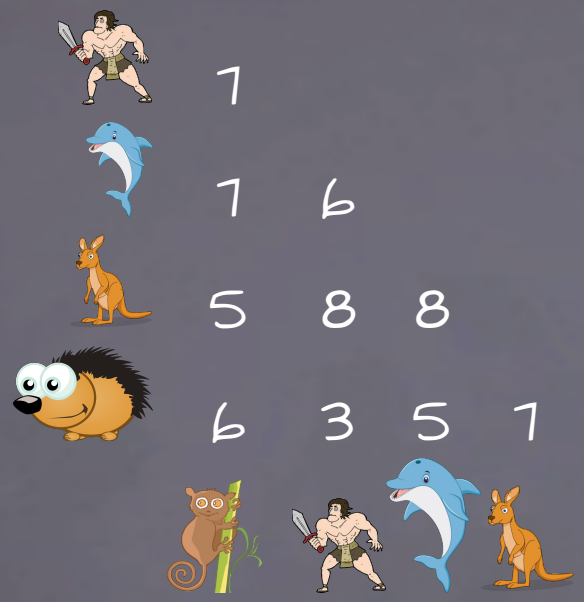

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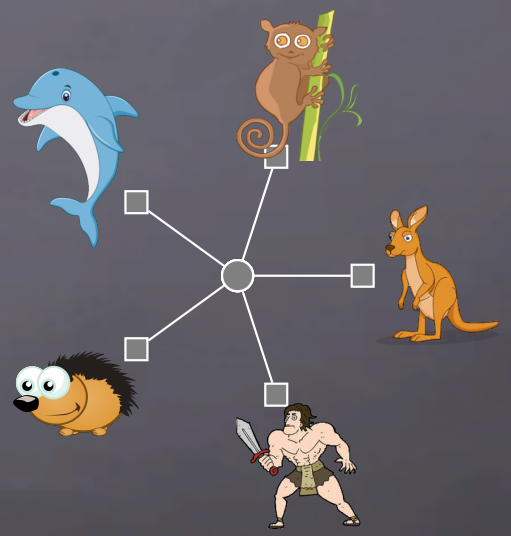
$$d_{X \cup Y,Z} = {}^1\!/_2 \left(d_{X,Z} + d_{Y,Z} - d_{X,Y}\right)$$

Branch lengths

$$2b(X) = \frac{\sum_Z (d_{X,Z} - d_{Y,Z} + d_{X,Y})}{n-2}$$



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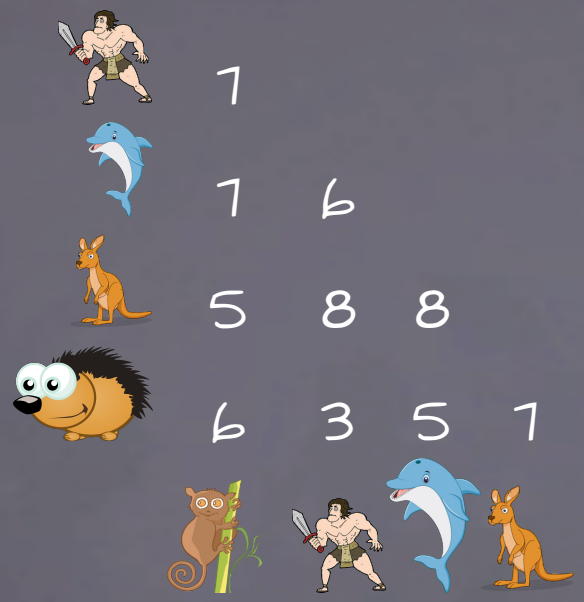

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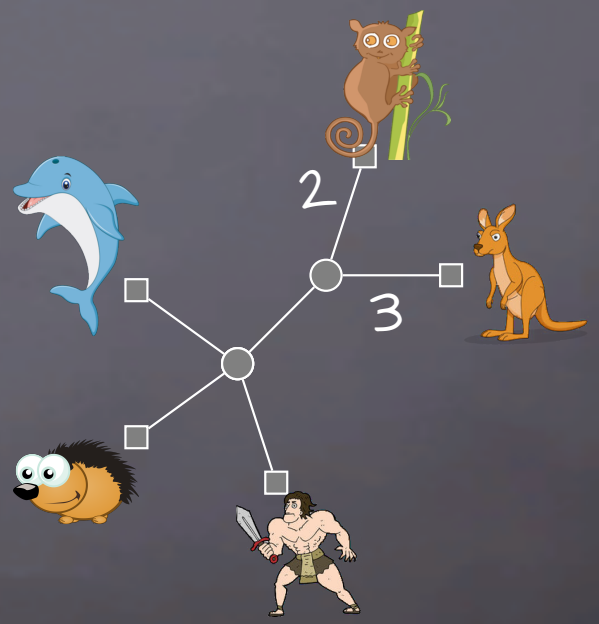

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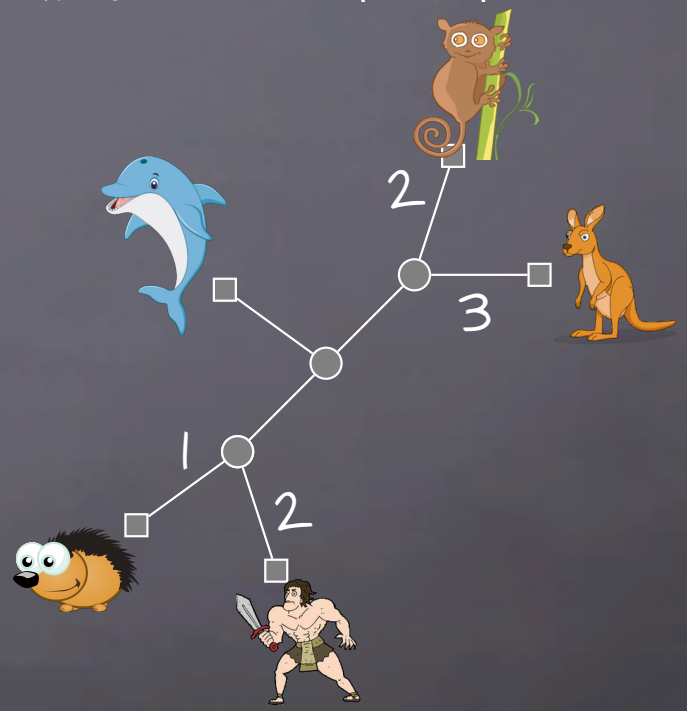

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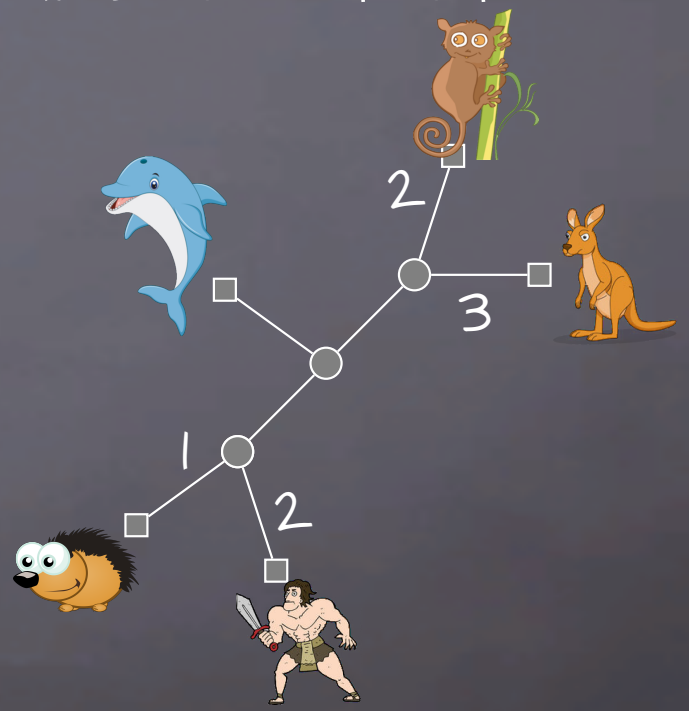

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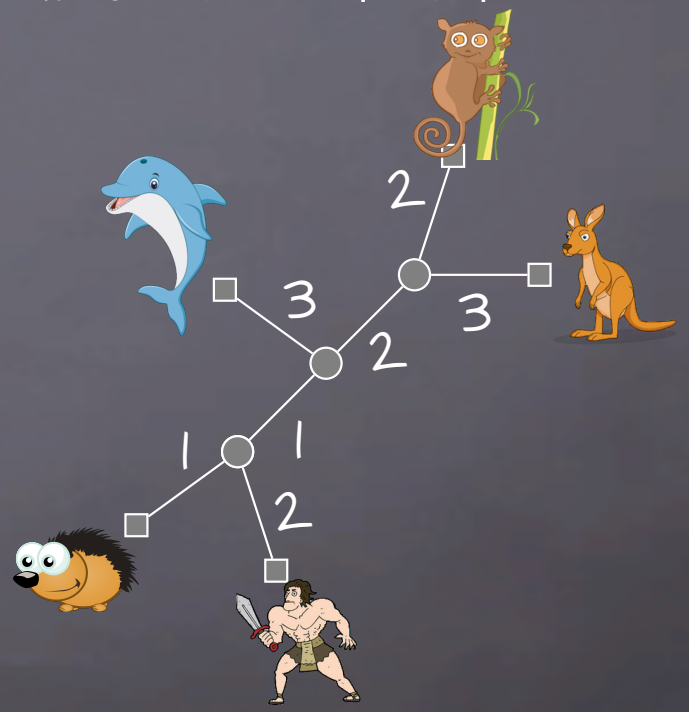

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Parsimony Reconstructing

Parsimony Reconstructing

	fur	AUS	pouch	land
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	✗	✓	✗	✓
	✗	✗	✗	✗
	✓	✓	✓	✓
	✓	✗	✗	✓

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	✓	✓	✓	✓
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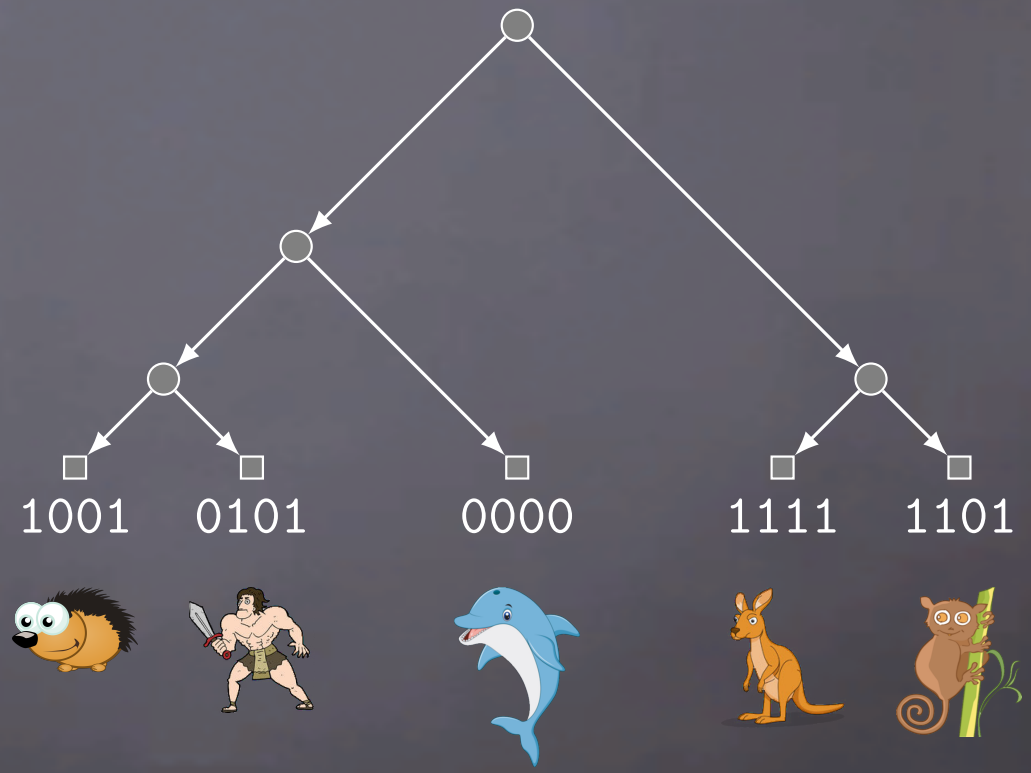

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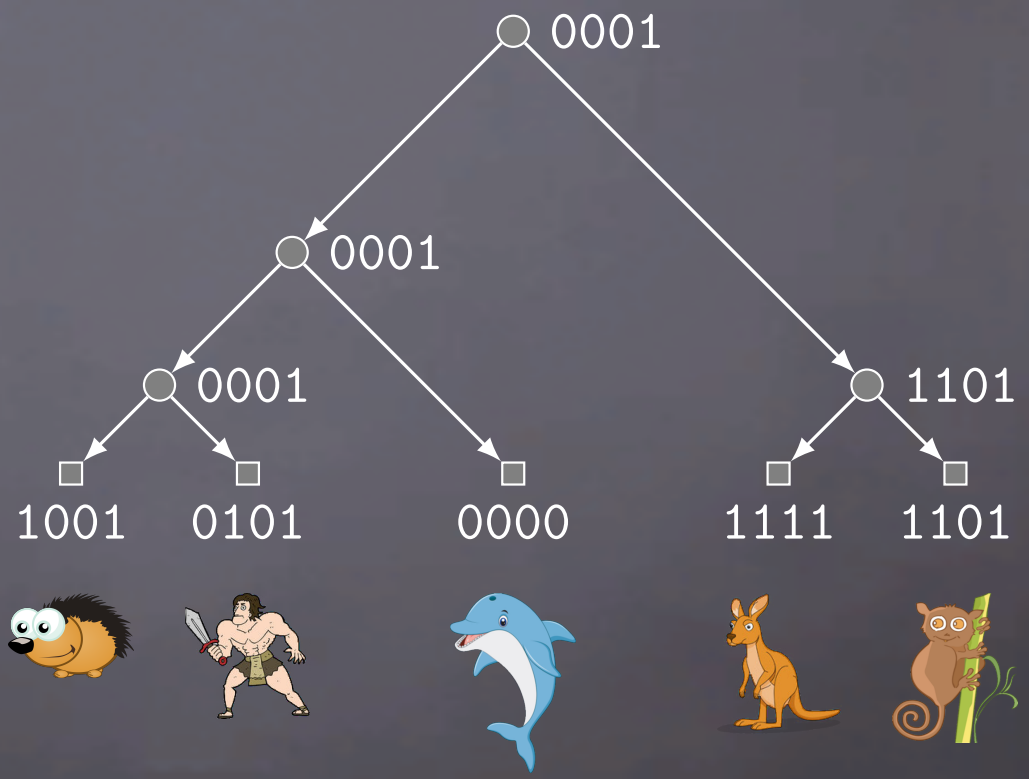
	✗	✓	✗	✓
	✗	✗	✗	✗
	✓	✓	✓	✓
	✓	✗	✗	✓



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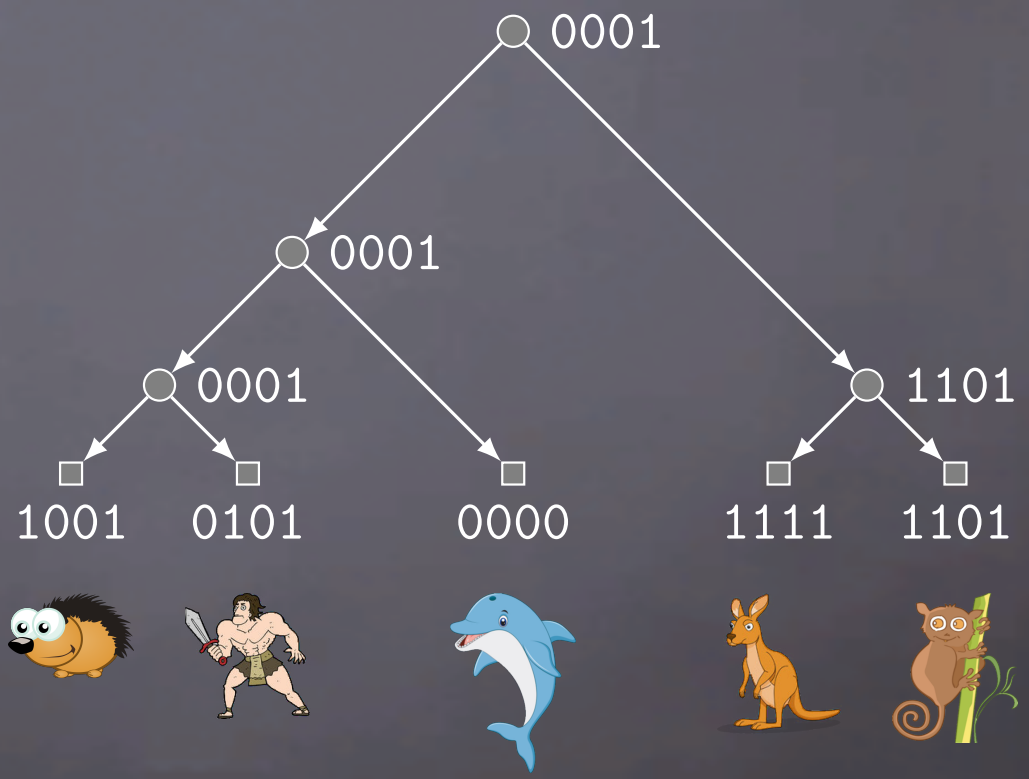
	fur	AUS	pouch	land
	✓	✓	✗	✓
	✗	✓	✗	✓
	✗	✗	✗	✗
	✓	✓	✓	✓
	✓	✗	✗	✓



sum "distance" of endpoints of each edge

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	✗	✗	✗	✗
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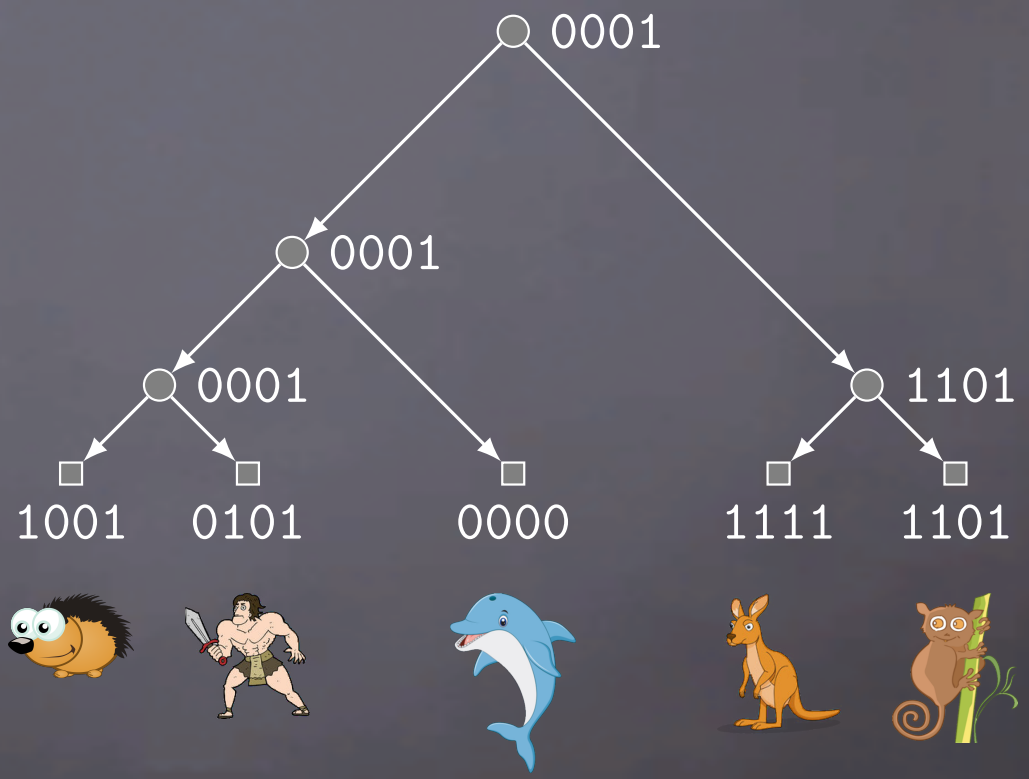

sum "distance" of endpoints of each edge ⇝ cost 6 (Hamming)

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	fur	AUS	pouch	land
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	✗	✓	✗	✓
	✗	✗	✗	✗
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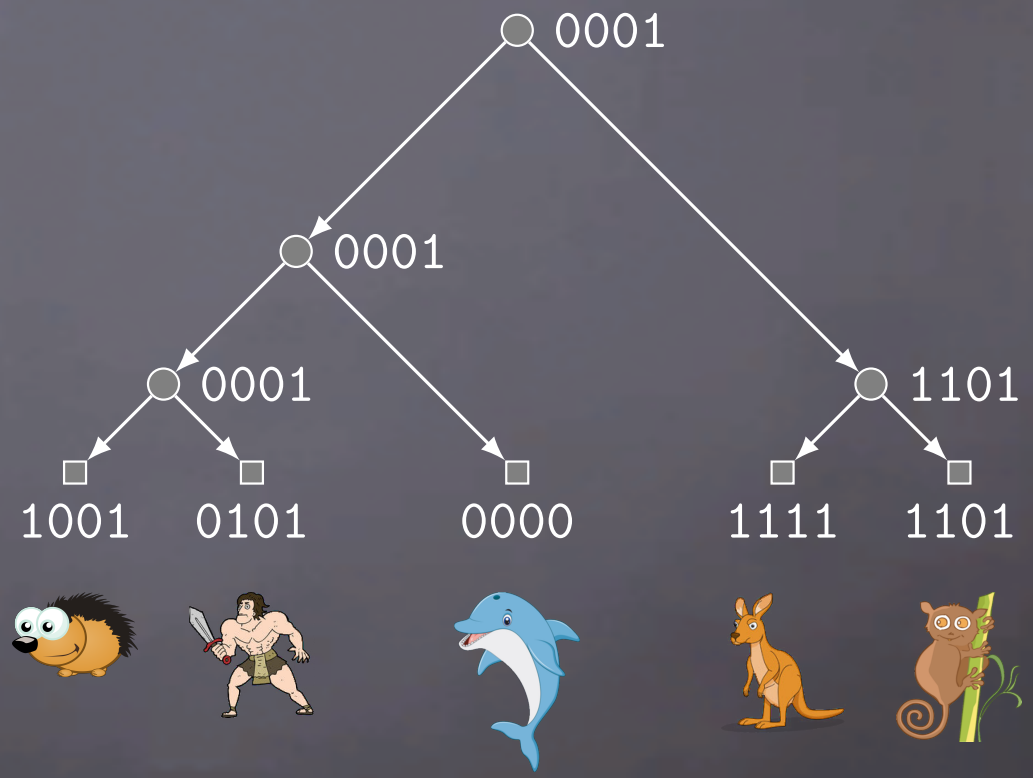
	✓	✗	✗	✓

Small Parsimony

Input: character state matrix M, rooted tree T

Task: assign characters to internal nodes minimizing total cost



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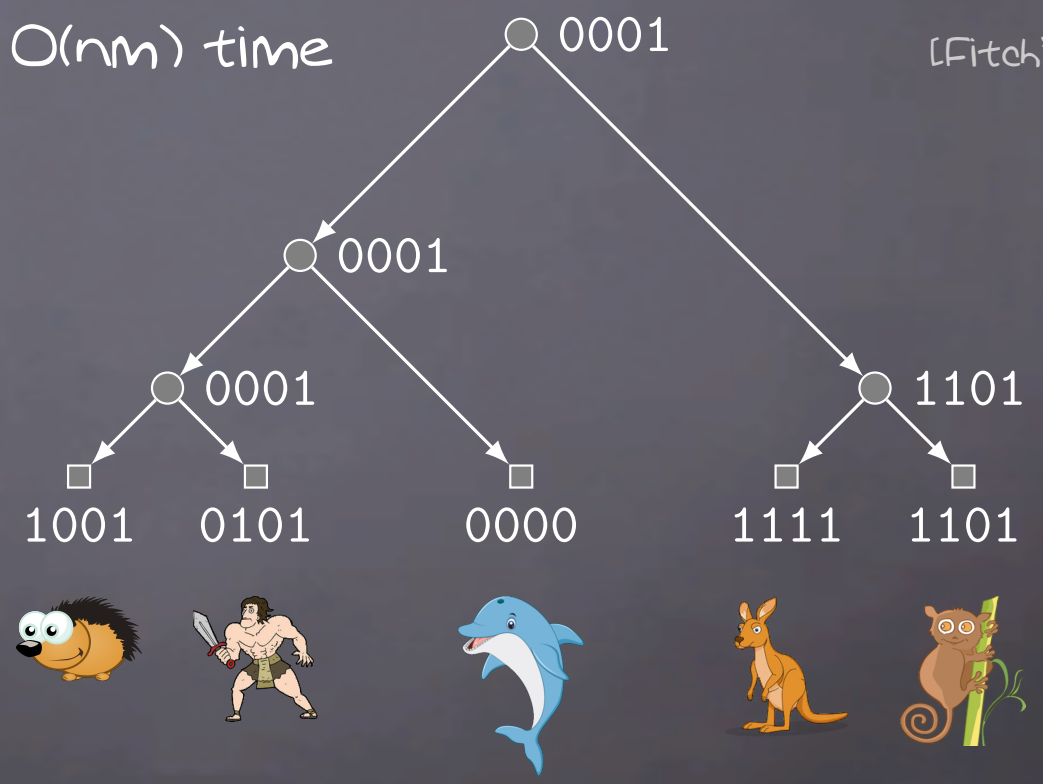
$\rightsquigarrow$ O(nm) time

[Fitch'71]



Algo (simple DFS):
Backtrack from v:
if v is leaf:
$\rightsquigarrow R(v) = \text{label}(v)$
else if $R(u) \cap R(w) = \emptyset$:
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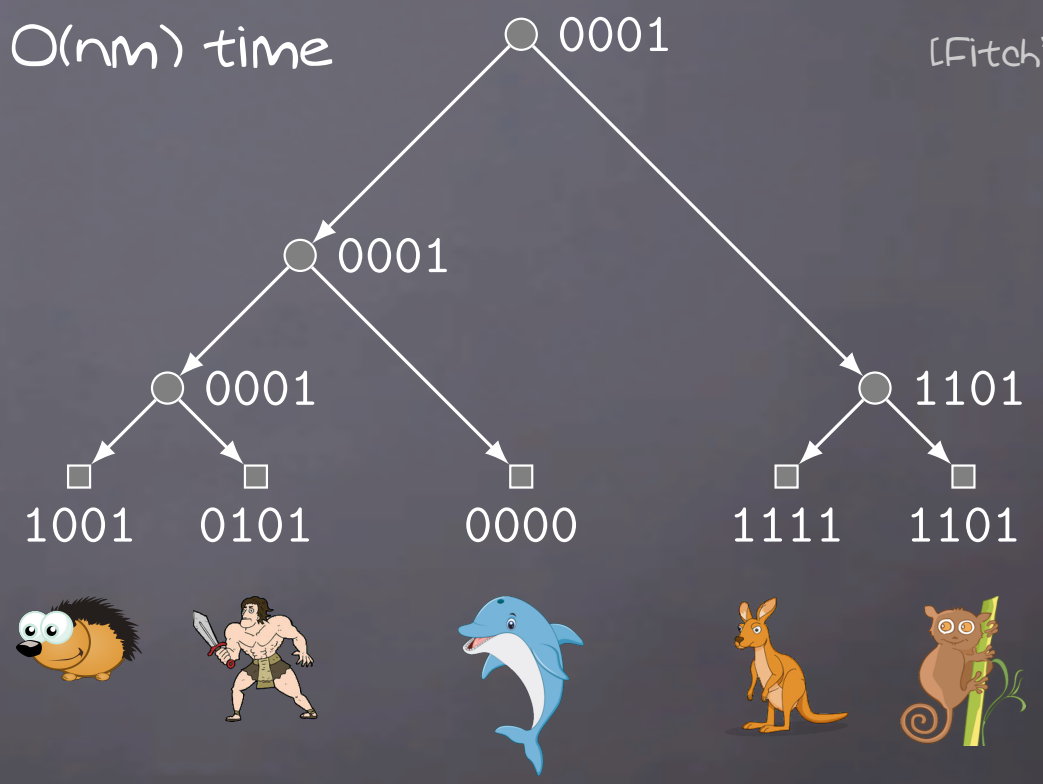

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Note: alignment is crucial!

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- each base occurs with equal frequency in the genome
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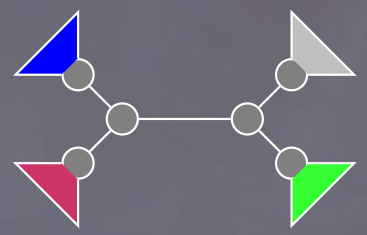
find best tree & parameters $\rightsquigarrow$ NP-hard
$\rightsquigarrow$ local search in the tree space

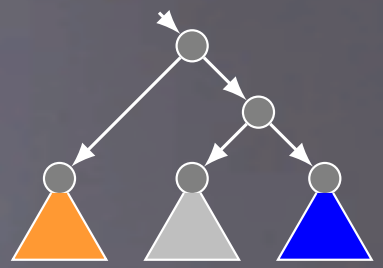
ML Reconstruction - Tree Spaces

Observe: a tree and a rearrangement operation span a space

Nearest Neighbor Interchange

change any configuration
of 4 (3) "neighboring"
subtrees into another





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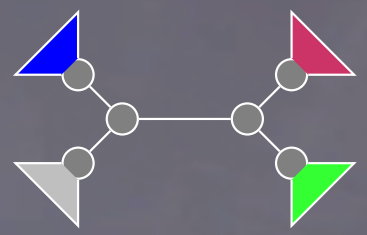

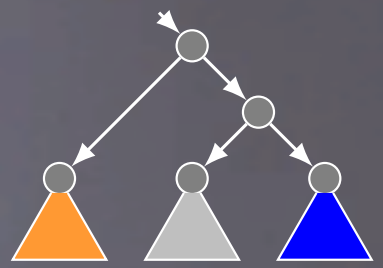

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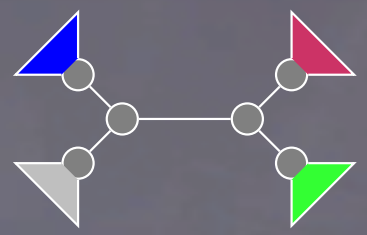

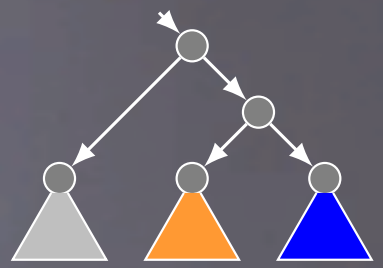

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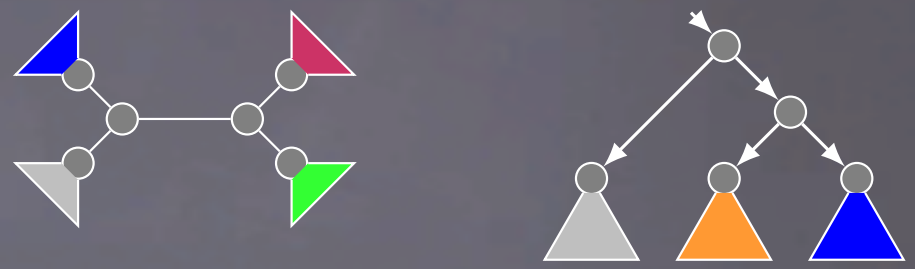

Subtree Prune & Regraft

Break any edge uv & connect v to any edge of the component of u

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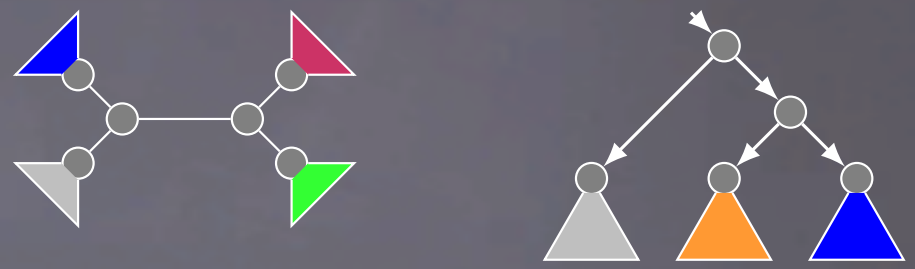

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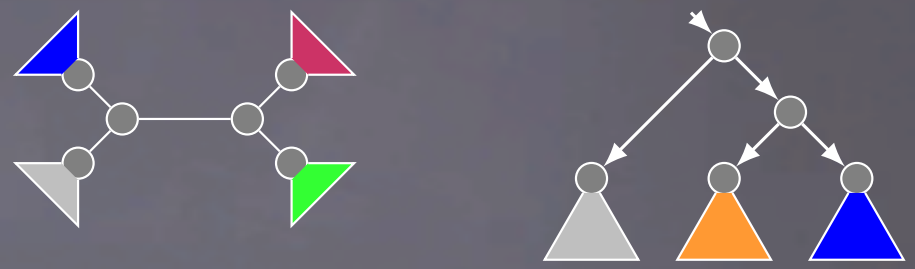

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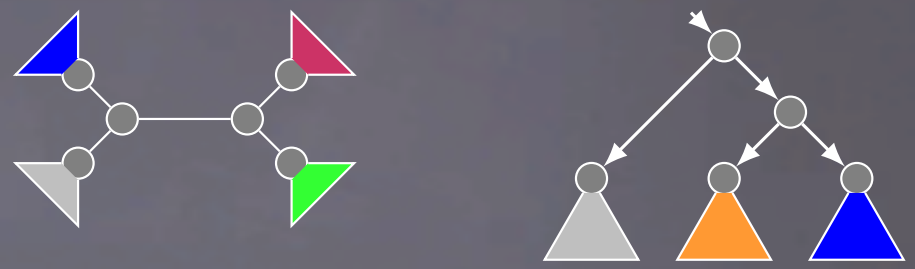

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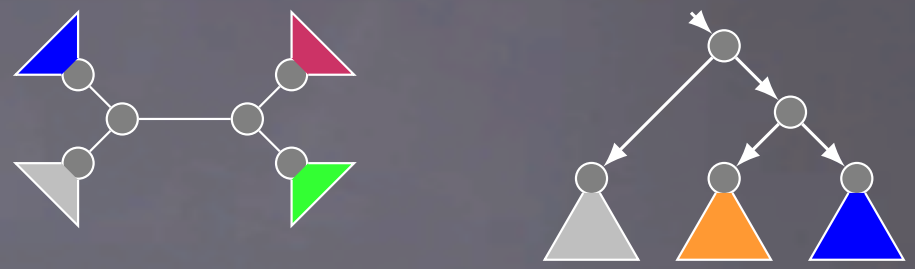

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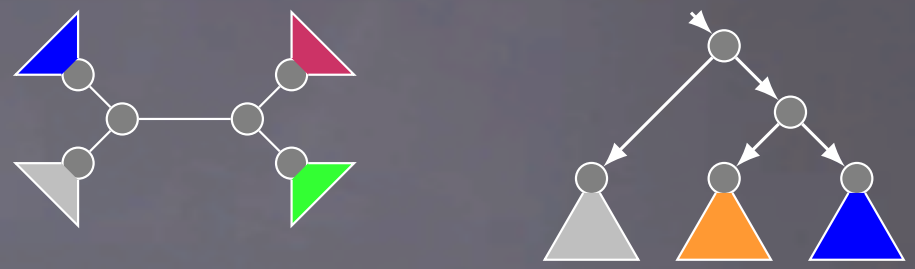

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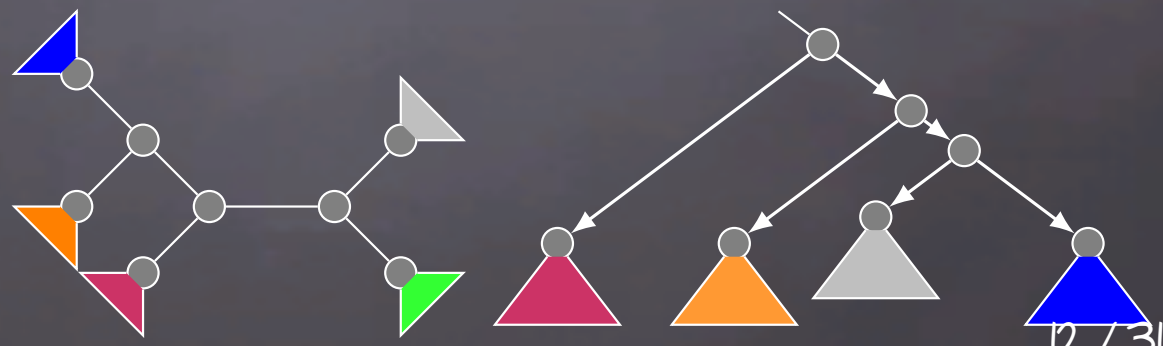

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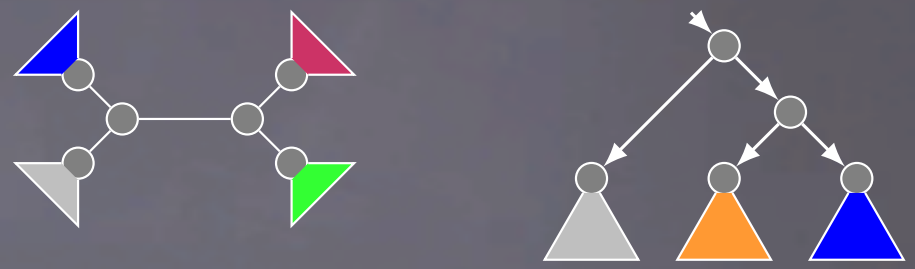

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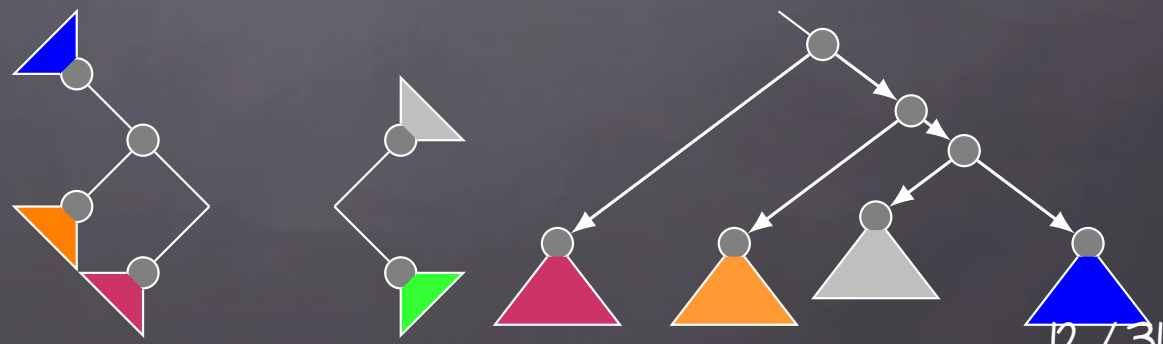

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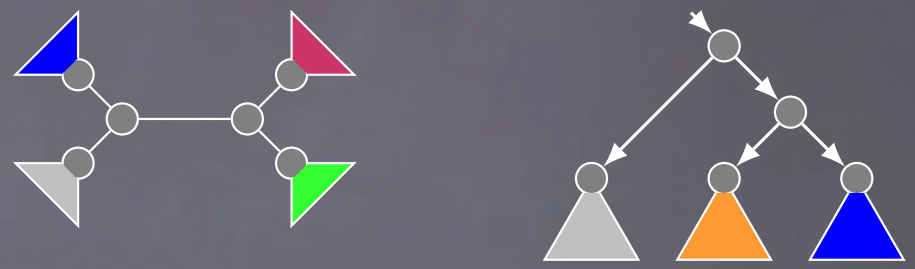

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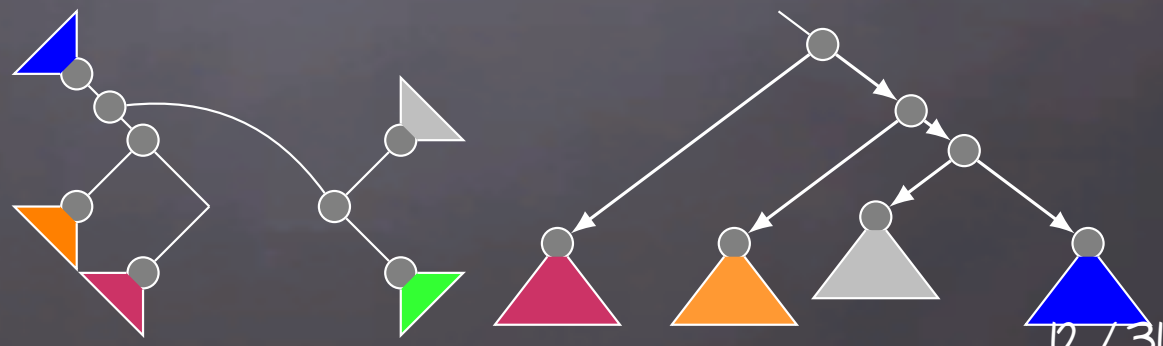

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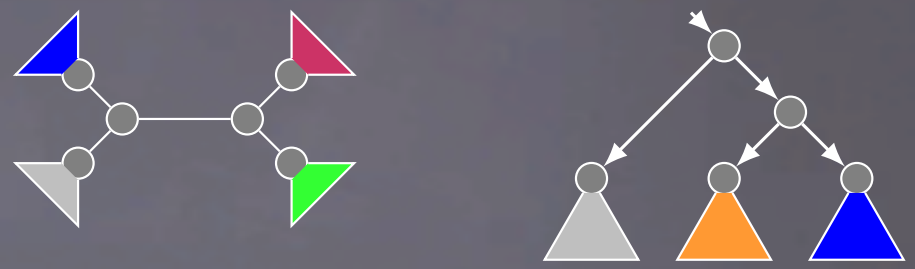

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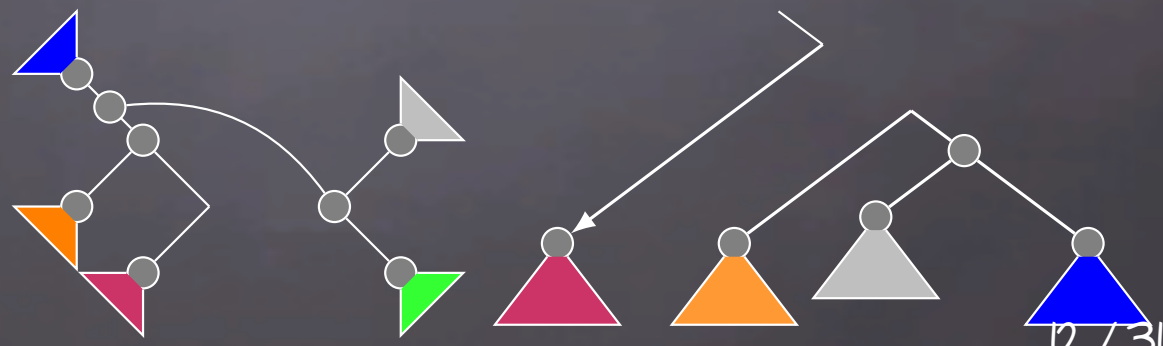

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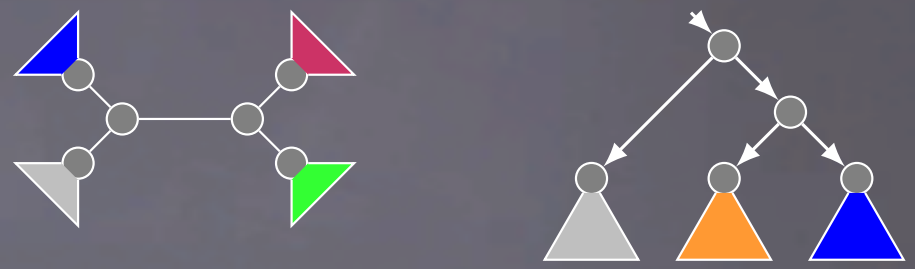

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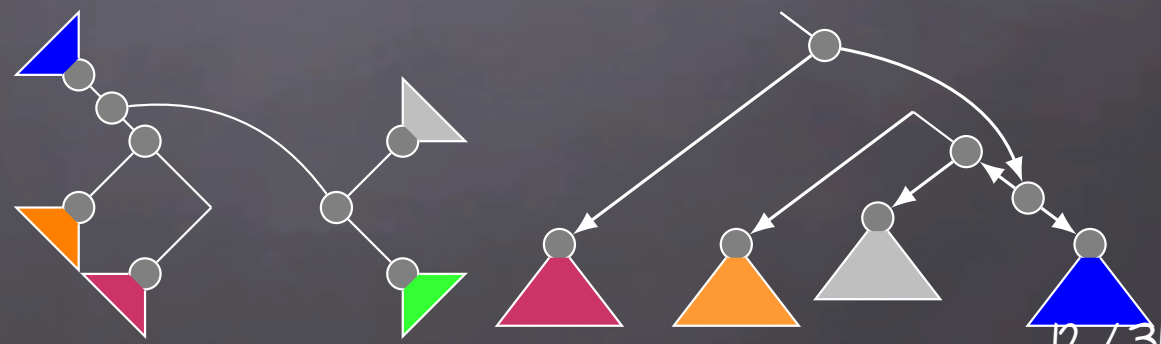
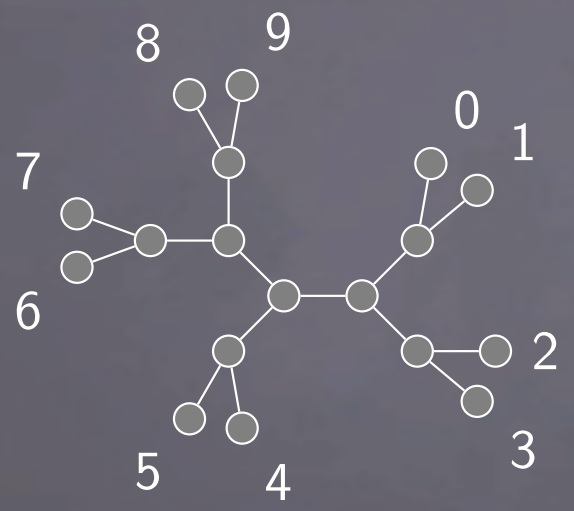


ML Reconstruction - Tree Spaces

Exercise: turn into (any) caterpillar:



Exercise: how are the distances related?

Checking Robustness – Bootstrap Method

suppose: method $\mathcal{X}$ yields tree T from $n \times m$ character-state matrix M
repeat k times the following experiment:

1. draw m columns from M (with repetition)
2. use $\mathcal{X}$ to compute T_i

Finally, for each branch of T, check how often it occurs in the T_i
$\rightsquigarrow$ "bootstrap value" measures robustness ("support") of each branch

Reconstruction by Gene Trees

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A Common Method For Reconstructing Trees

1. get genomes of multiple species
2. extract "genes" using START & STOP codons
3. cluster genes in "families" of similar genes
4. within each family, infer a "gene tree" using dissimilarities
5. Build a consensus among the gene trees $\rightsquigarrow$ "species tree"
   (Note: species tree may differ significantly from individual gene trees)
6. reconcile all gene trees with the species tree to learn the evolution of those genes

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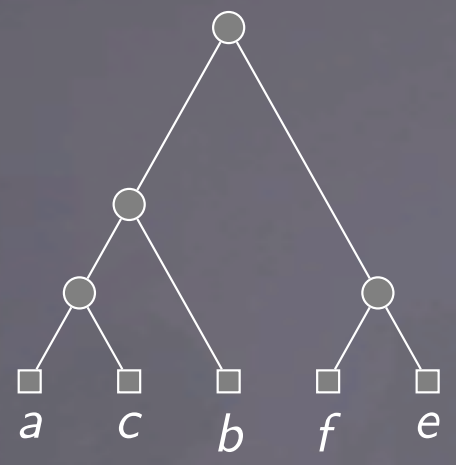
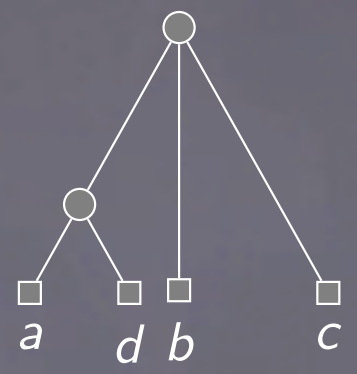
Supertrees - "Build" Algorithm

Idea: find root partition & recurse (as long as there are ≥ 3 taxa)





Algo [Aho et al'81]

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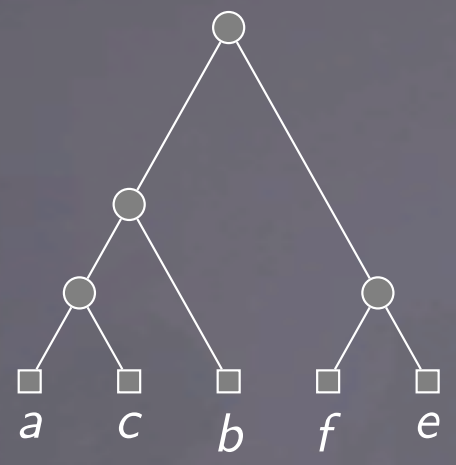

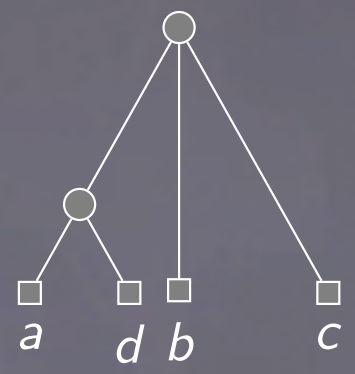

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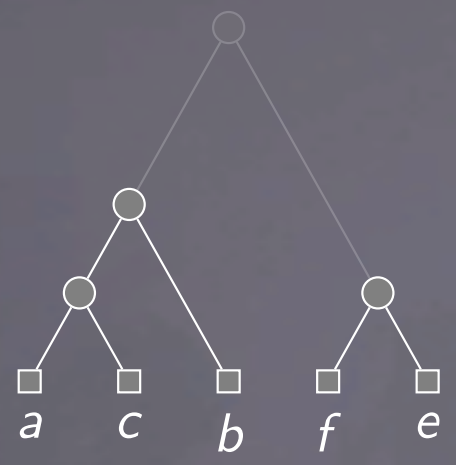

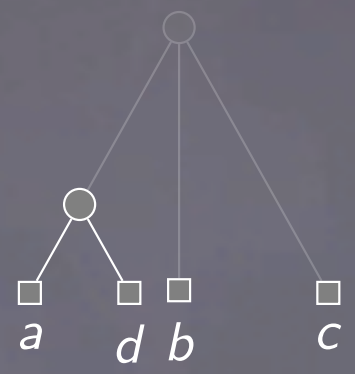

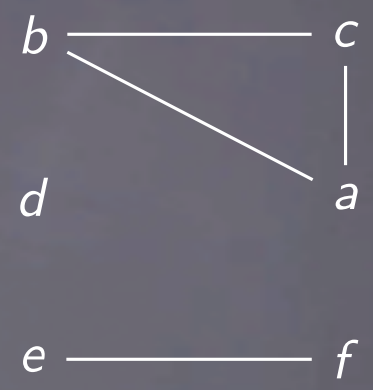

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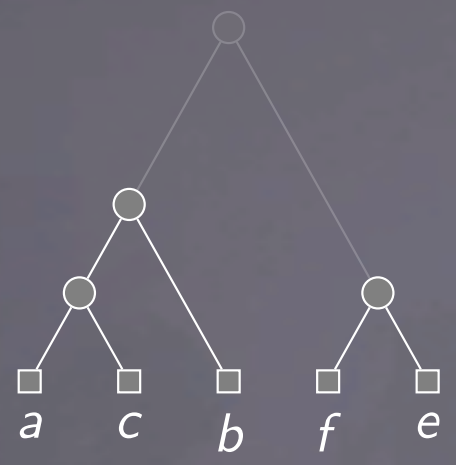

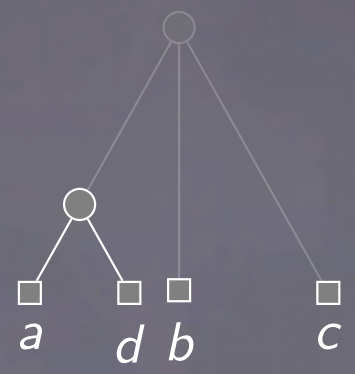

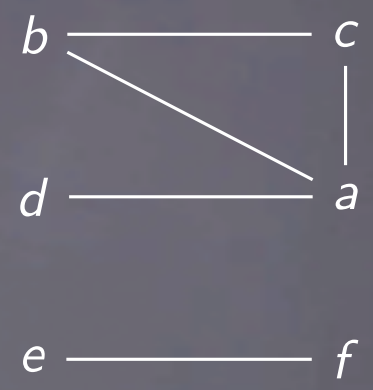

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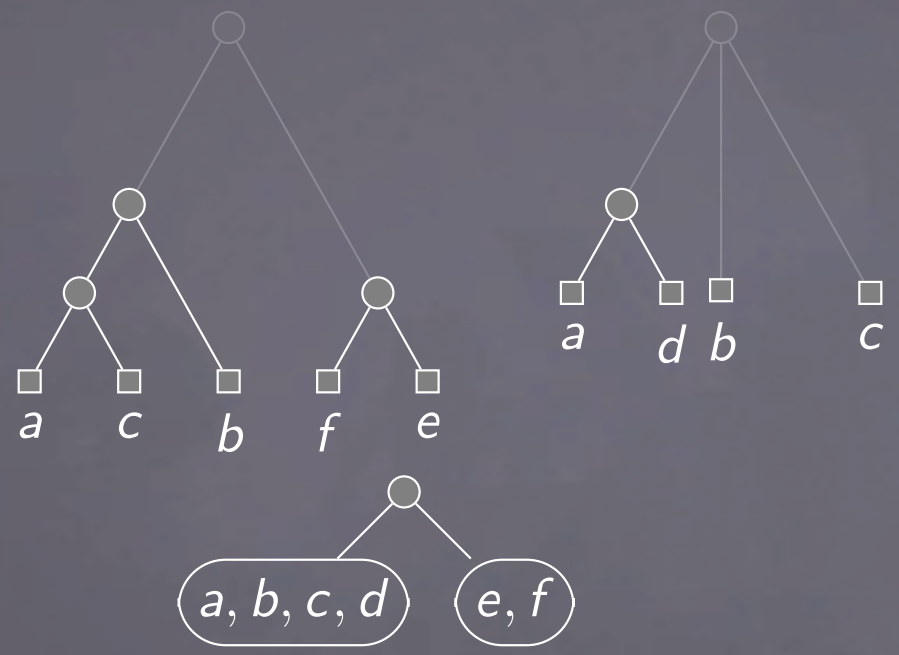

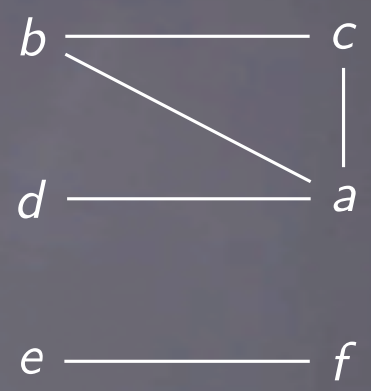

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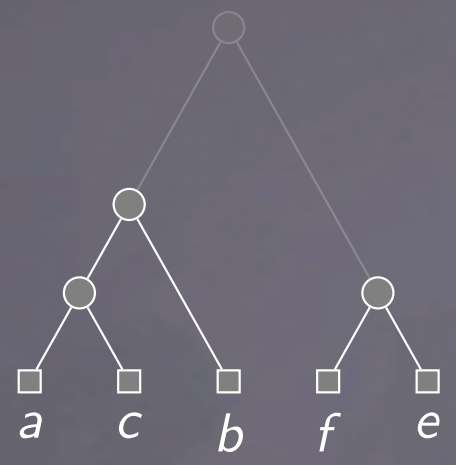

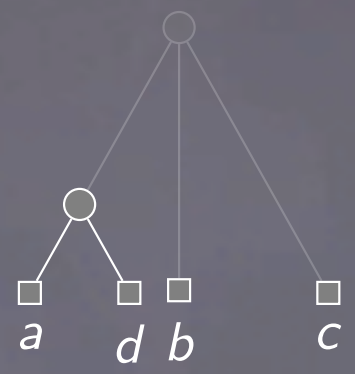

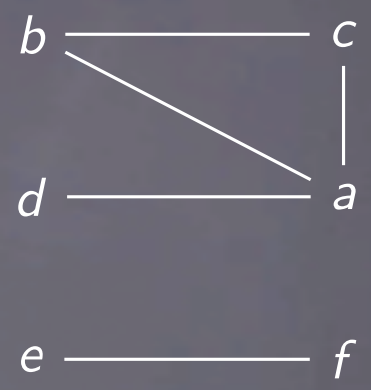

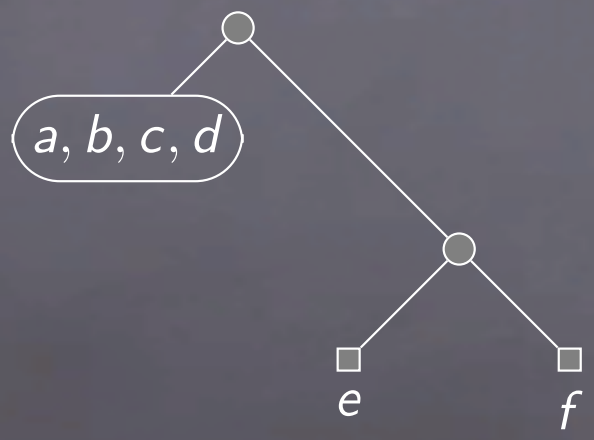

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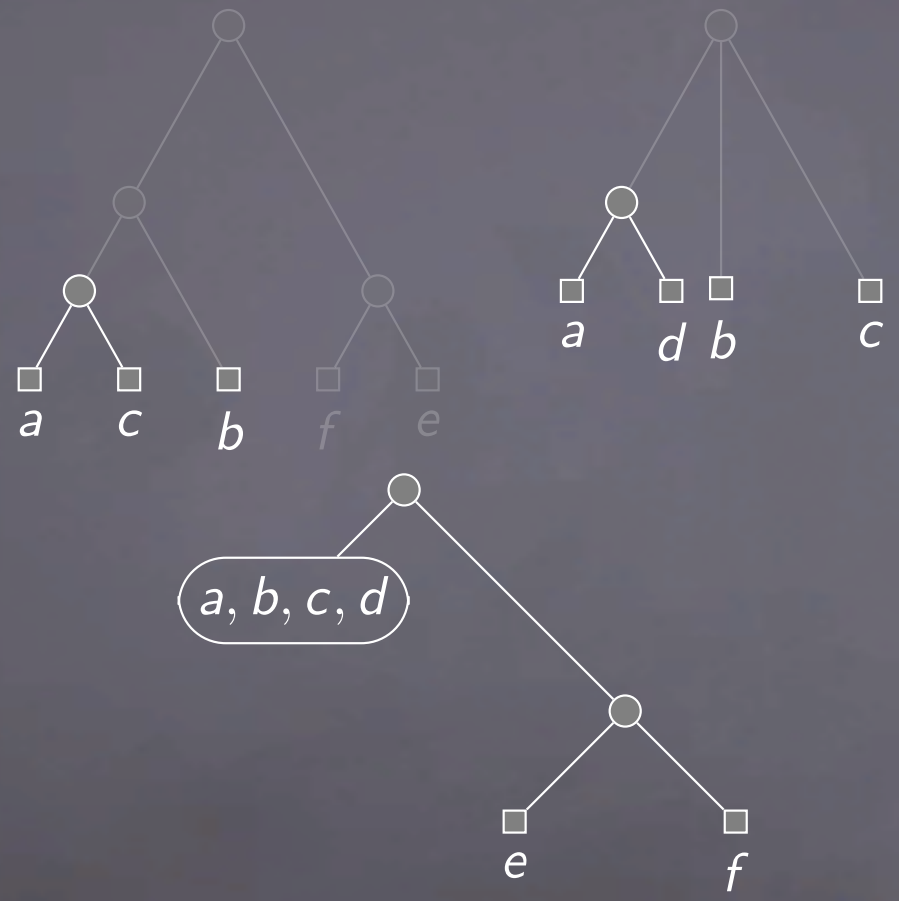

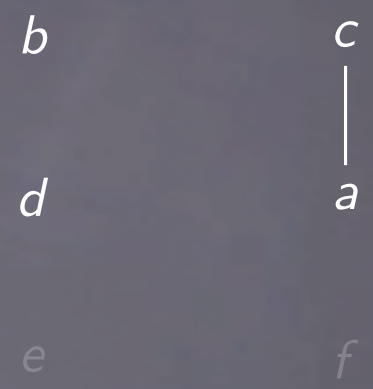

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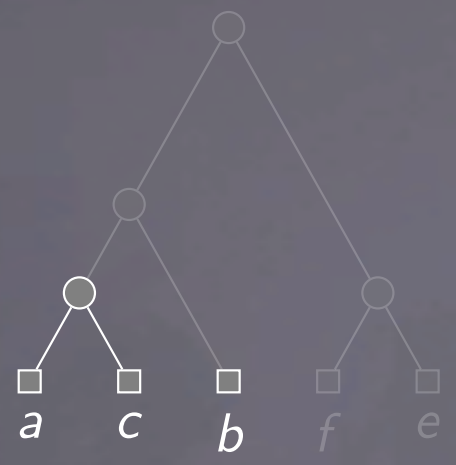

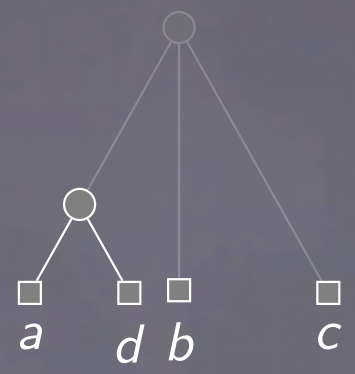

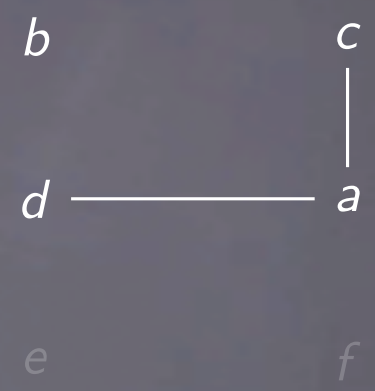

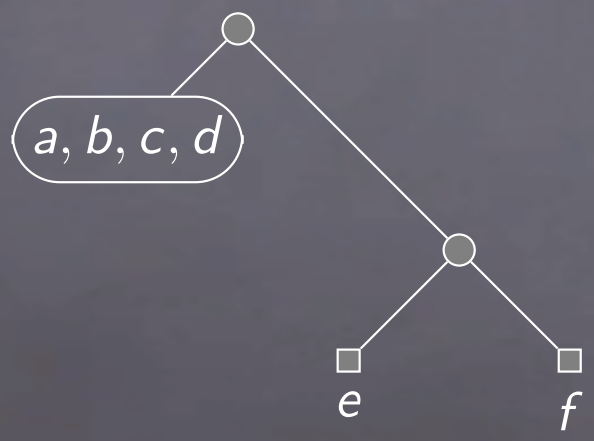

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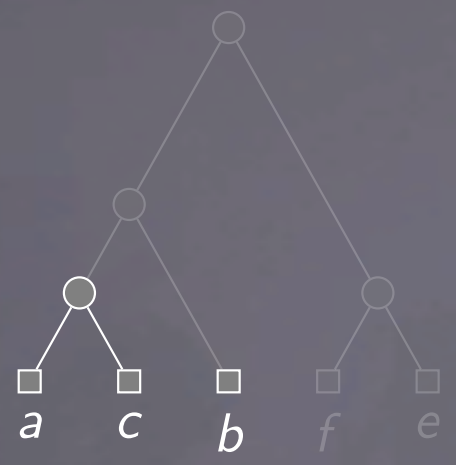

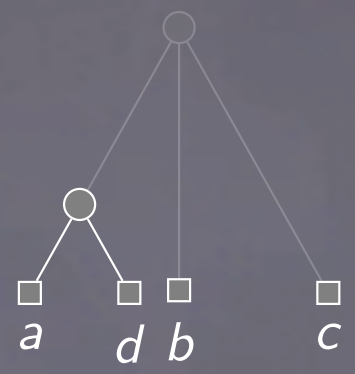

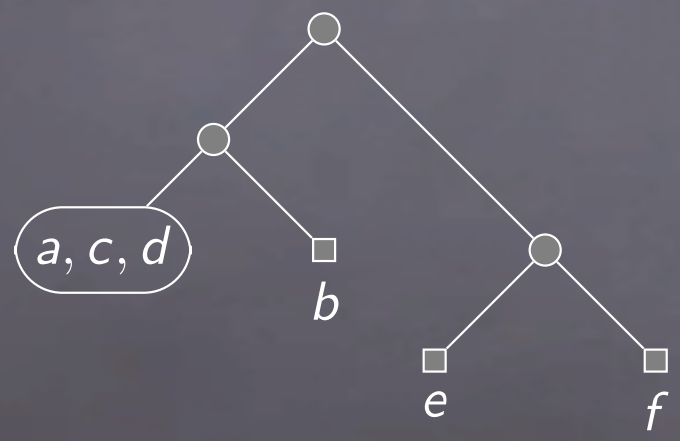

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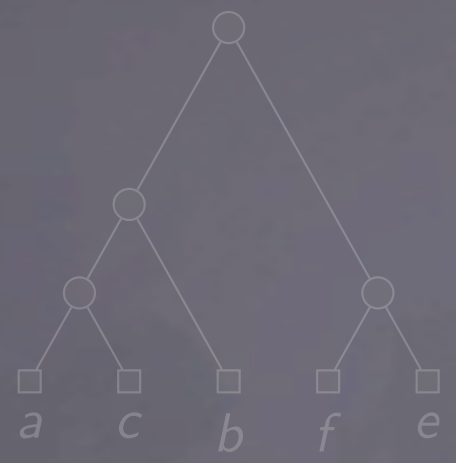

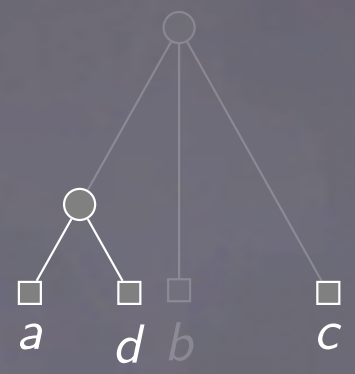

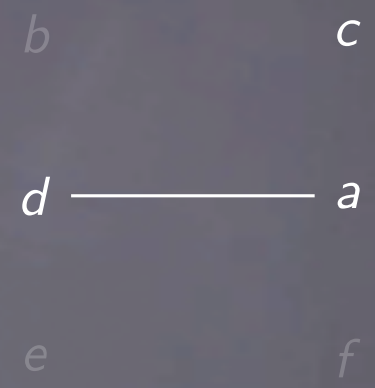

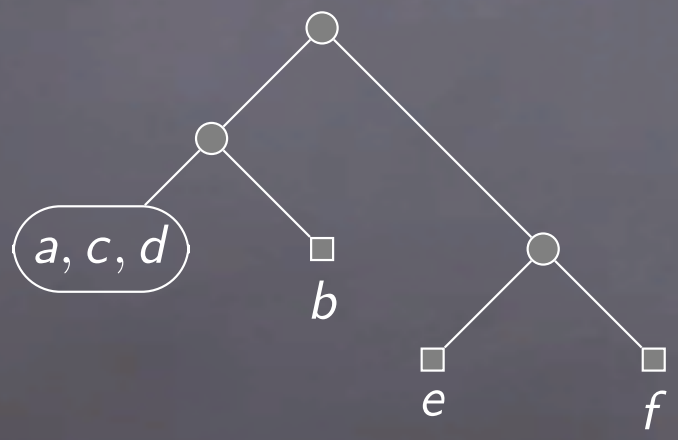

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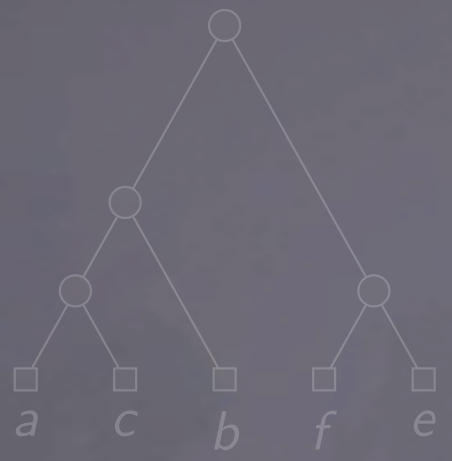

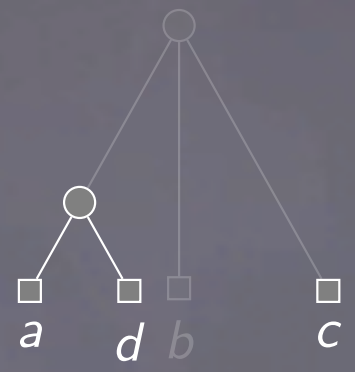

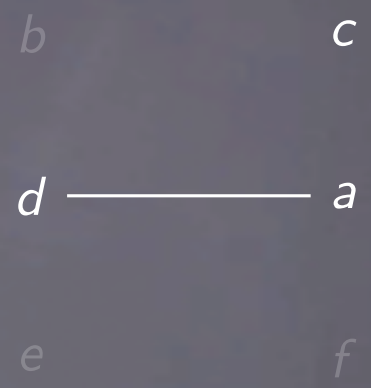

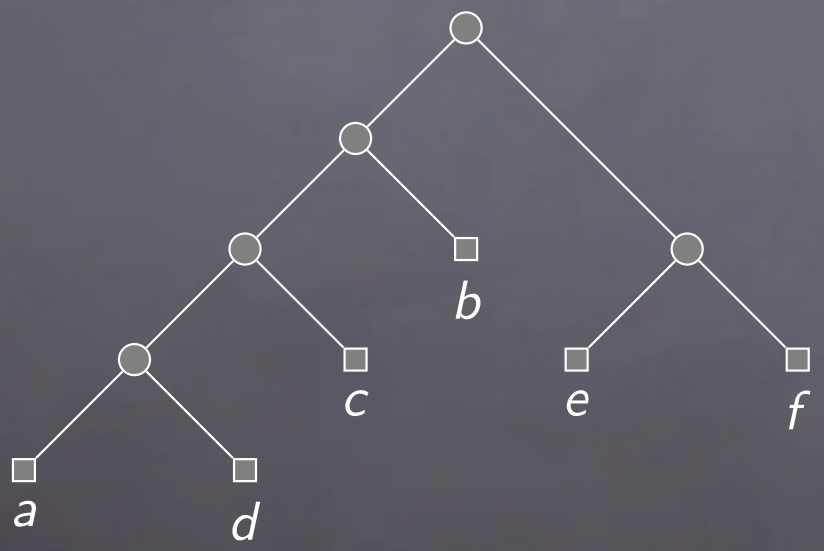

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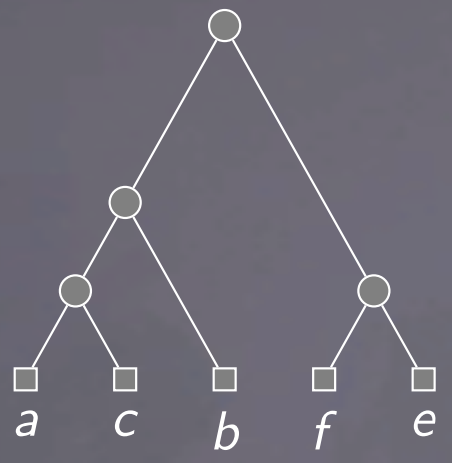
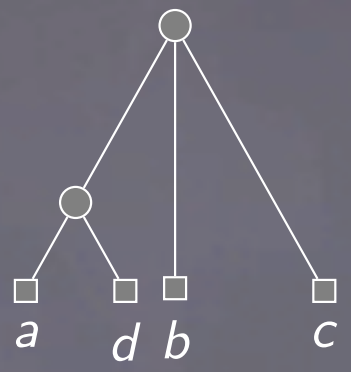
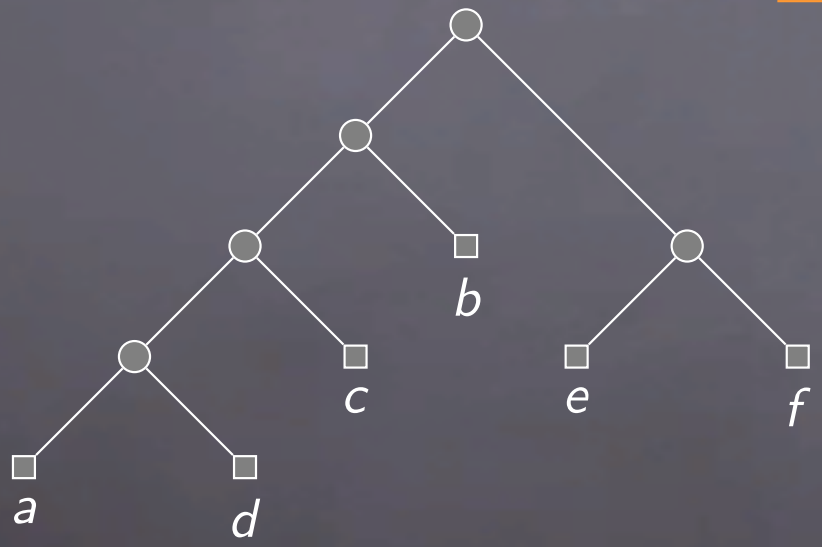




Note: always works if trees are compatible



Supertrees – "Build" Algorithm

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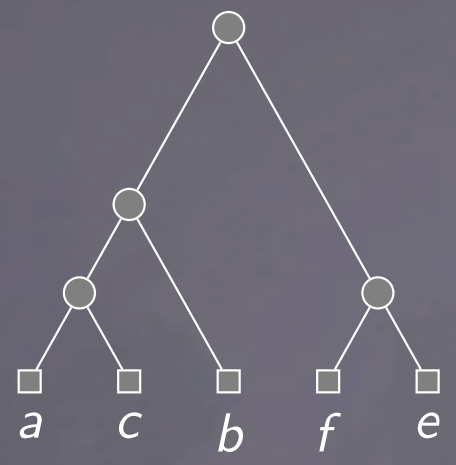

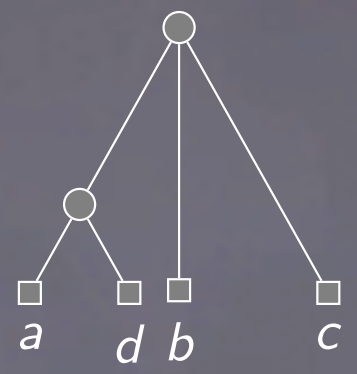

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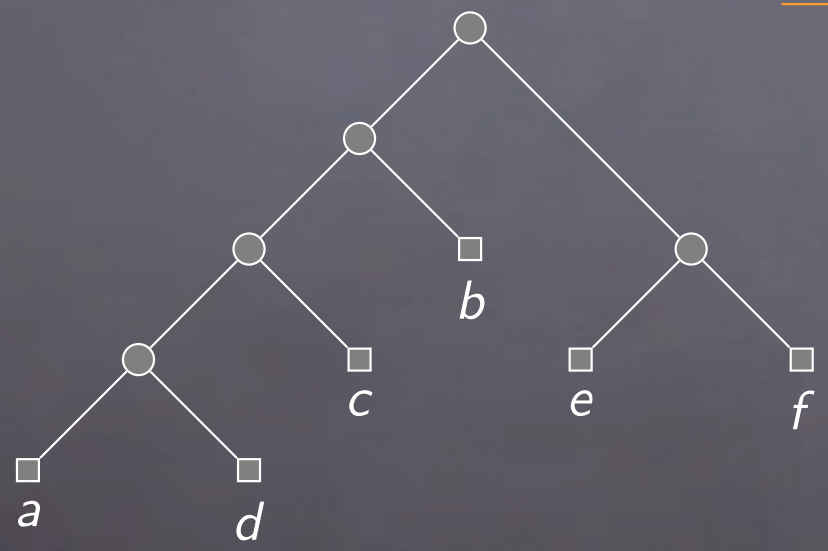


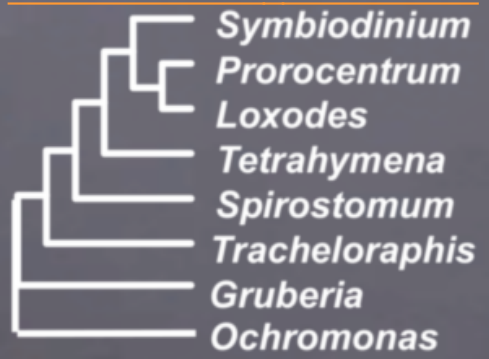
incompatible?

- largest compatible subset
  $\rightsquigarrow$ NP-hard (even for triplets)
- voting schemes
  (each tree votes for their clades)
- reinterpret clades as characters,
  combine into matrix & reconstruct

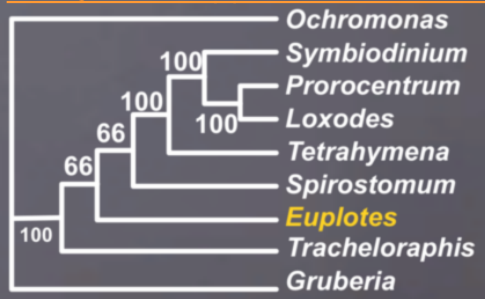
Consensi of Non-Agreeing Trees

strict consensus

consensus subtree



majority consensus



Reconstruction By Gene Trees

A Common Method For Reconstructing Trees

1. ~~get genomes of multiple species~~
2. ~~extract "genes" using START & STOP codons~~
3. ~~cluster genes in "families" of similar genes~~
4. ~~within each family, infer a "gene tree" using dissimilarities~~
5. Build a consensus among the gene trees $\rightsquigarrow$ "species tree"
   (Note: species tree may differ significantly from individual gene trees)
6. reconcile all gene trees with the species tree to learn the evolution of those genes

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The History of a Gene Family

Recall

gene = "functional element" of DNA, clustered into gene-families

```
Mouse  GGAGCTTGAGCCGGAATAGTAGGAACATCTTTAAGAATTTTAATTCGAGC
Dog    GGAATCTGAACAGGCTTAGTAGCCACTAGAATAAGACTTTTAATTCGAGC
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```
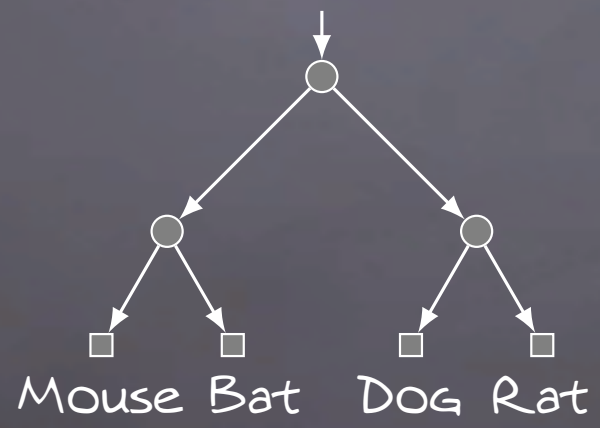
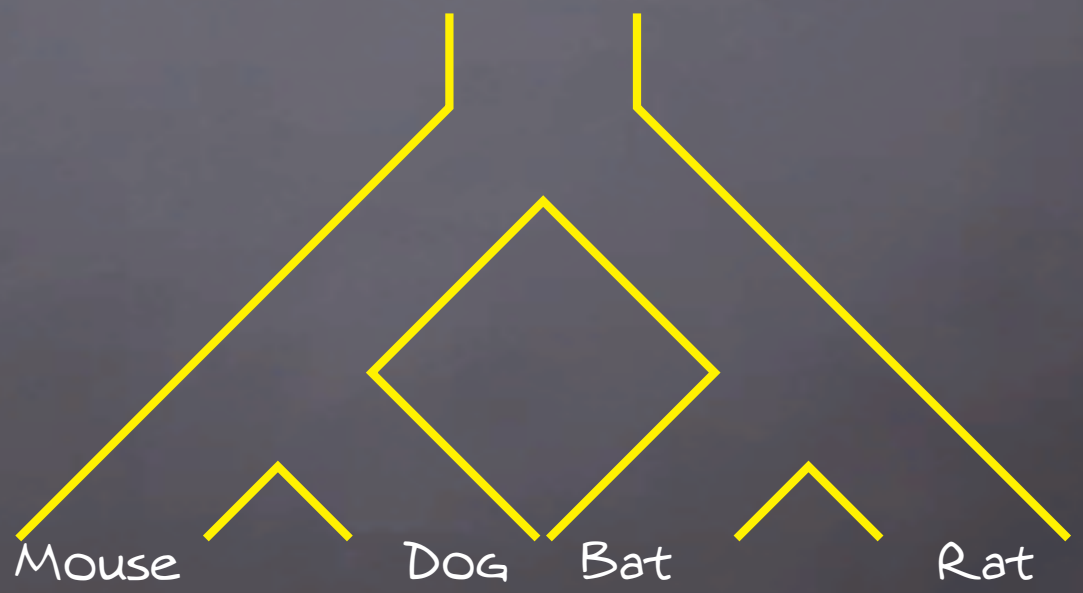

each family yields a tree depicting its history ⇝ "gene tree"
consensus of the gene trees yields "species tree"
But: what did really happen???





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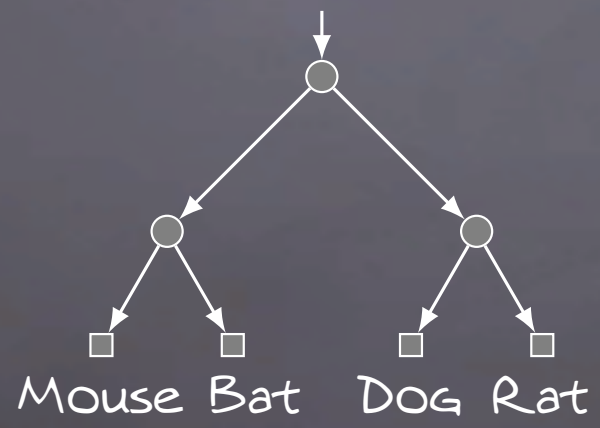

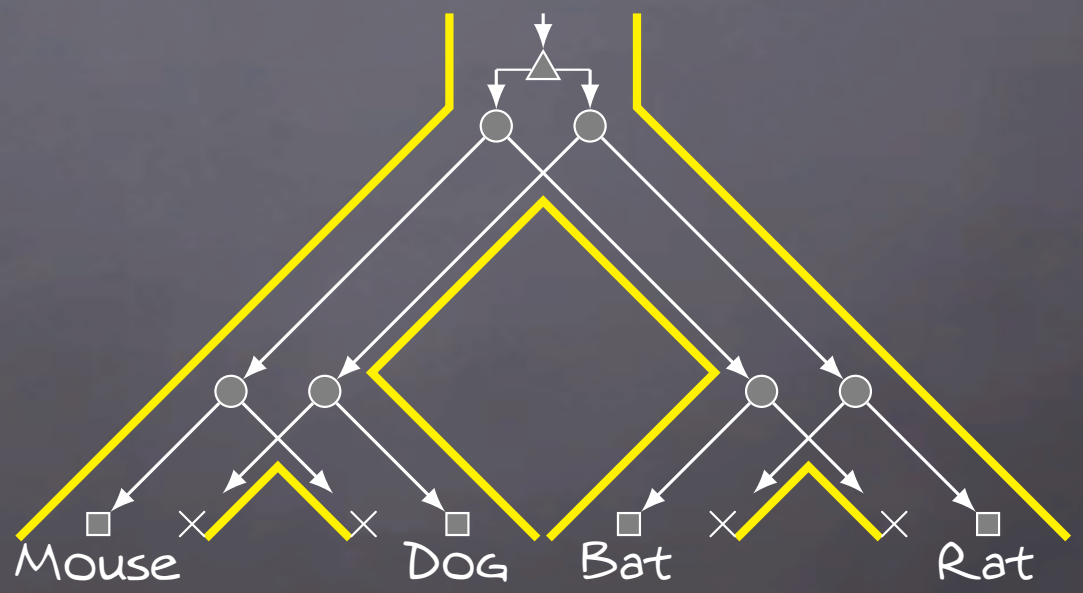

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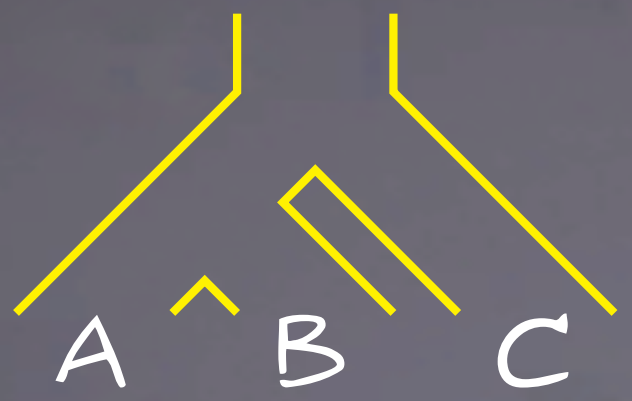
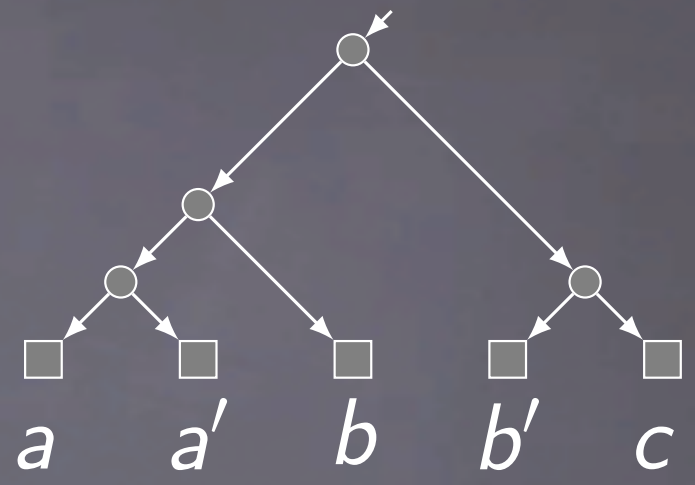


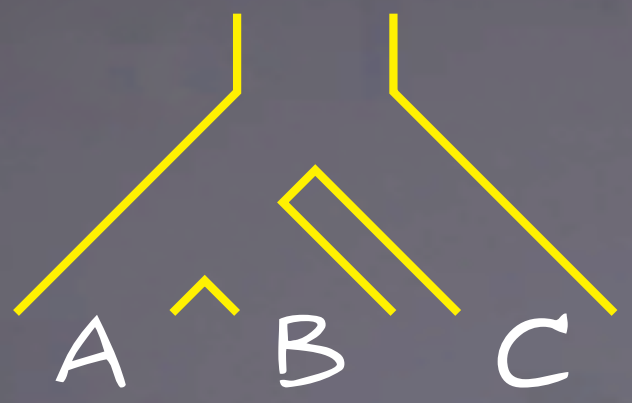


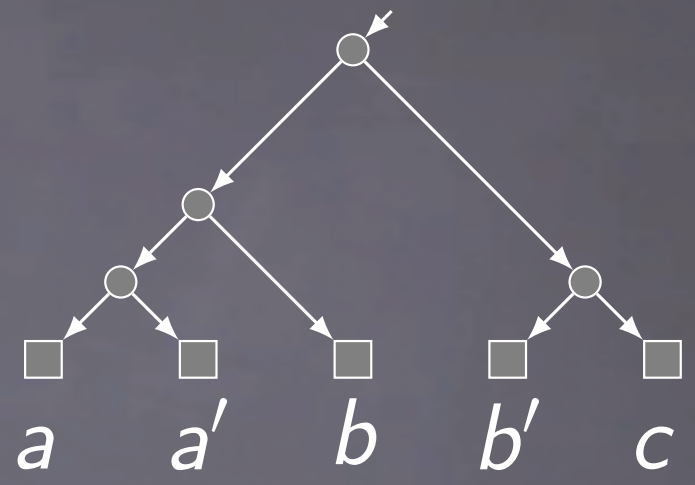
Embedding Rules

gene tree G, species tree S

- mapping $\rho : V(G) \to V(S)$
- ℓ is leaf in $G \rightsquigarrow \rho(\ell)$ "corresponds" to ℓ ($a \to A$, $a' \to A$, etc.)
- $u \in V(G)$ is called duplication if $\rho(u) = \rho(c)$ for any child c of u in G
- all non-leaves of G that not duplications are called speciations
- each edge uv of G incurs a loss-cost equal to the number of edges in the $\rho(u)$-$\rho(v)$-path in S minus 1 if v is a speciation or 0 if v is a duplication

Reconciliation



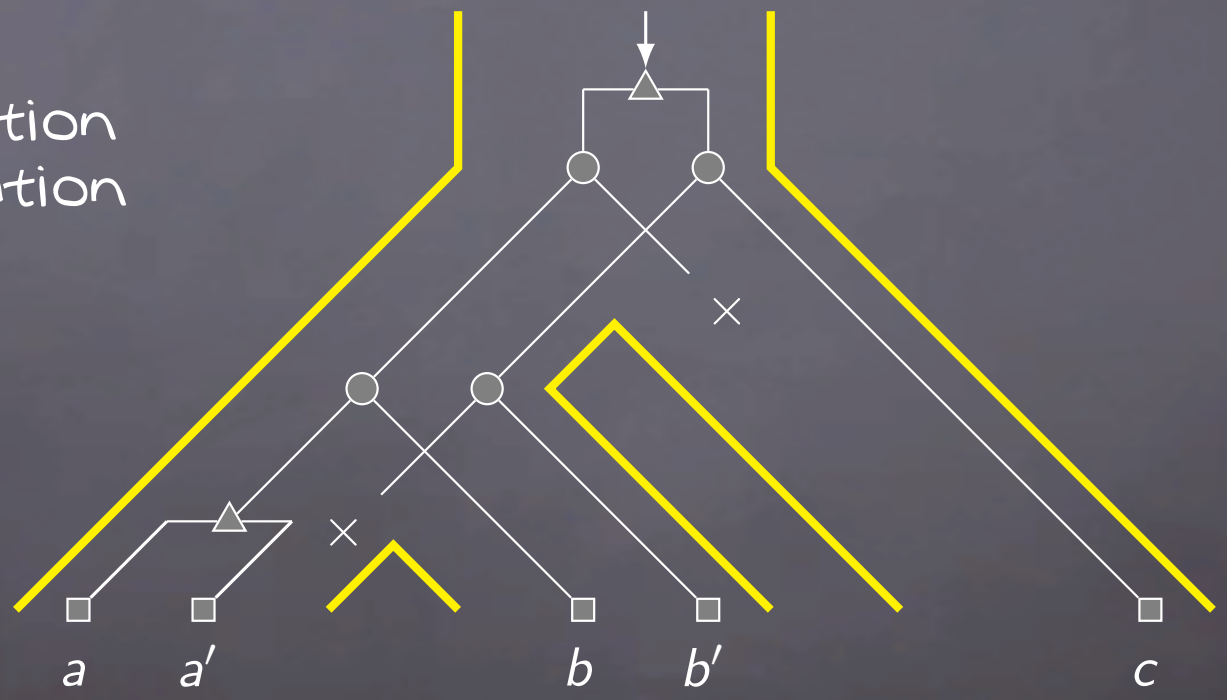


DL-model

○ = speciation

△ = duplication

× = loss



Reconciliation

Goal: embed gene tree into species tree
(extant genes must map to their species)

Max. Likelihood

find most probable embedding
(computationally expensive)

Parsimony

find embedding minimizing
#events (possibly weighted)

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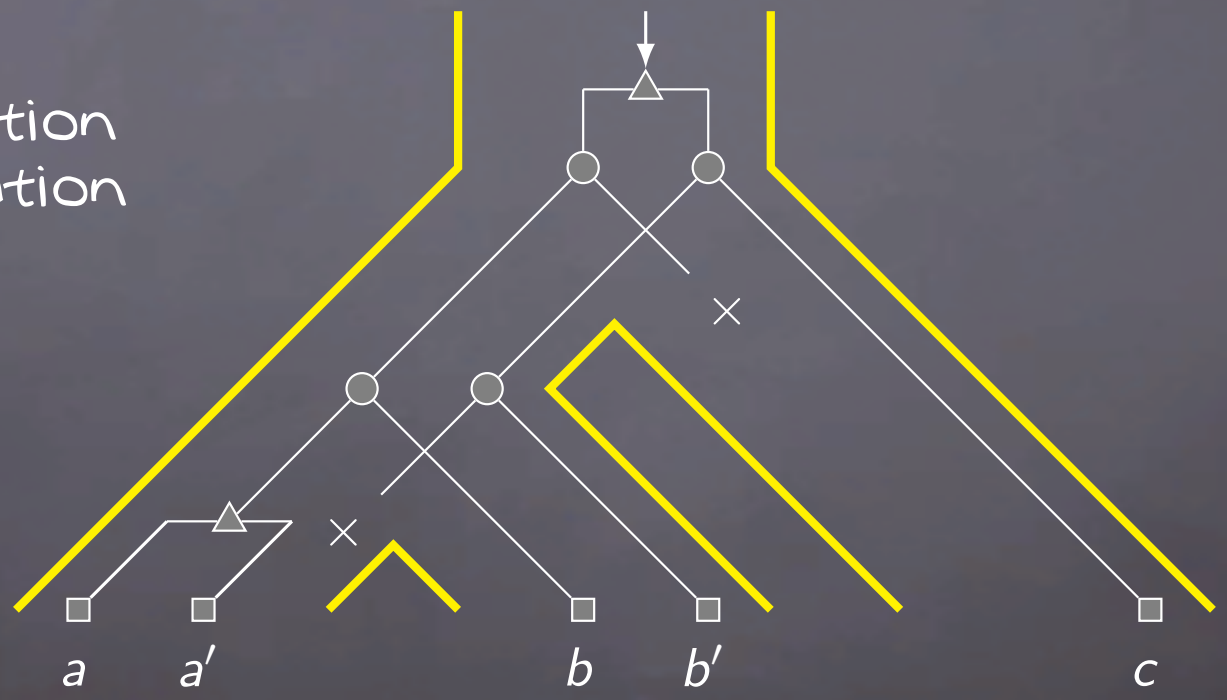

Reconciliation

Parsimonious Reconciliation

Input: species tree S, gene tree G, $\delta, \lambda \in \mathbb{N}$

Task: embed G in S, minimizing the weighted sum of events

Result: LCA-assignment solves this optimally in $O(|S|+|G|)$

DL-model

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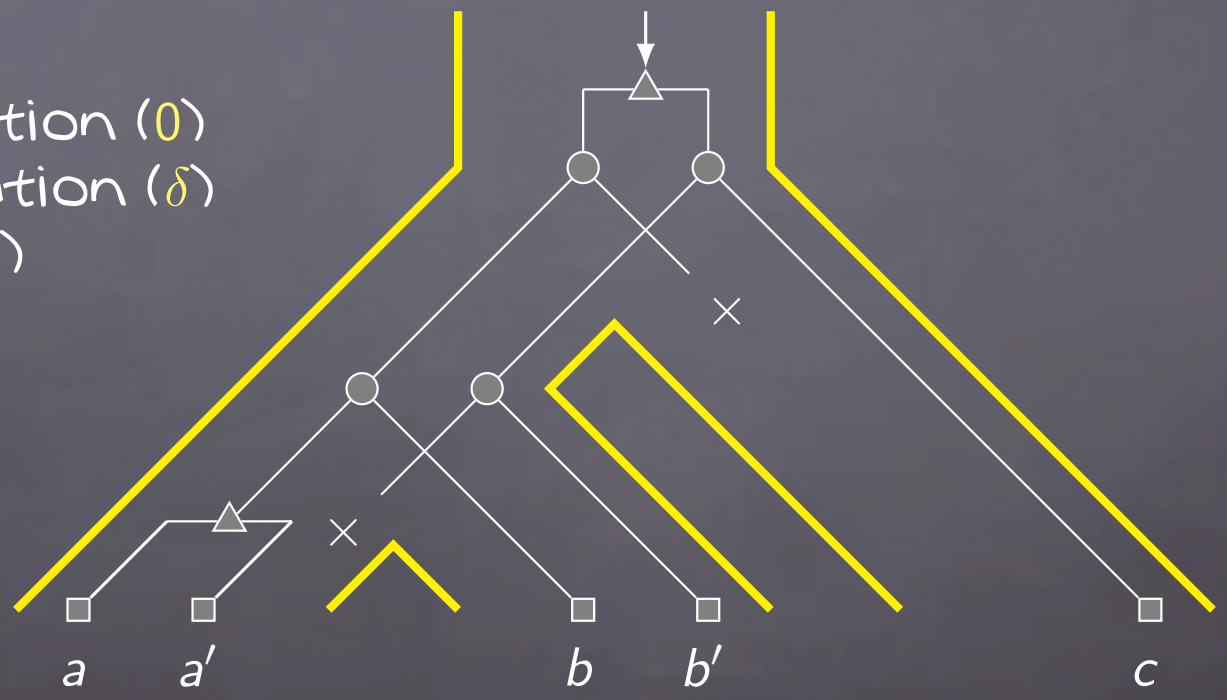

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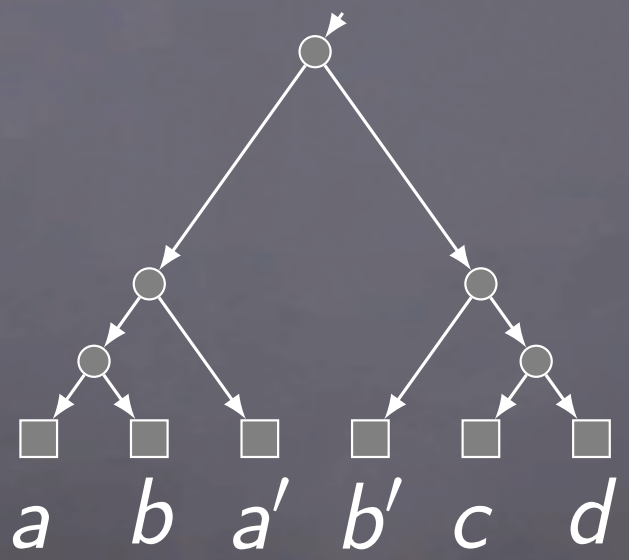

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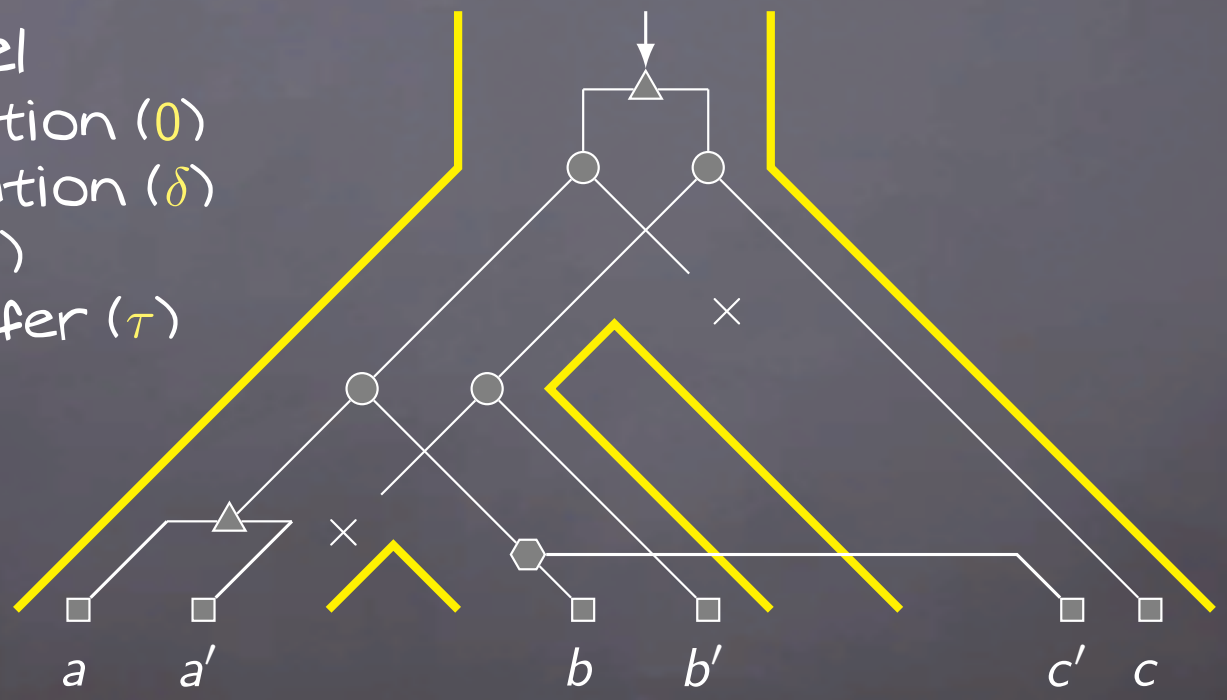

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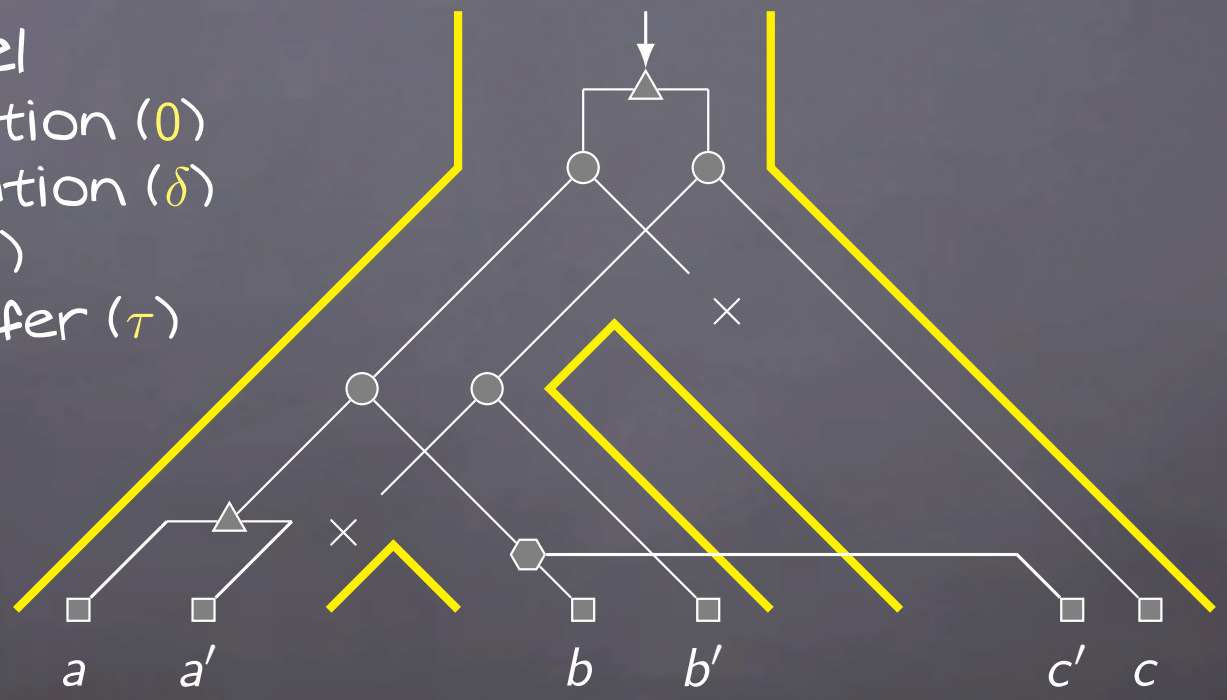

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Idea: take dated species tree $\rightsquigarrow$ $O(|S|^2|G|)$ time [Doyon et al.'10]

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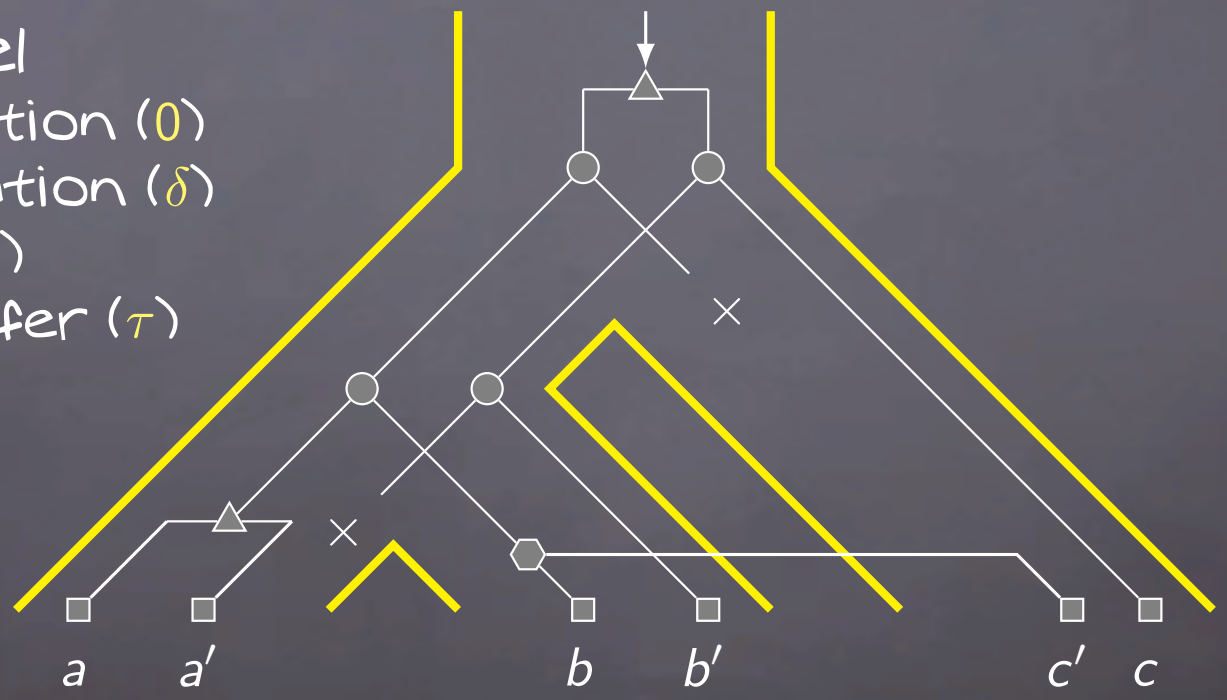

Comparing Phylogenetic Trees

Distance Measures

- Nearest Neighbor Interchange
- Subtree Prune & Regraft
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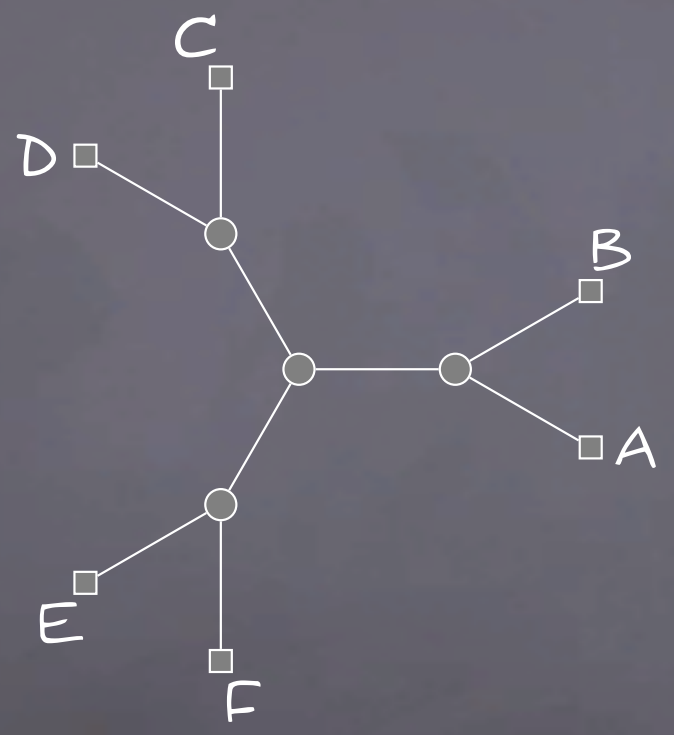
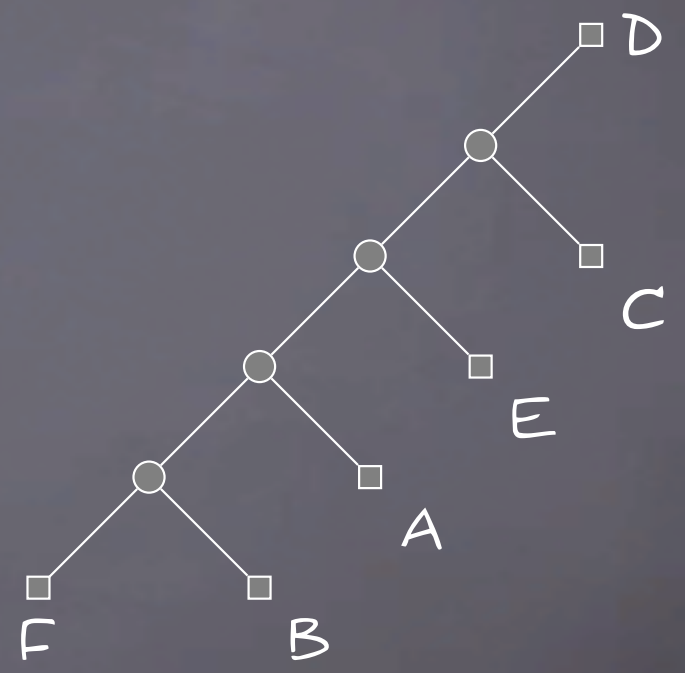
- quartet/triplet distance

Agreement Forests

Definition

A forest F is called **agreement forest** of trees T_1 and T_2 if F can be obtained from T_1 and T_2 by removing edges.





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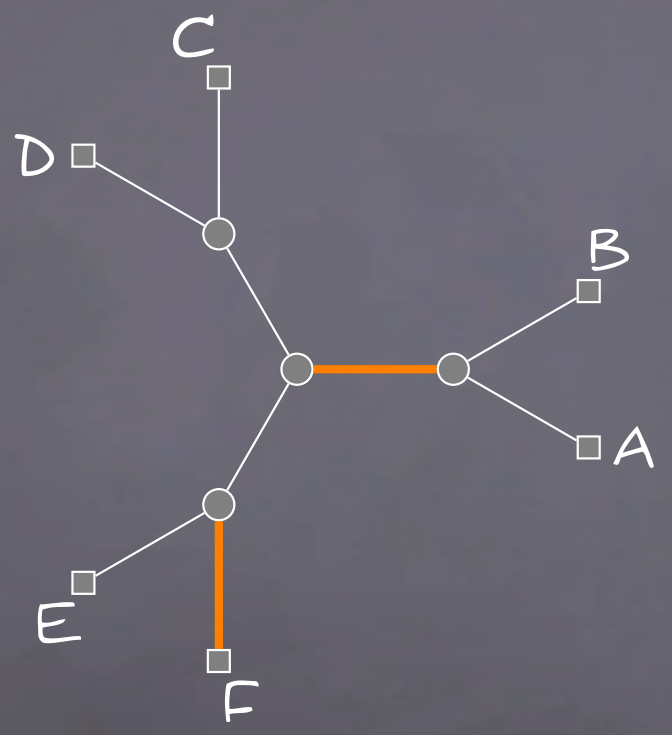

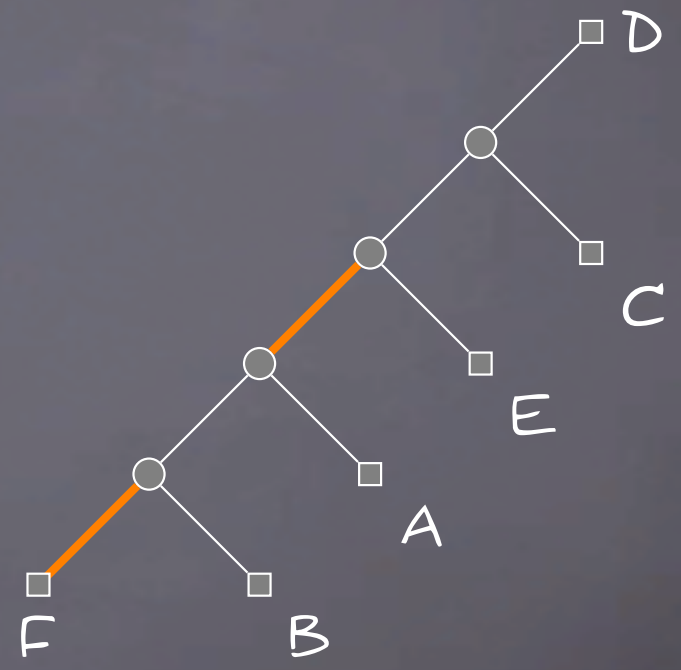

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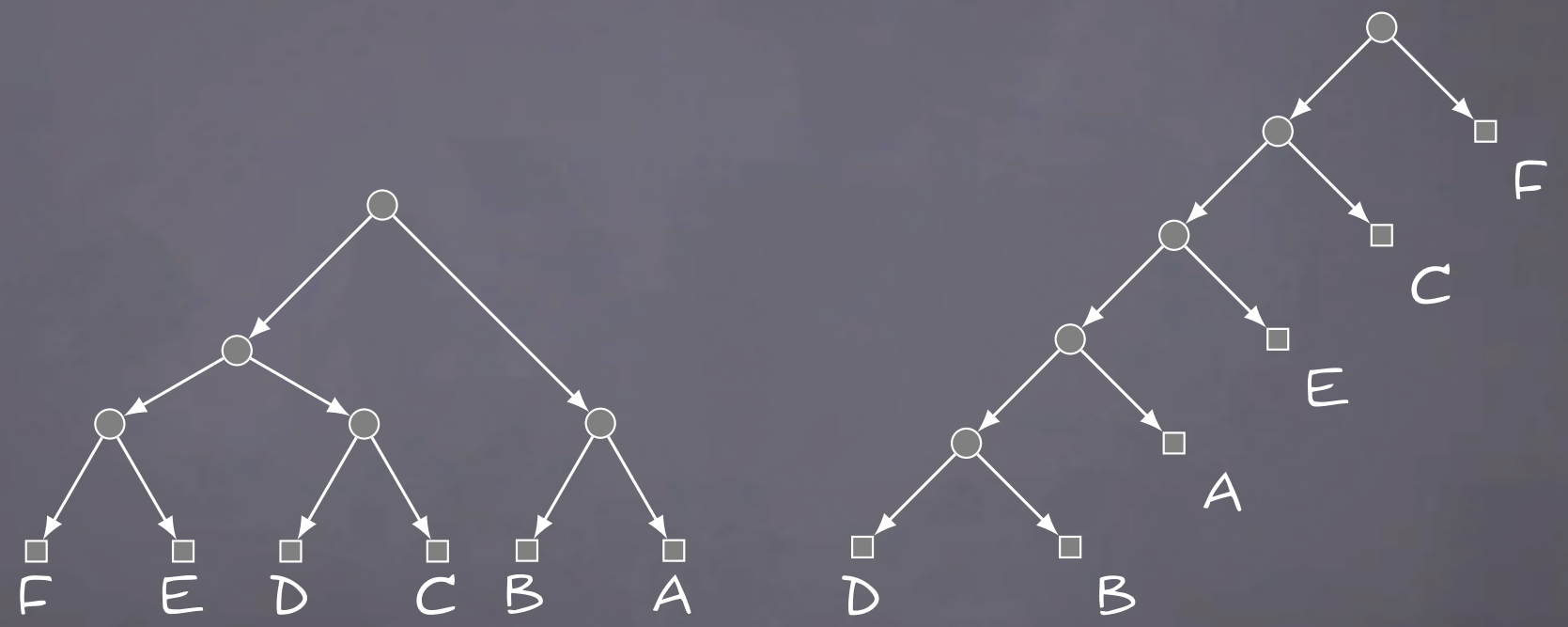

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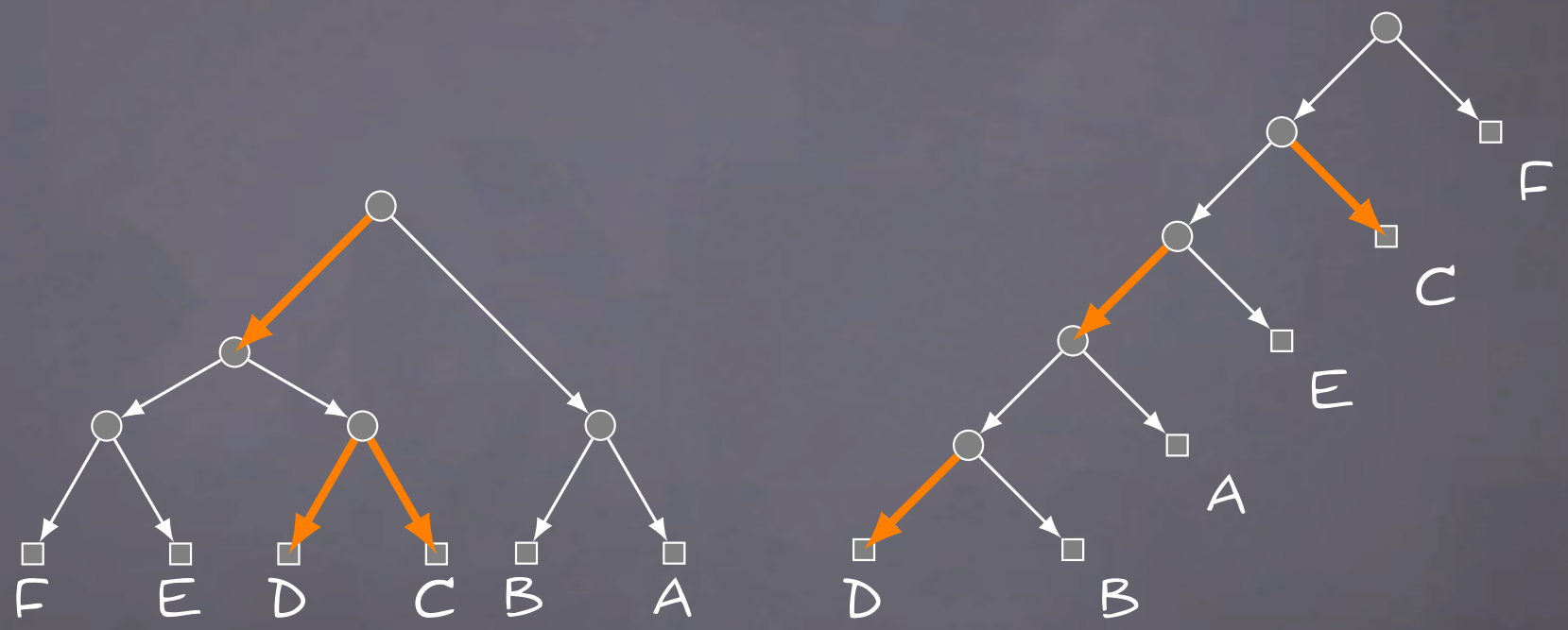

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Theorem [Allen & Steel, '01]

TBR-distance(T_1, T_2) = #trees in smallest agreement forest - 1
NP-hard to compute

Theorem [Bordewich & Semple, '04]

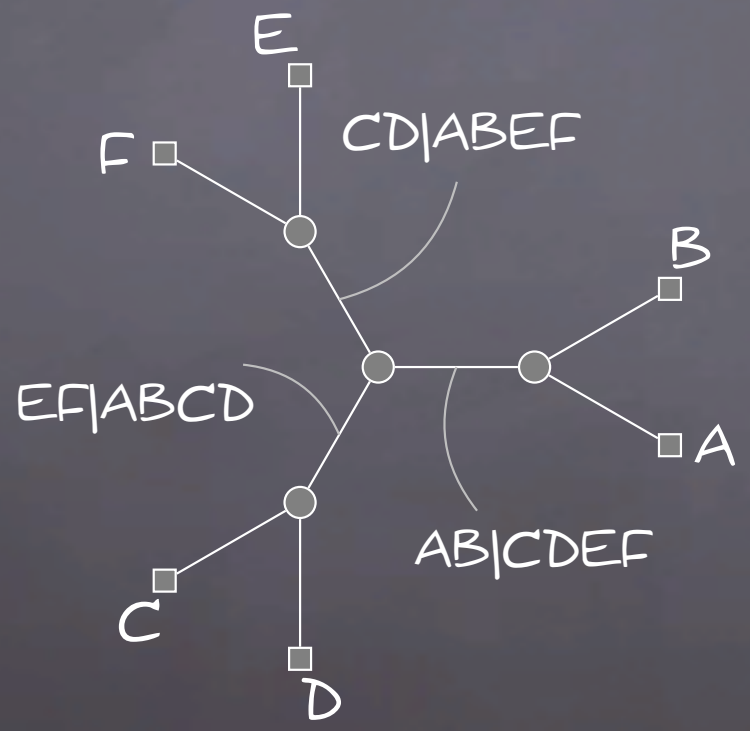
rSPR-distance(T_1, T_2) = #trees in smallest rooted agreement forest - 1
NP-hard to compute

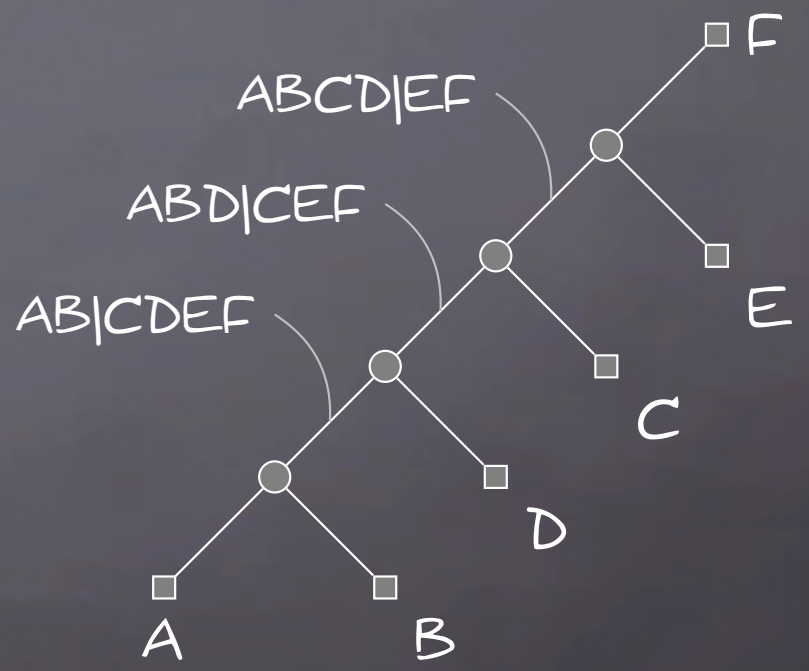
Robinson-Foulds Distance

Definition

$RF(T_1, T_2)$ = #splits/clusters occuring in exactly one of T_1 and T_2
= edge-contraction distance a common tree

Note: observe relation to NNI: $RF(T_1, T_2) \leq 2\ NNI(T_1, T_2)$





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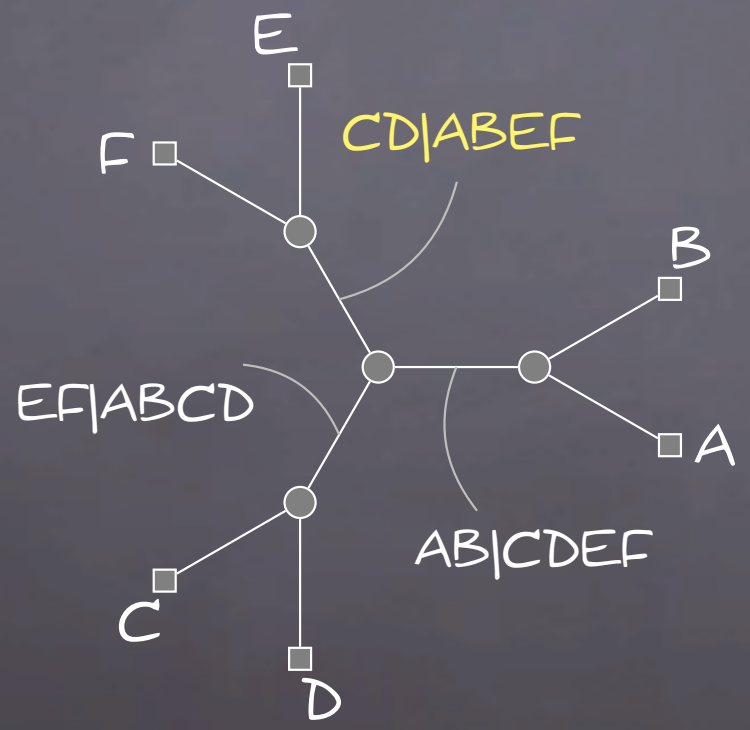

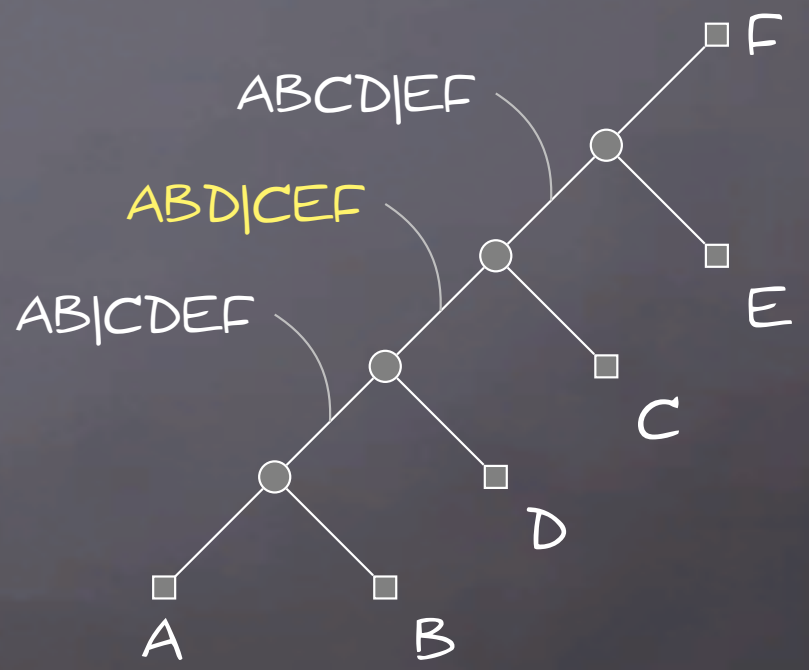

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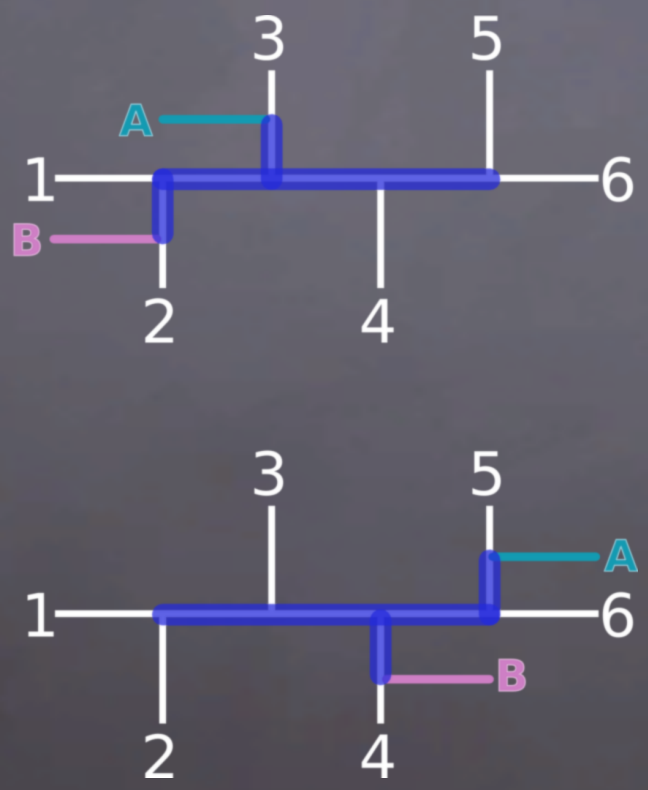

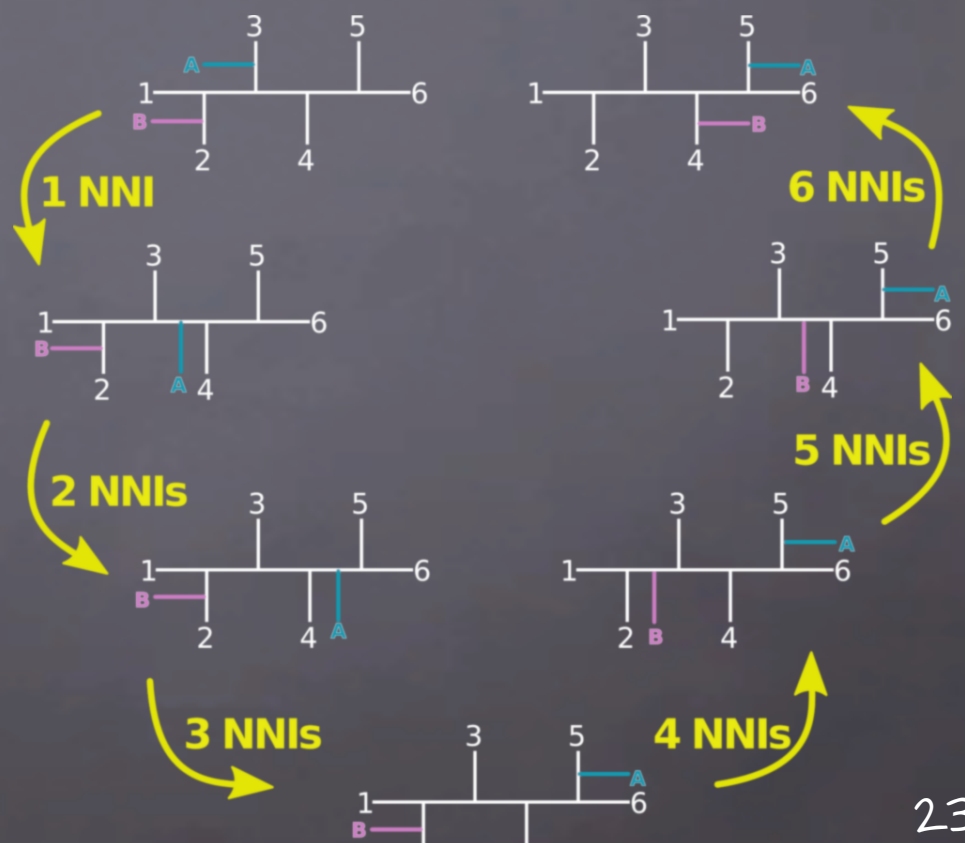

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Note: splits correspond to clusters when rooted at last leaf

Day's Algorithm (common clusters in $O(n)$)

[Day'85]

1. relabel all leaves such that leaves continuous in T_1
2. each node in T_1 knows:
   L = smallest leaf in cluster & R = largest leaf in cluster
   $\rightsquigarrow$ note T_1's clusters in hash-set
3. each node in T_2 knows: L, R, and size N of its cluster
4. each node in T_2 checks $[L, R]$ in table only if $R - L = N - 1$
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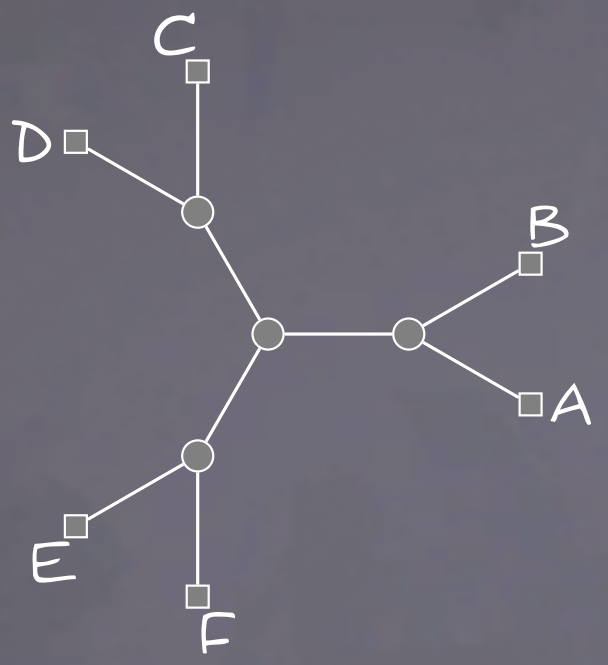
Robinson-Foulds Distance



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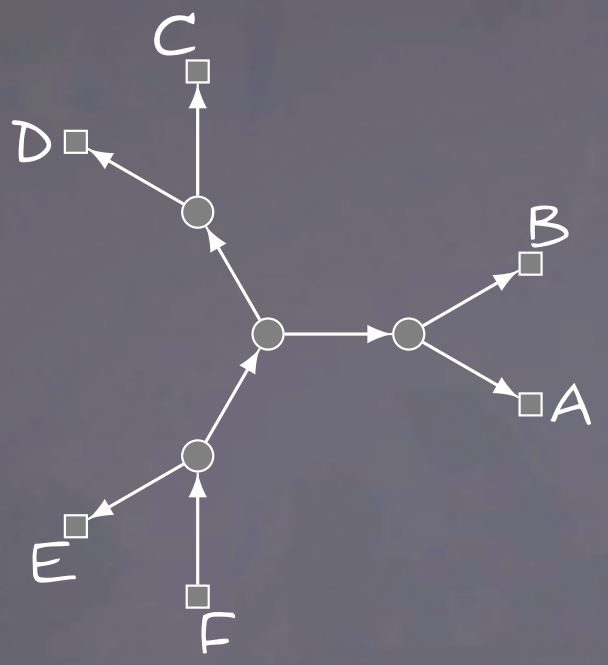

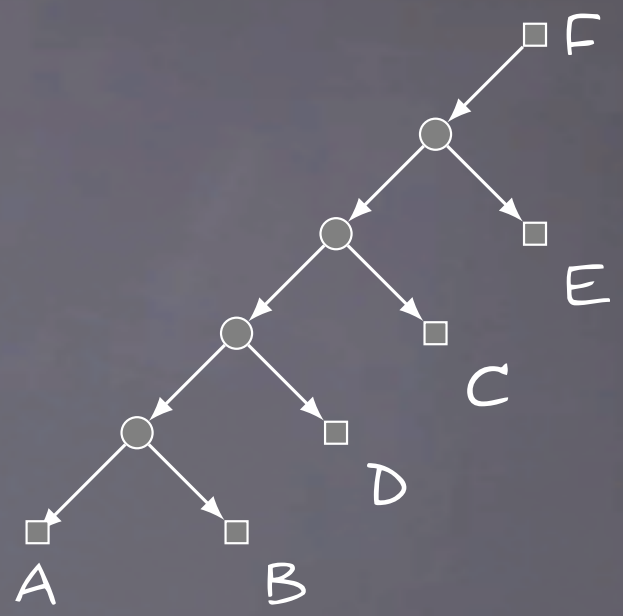

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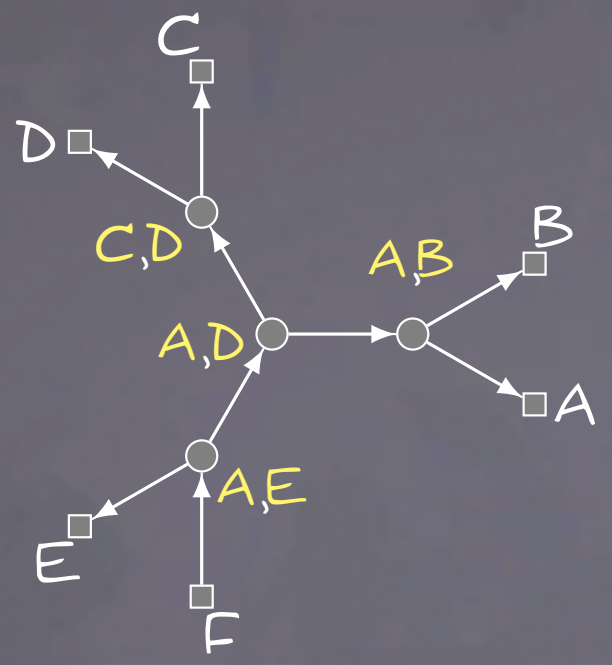

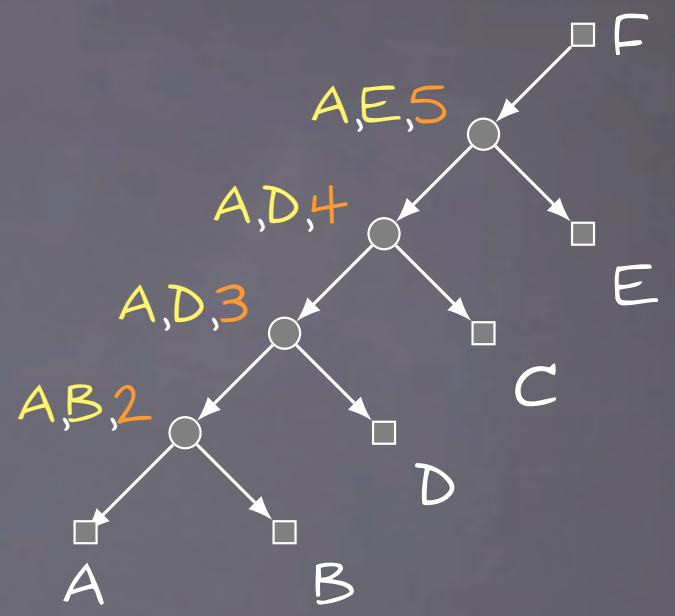

Day's Algorithm (common clusters in $O(n)$)

[Day'85]

1. relabel all leaves such that leaves continuous in T_1
2. each node in T_1 knows:
   L = smallest leaf in cluster & R = largest leaf in cluster
   $\rightsquigarrow$ note T_1's clusters in hash-set
3. each node in T_2 knows: L, R, and size N of its cluster
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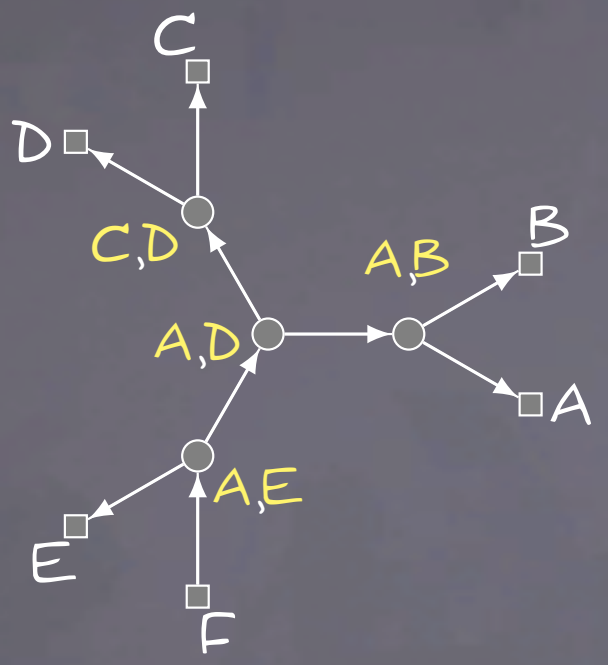

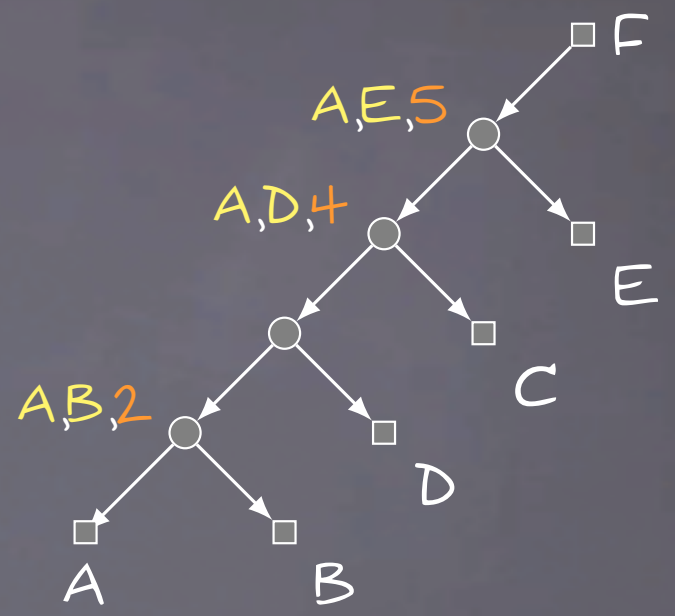

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computing Q-distance (Binary trees) [Bryant et al.'00]

1. each edge uv has 4 sets (2 clusters for each of u & v)
2. quartet AB|CD "belongs" to edge e if e splits AB|CD and e touches AB-path $\rightsquigarrow$ each quartet is owned exactly once
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State of the Art

count conflict quartets/triplets $\rightsquigarrow$ $O(n \log n)$ time [Brodal et al.'13]
enumerate conflict quartets $\rightsquigarrow$ $O(n^2 + d)$ time [Bryant et al.'00]
enumerate conflict triplets $\rightsquigarrow$ $O(n + d)$ time [Weller'17]

Phylogenetic Networks

Observation

Trees cannot capture hybridization

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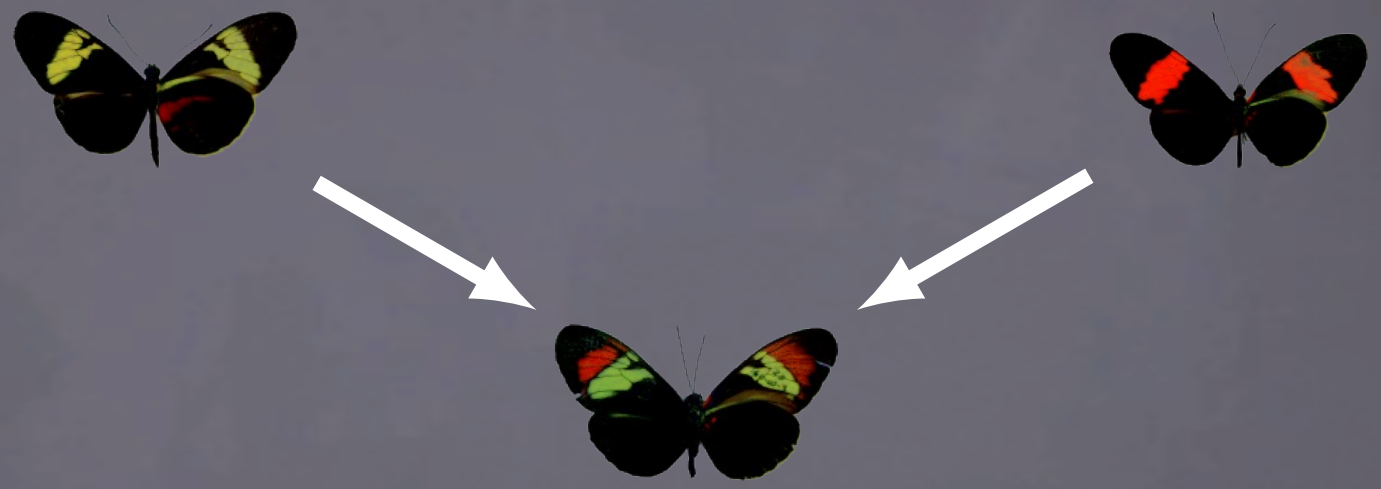

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evolutionary network N = rooted DAG, leaves labeled (taxa)
reticulations R = vertices of in-degree ≥ 2
binary = all inner vertices degree 3
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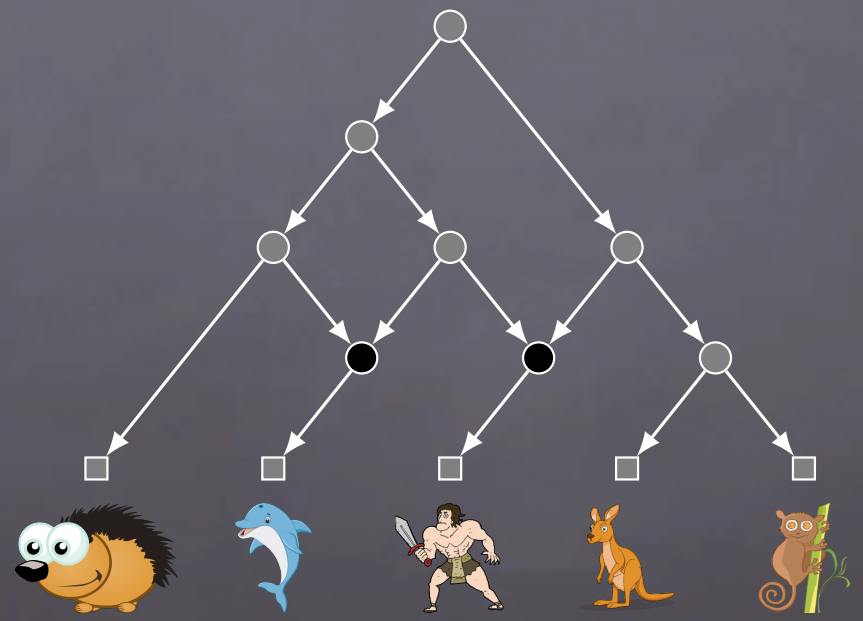
display T = subdivision of T is a subgraph



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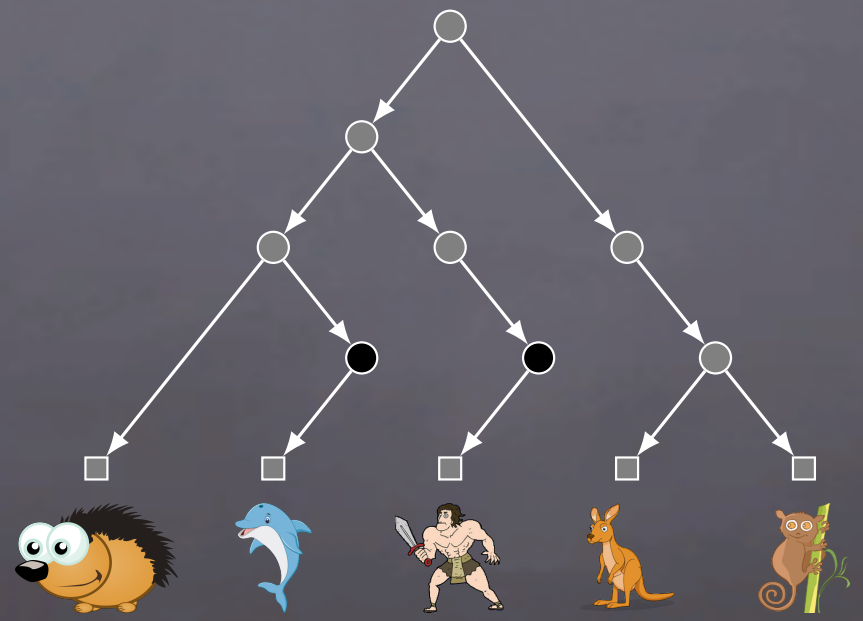
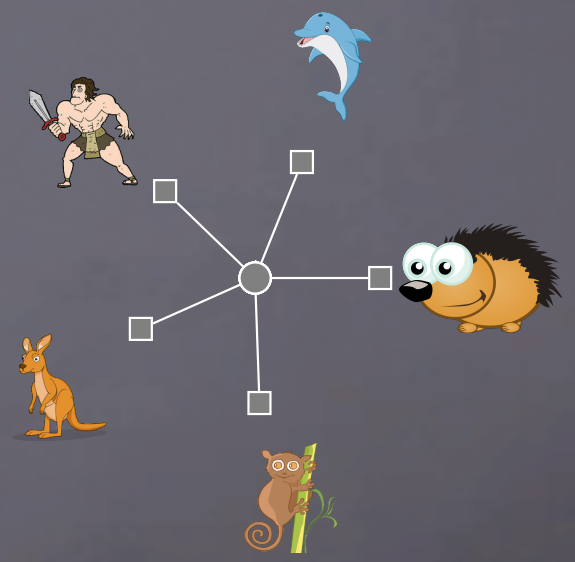


Split Networks

split = bipartition of set of taxa

splits A|B & X|Y incompatible if both A & B intersect both X & Y

Convex Hull Algorithm [Holland et al.,'04]



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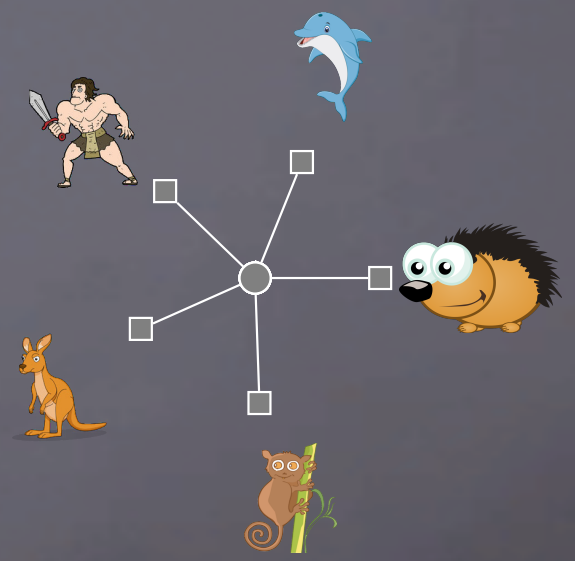

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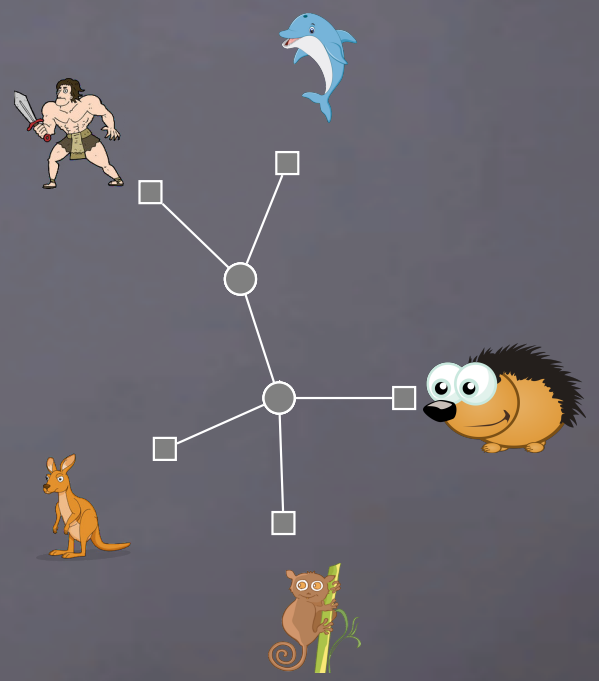

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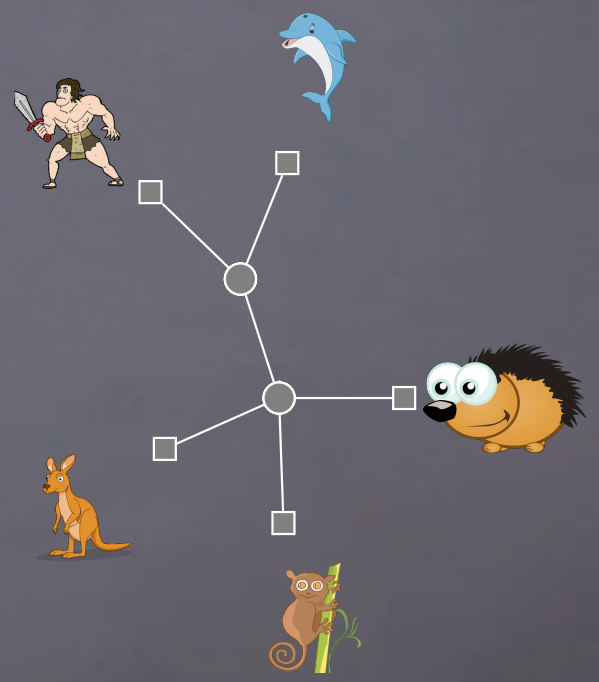

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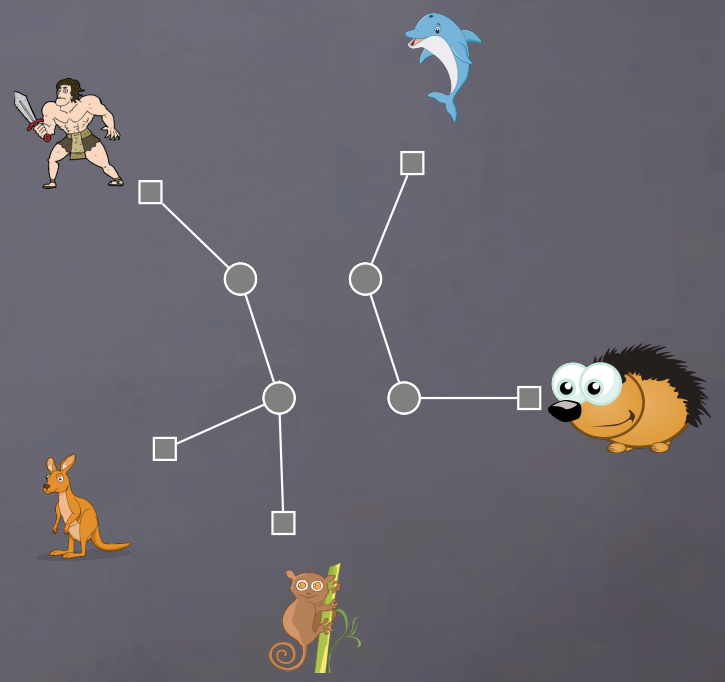

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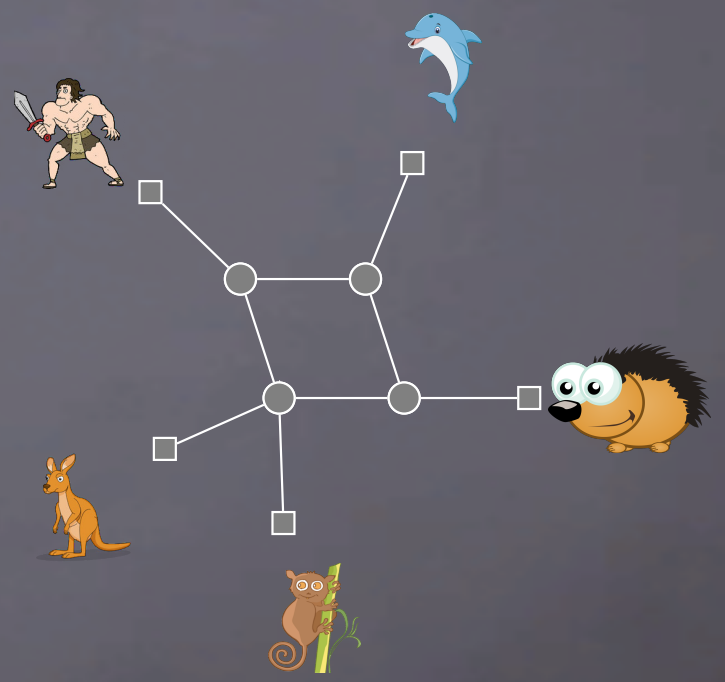

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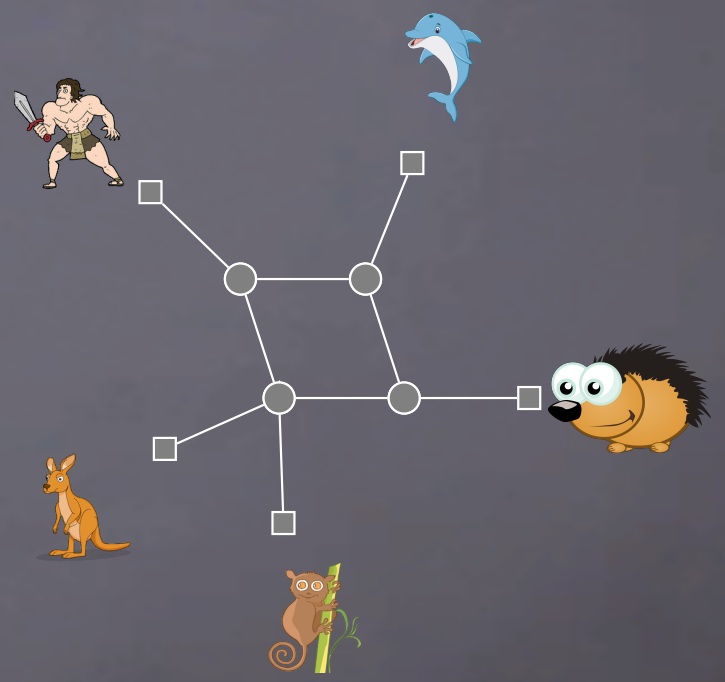

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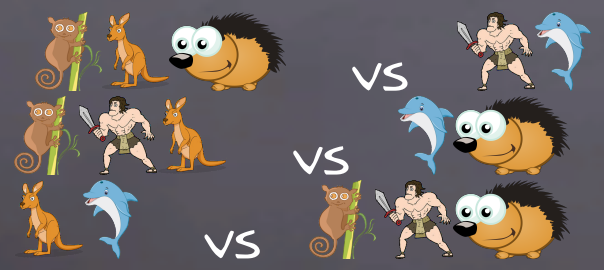

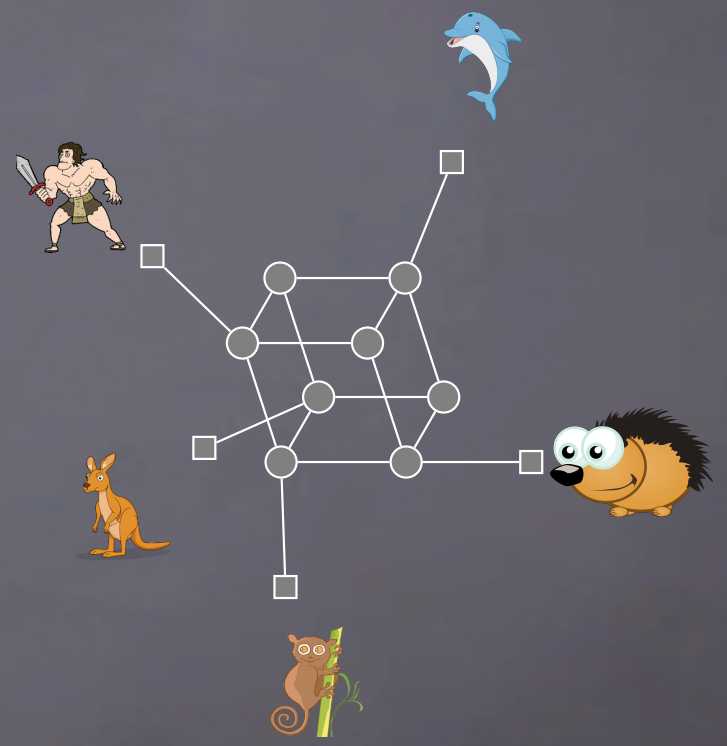

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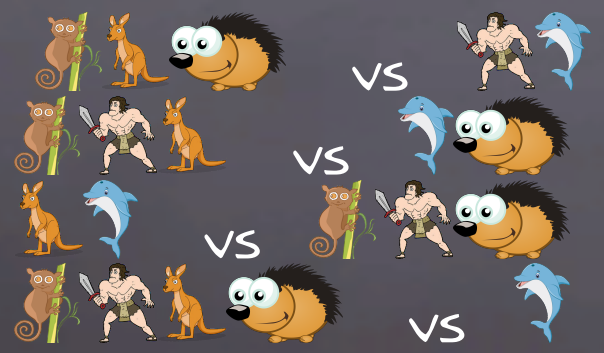

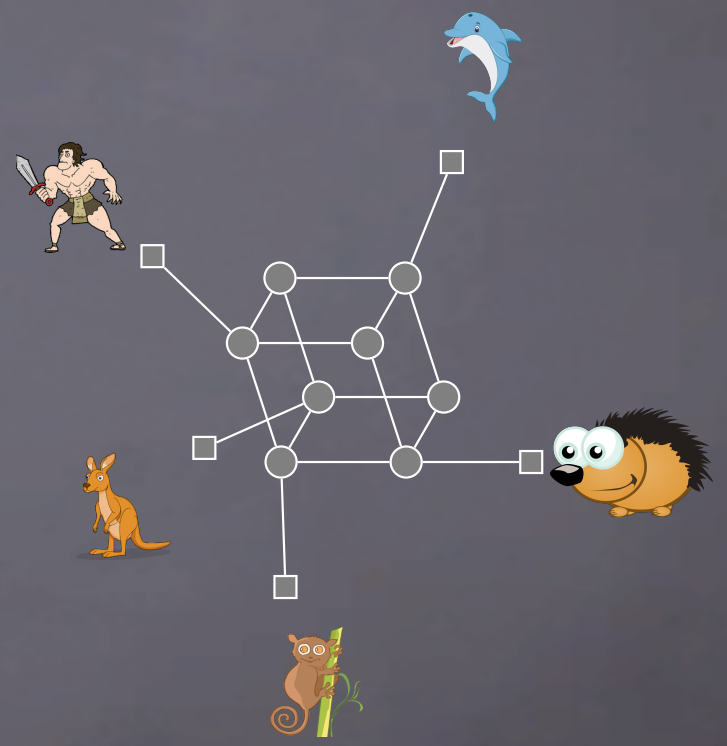

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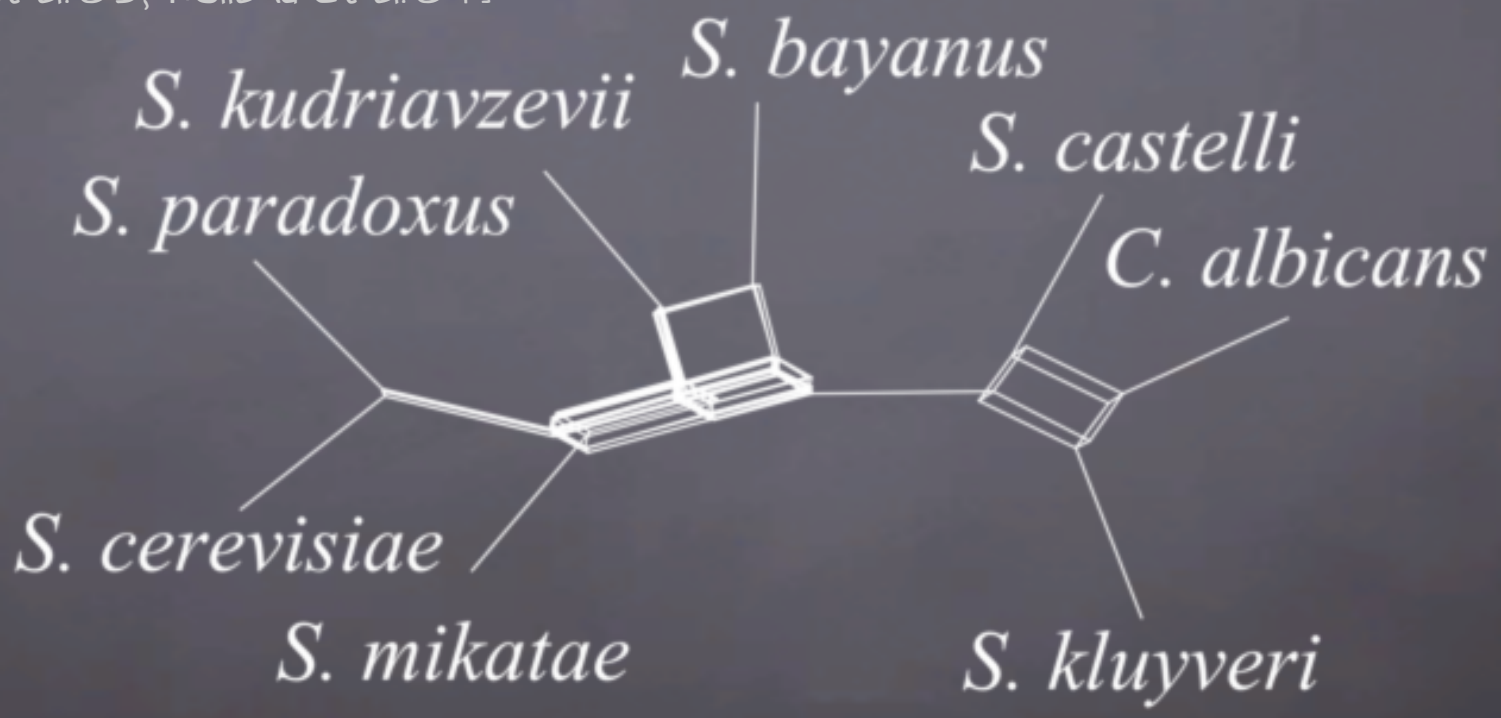

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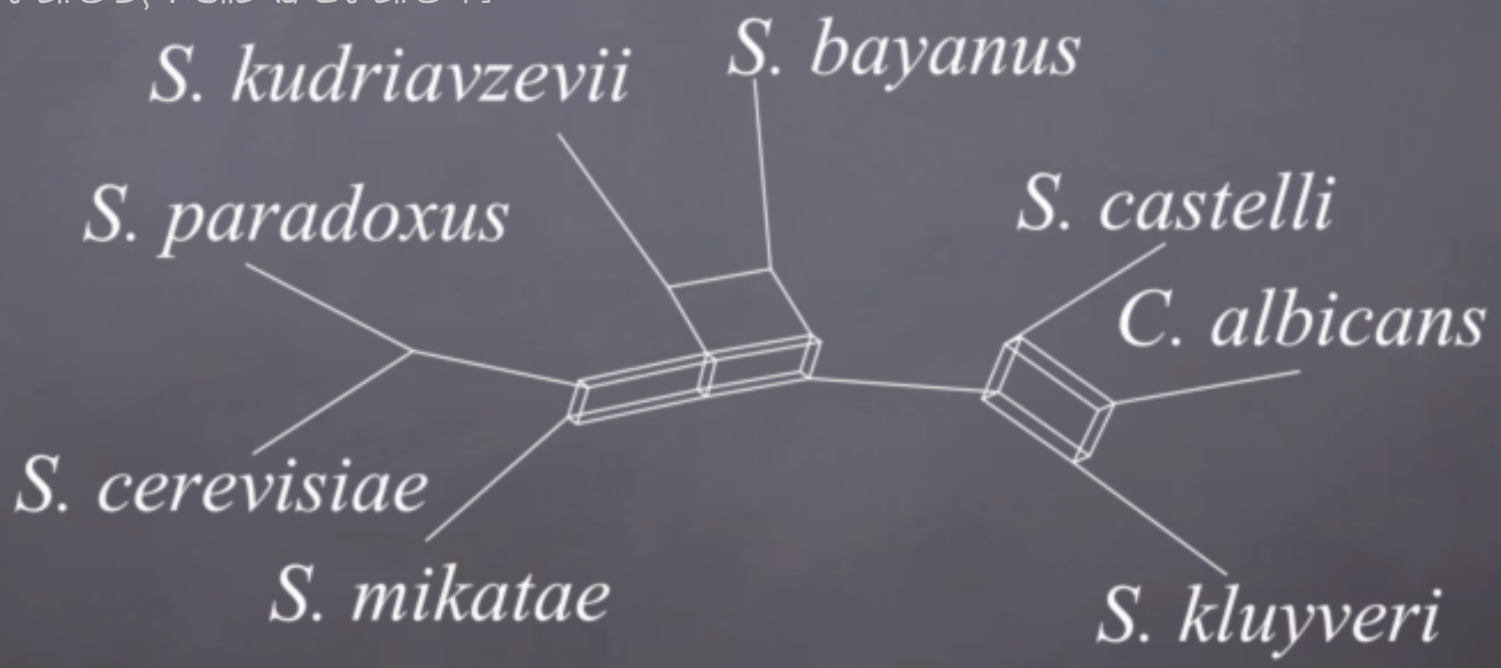

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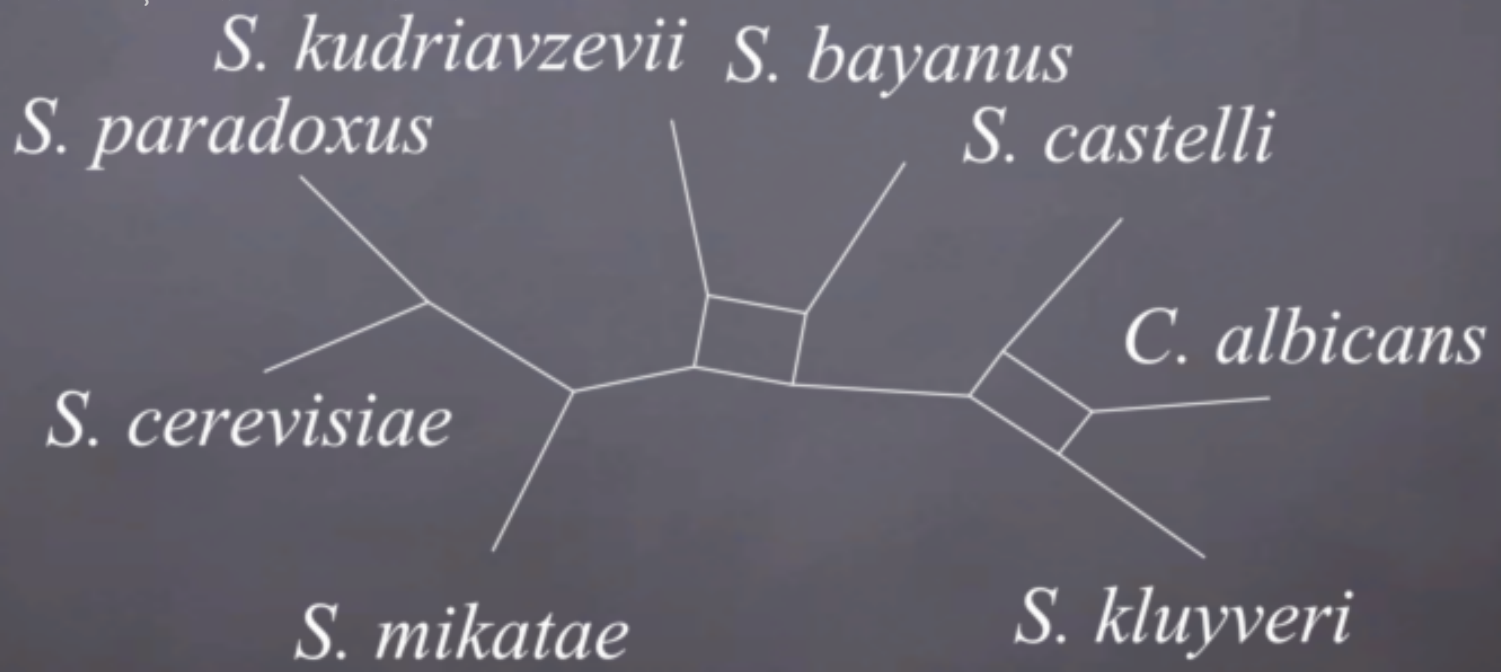

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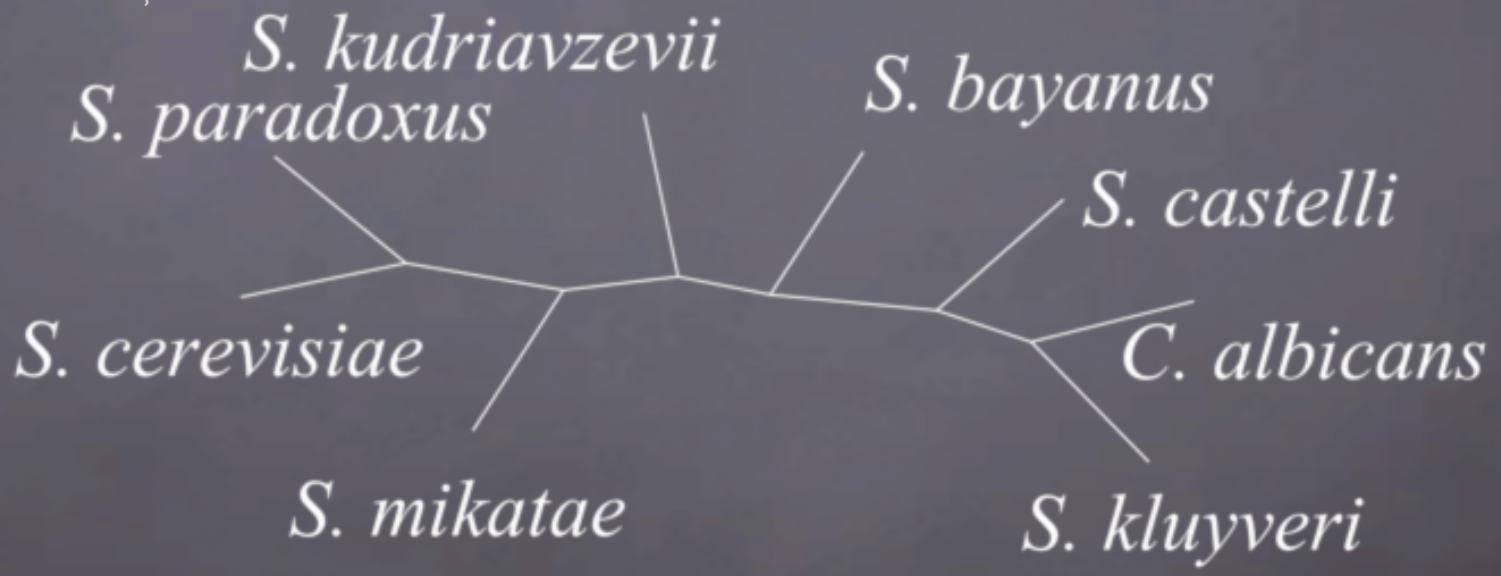

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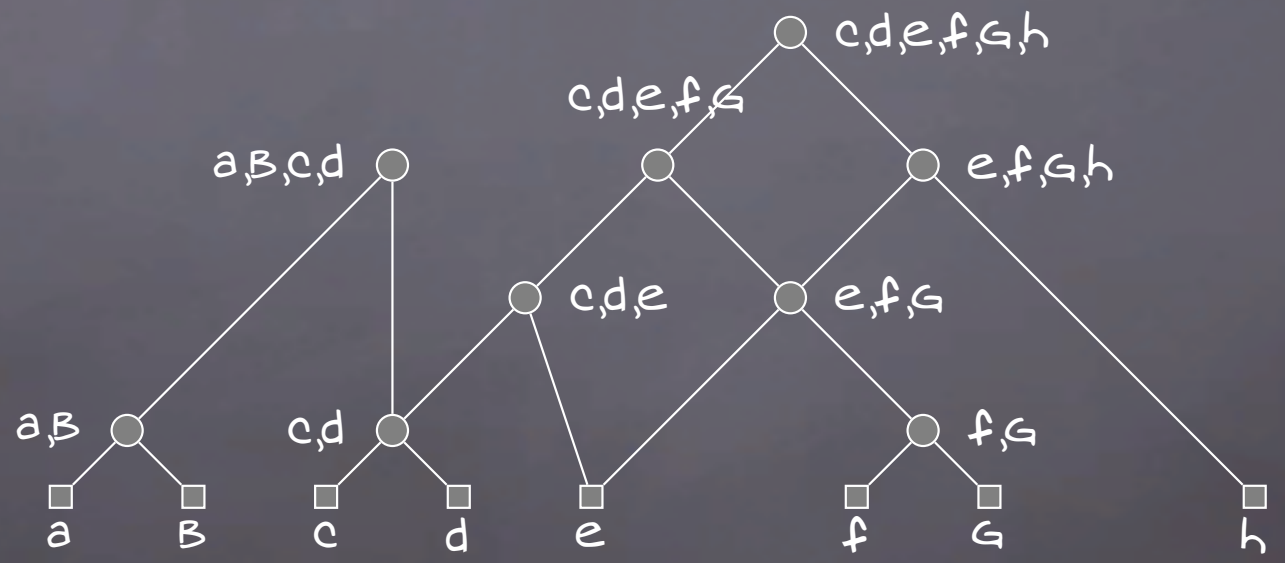

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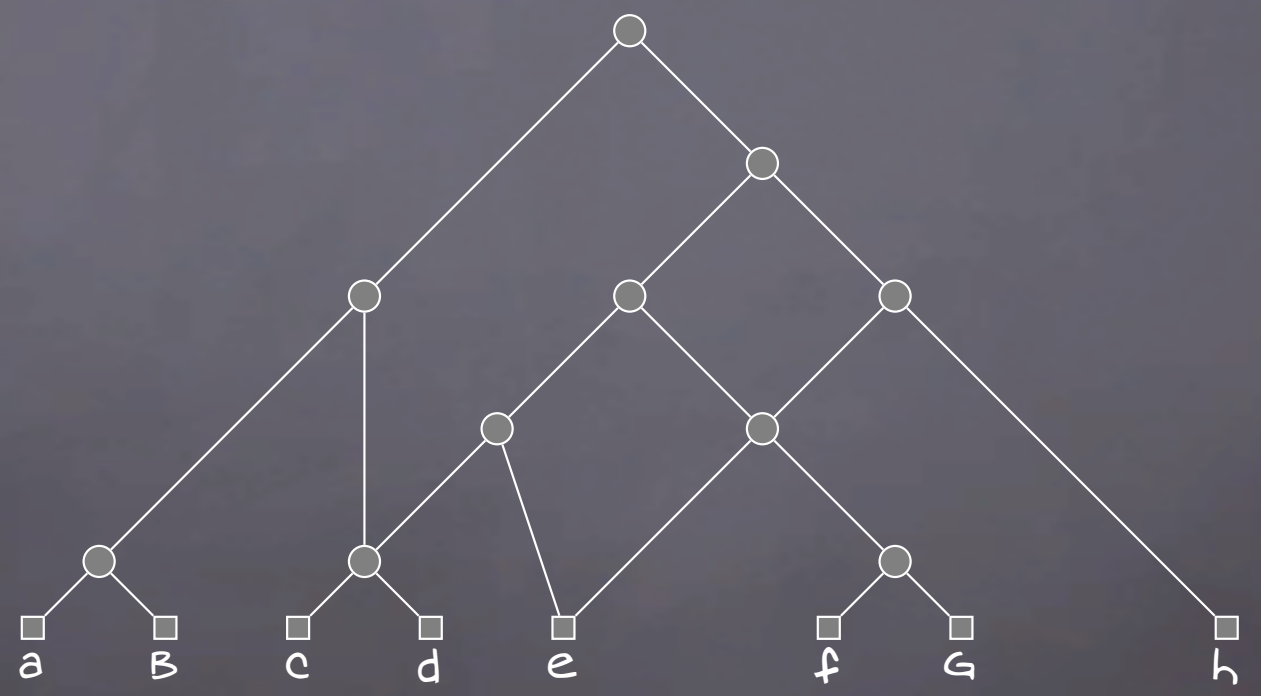

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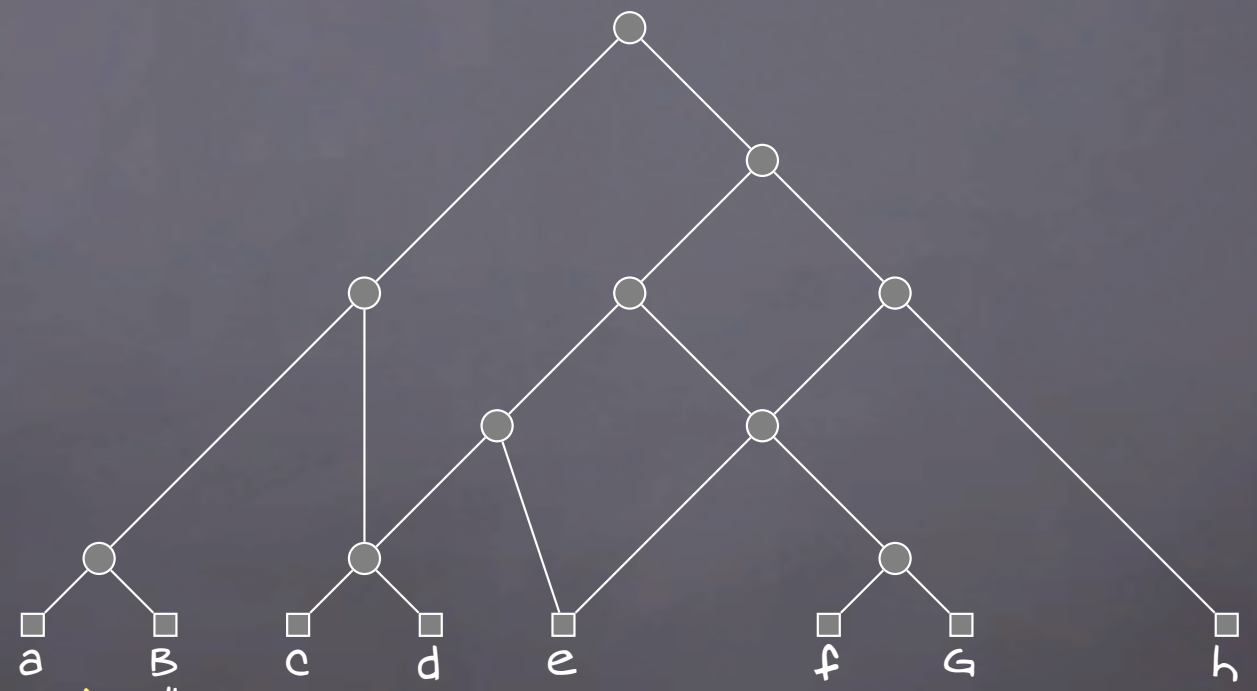

c.f. "cluster popping" [Huson & Rupp,'08]

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Note: $HN(T_1, T_2)$ = max. acyclic agreement forest − 1 [Baroni et al.,'05]

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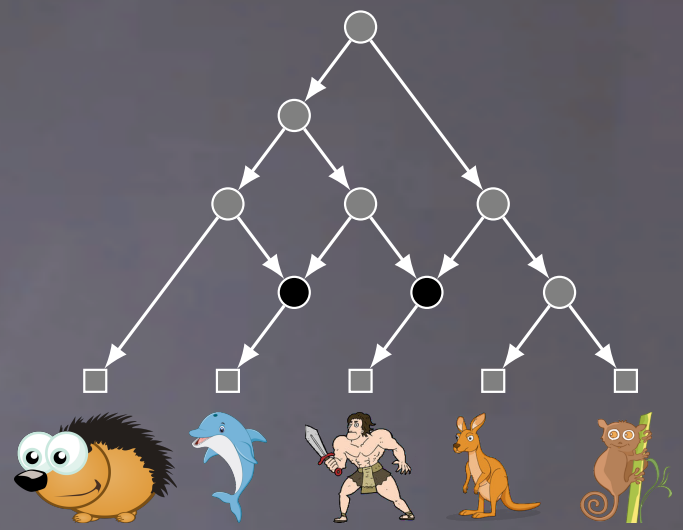
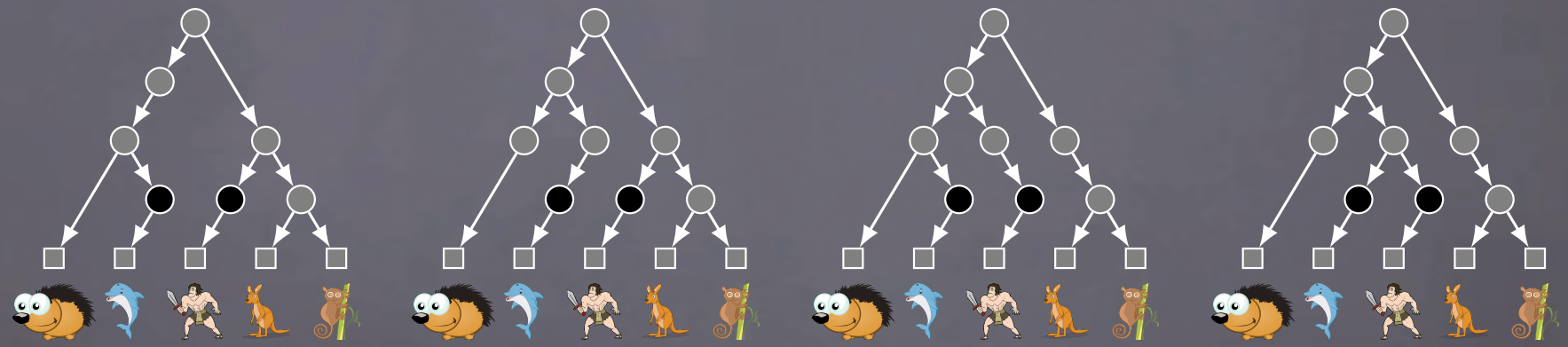
A network may display up to $2^{|R|}$ trees.





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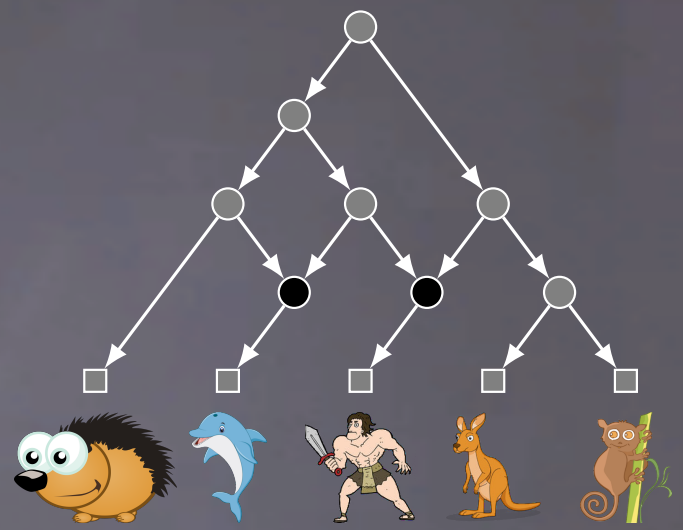

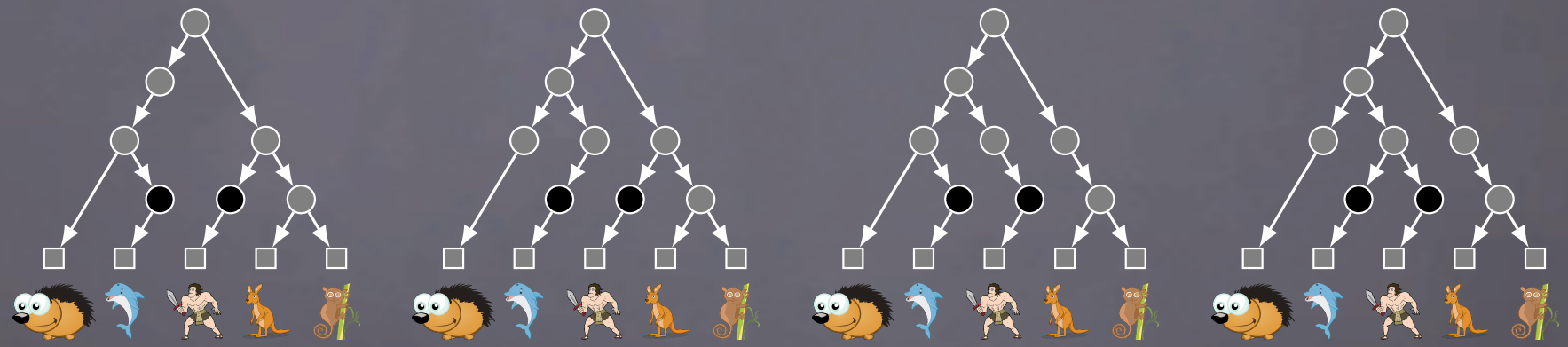

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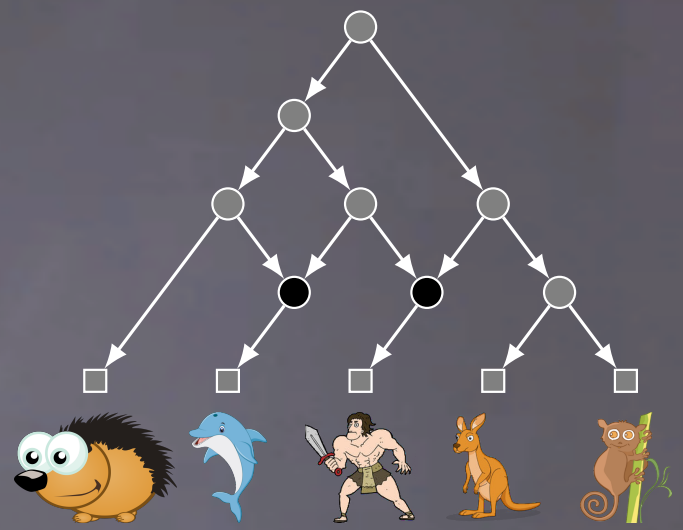

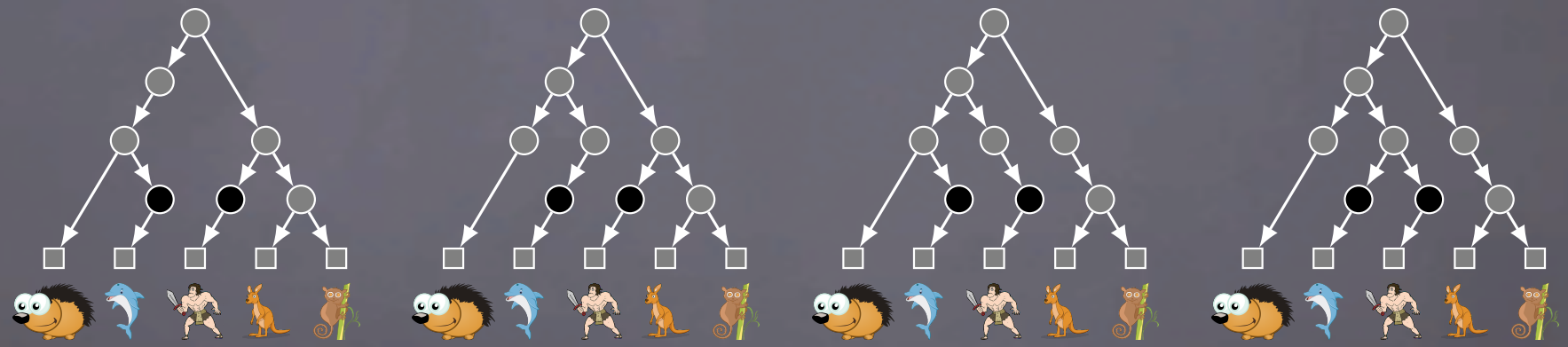

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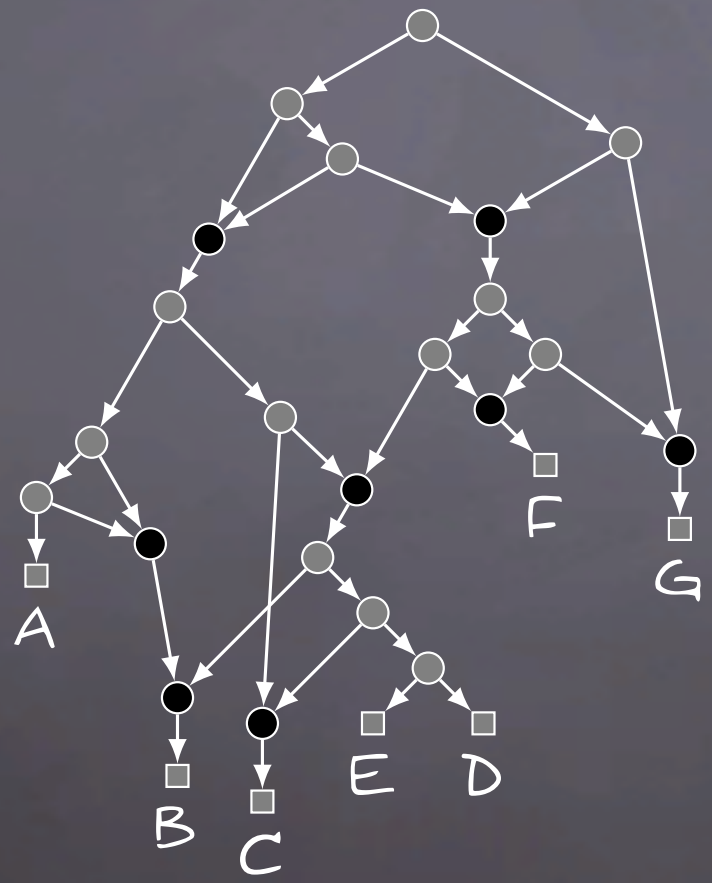
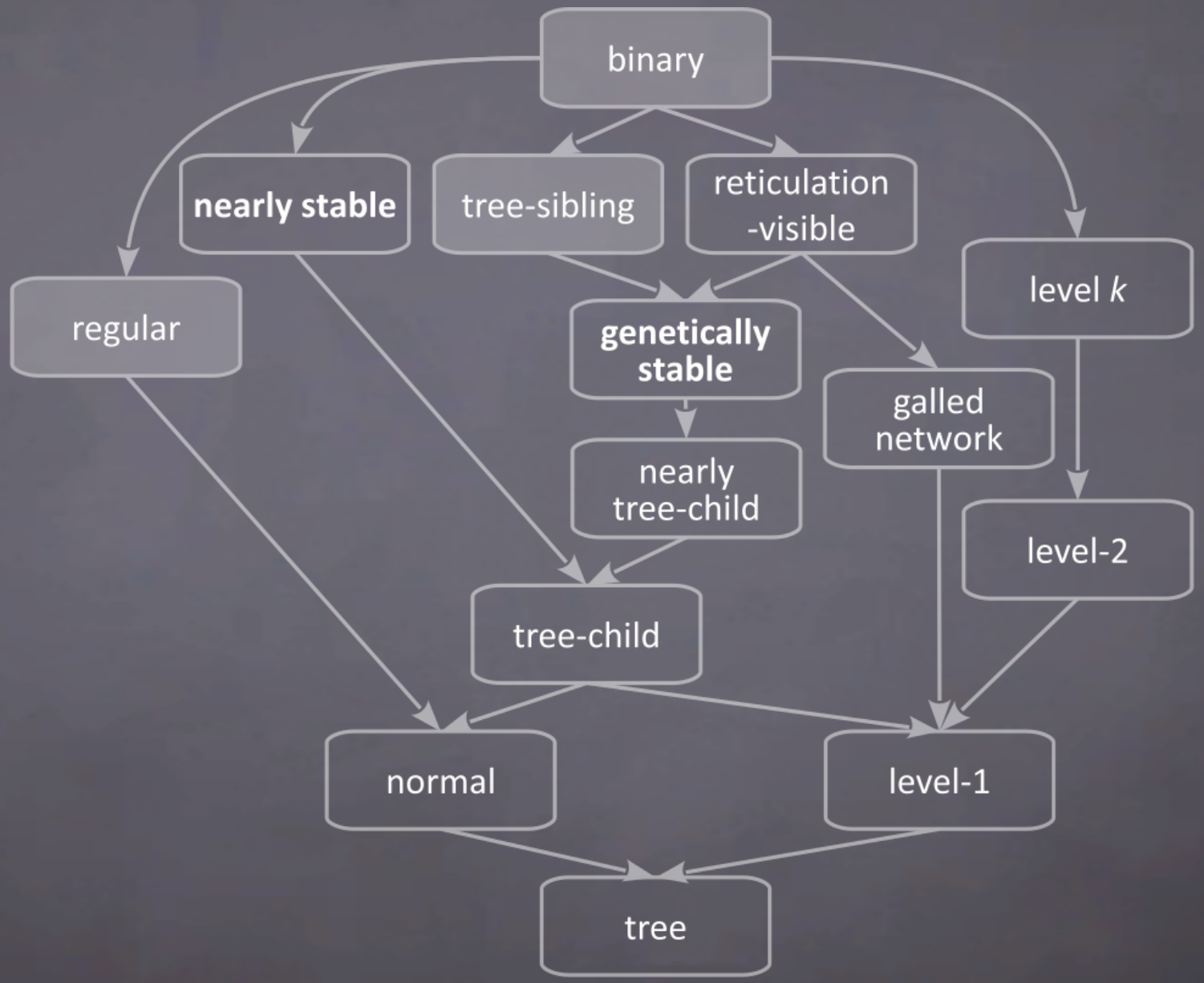


Small Taxonomy of Network Classes



c.f. "Who is Who in Phylogenetic Networks" (http://phylnet.univ-mlv.fr/)


Thanks
& Enjoy
Part III