Phylogenetic Reconstruction (2)

TREE-PUZZLE, parallel computing, obstacles, problems, wishes. . .

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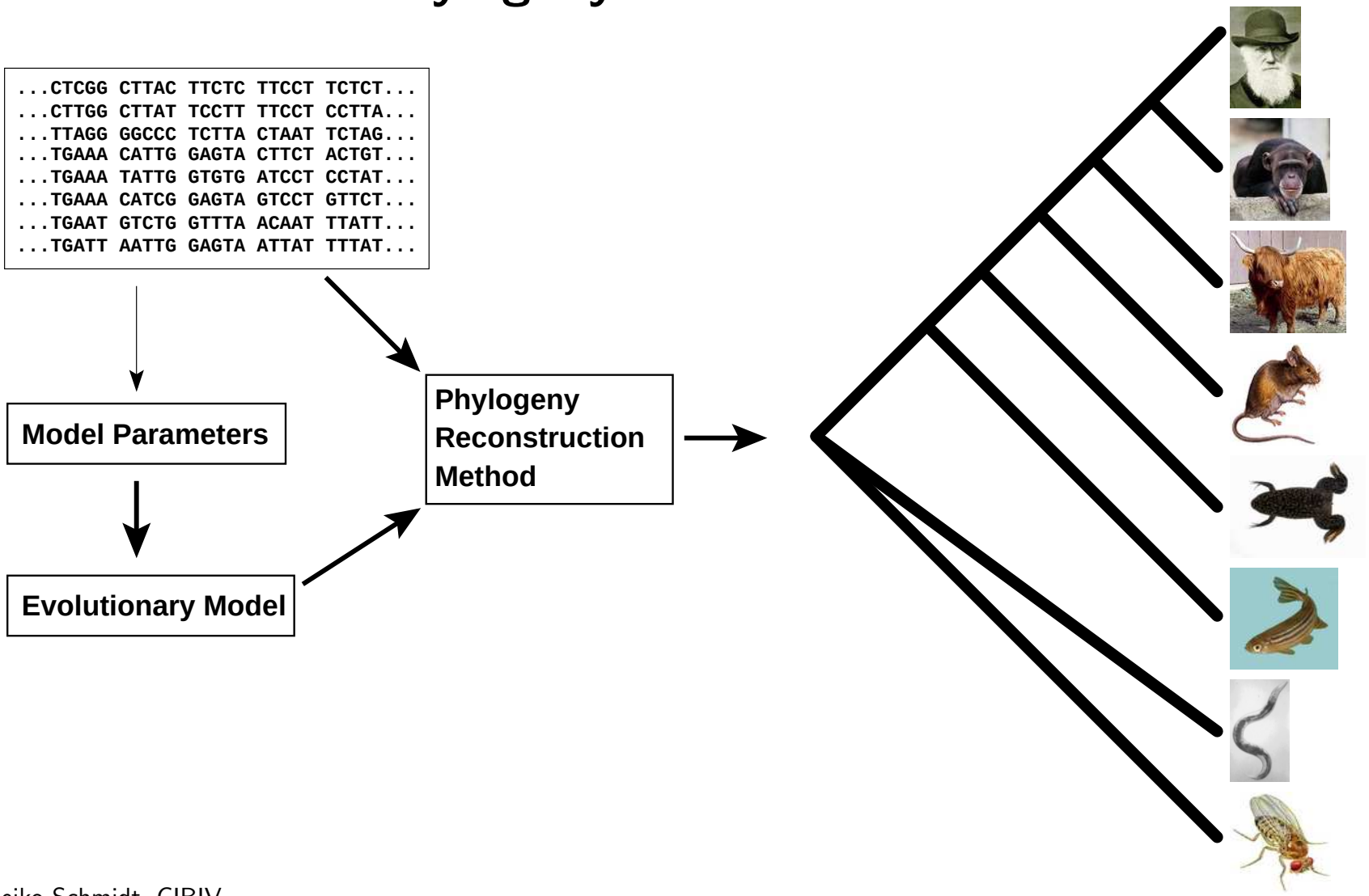
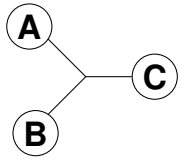
Phylogeny-Reconstruction



Binary Unrooted Trees



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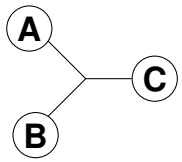

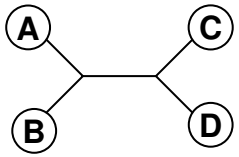

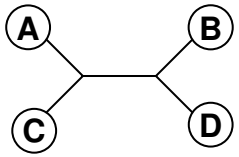

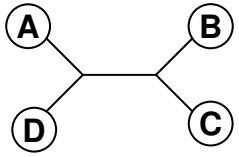

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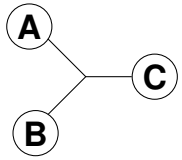

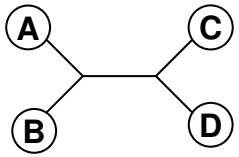

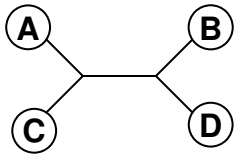

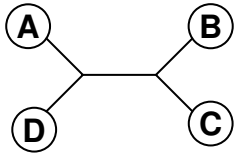

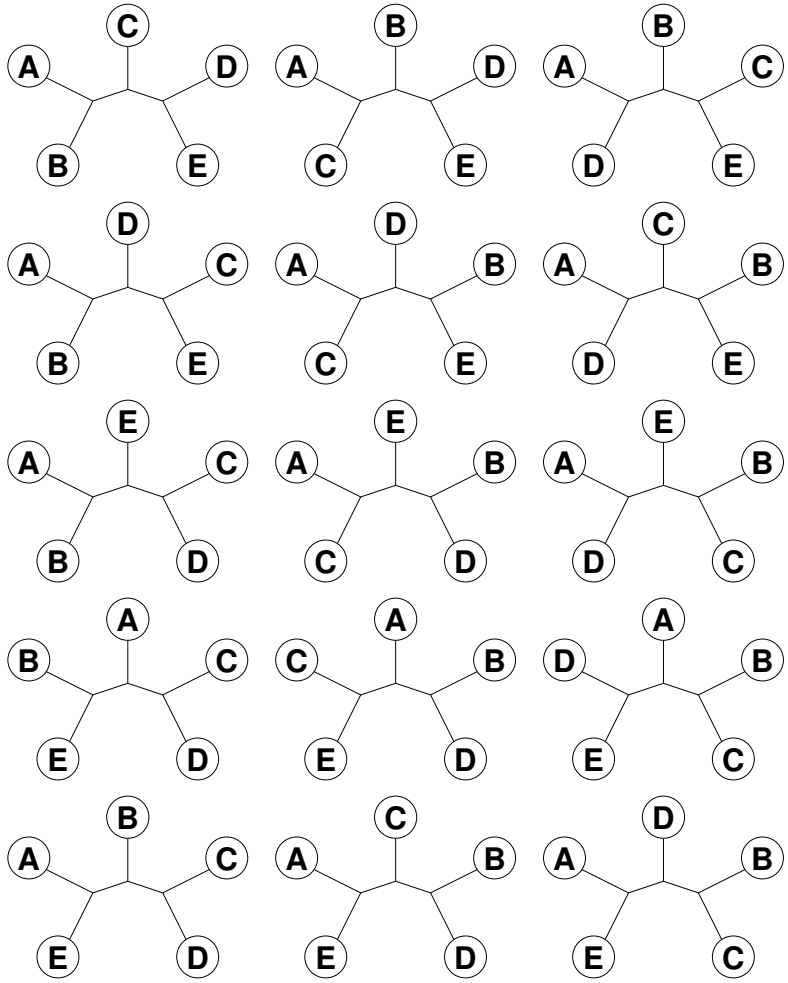

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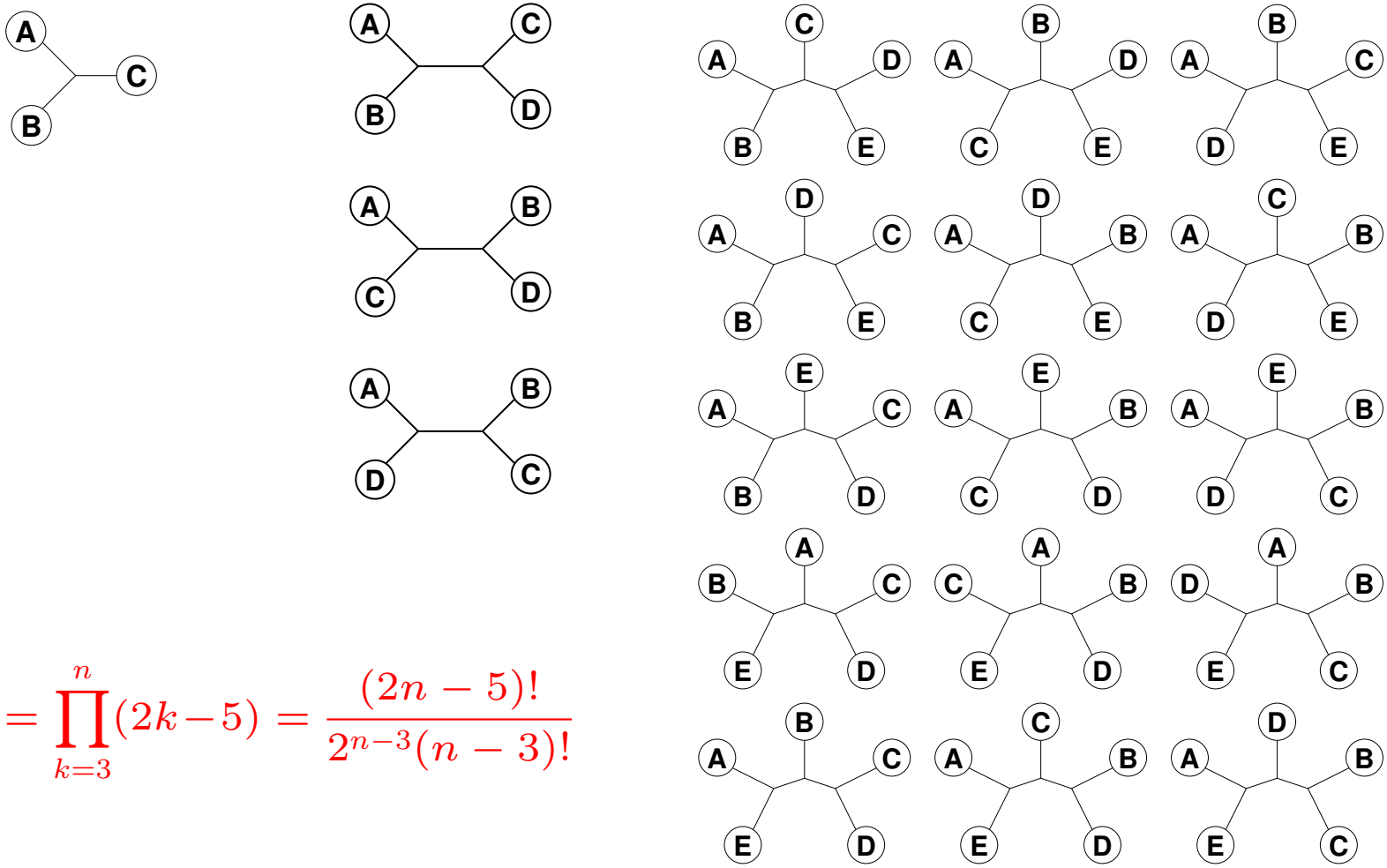

$$B(n) = \prod_{k=3}^{n}(2k-5) = \frac{(2n-5)!}{2^{n-3}(n-3)!}$$

Quartet Methods

```
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...TGAAT GTCTG GTTTA ACAAT...
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Data

Heiko Schmidt, CIBIV

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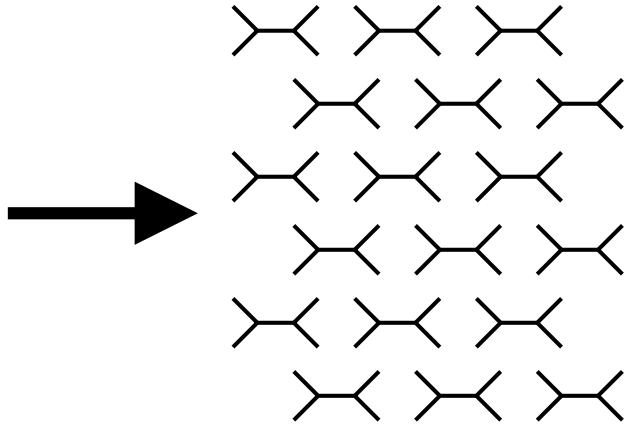
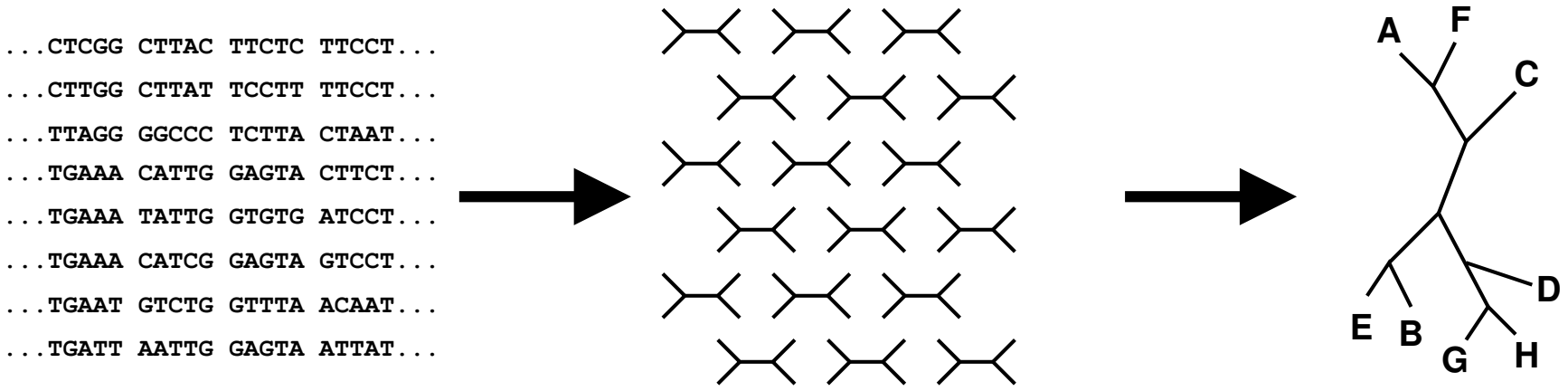


Data **Quartet trees**

Quartet Methods



Data **Quartet trees** **Tree**

Why Quartets?

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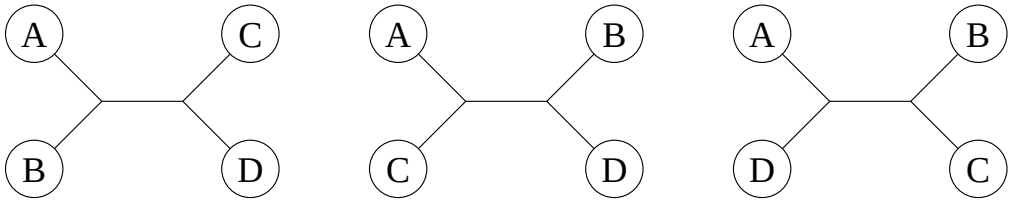
- There are only 3 topologies for 4 sequences.



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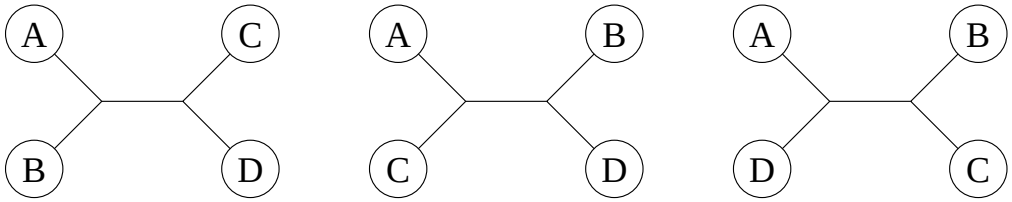

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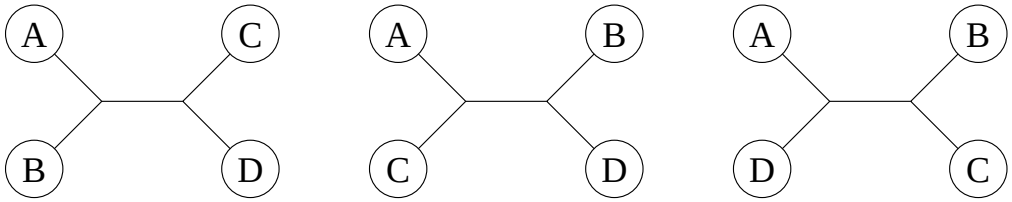

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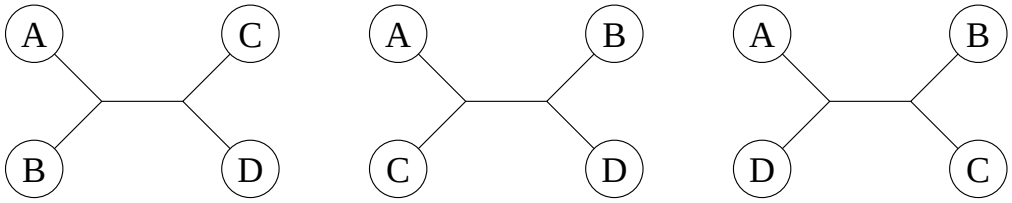

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- Hence, the computational burden is reduced from huge equations on huge numbers of large trees to 'small' equations on a large number of 4-trees

Quartet Puzzling

The Quartet Puzzling algorithm implemented in the TREE-PUZZLE program is a four-step procedure:

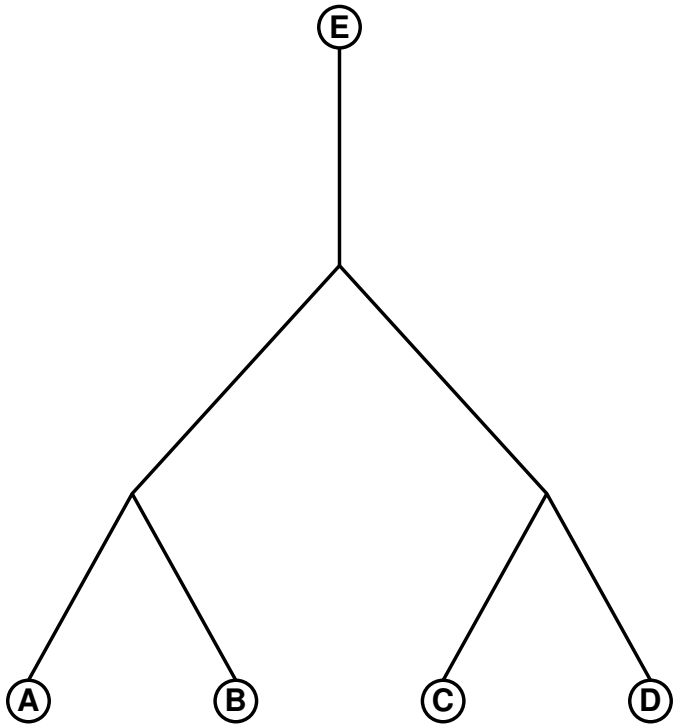
1) model parameter estimation

2) maximum-likelihood step: compute ML trees for all quartets of an alignment.

3) puzzling step: compose an intermediate tree from quartet trees.
Starts with a quartet topology and adds sequences by stepwise insertion. (this is done multiple times).

4) consensus step: construct a majority rule consensus tree from the intermediate trees and evaluate the branch lengths.

Puzzling Step: Quartets $\longrightarrow$ Full Tree



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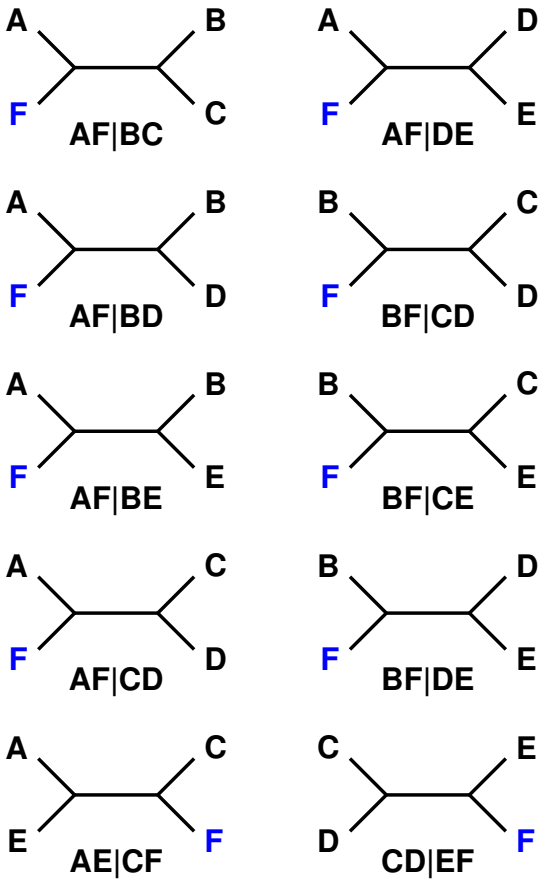

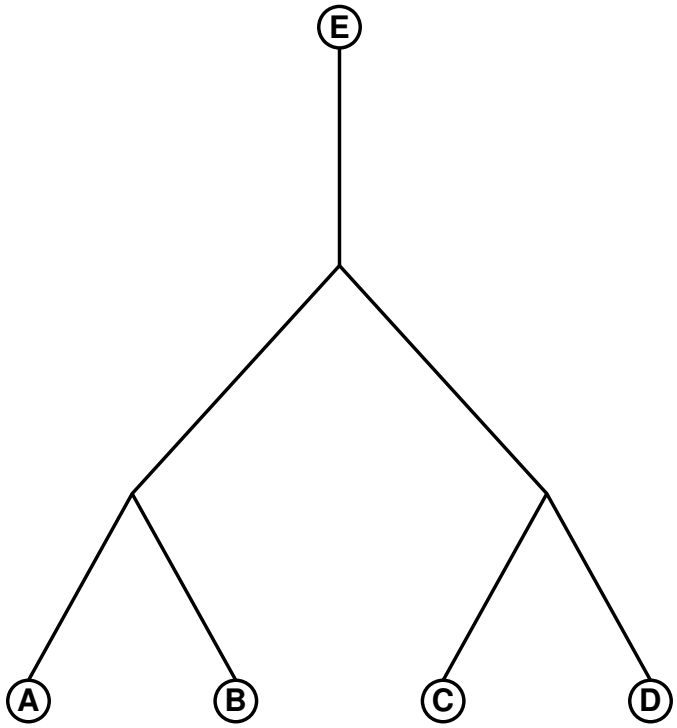

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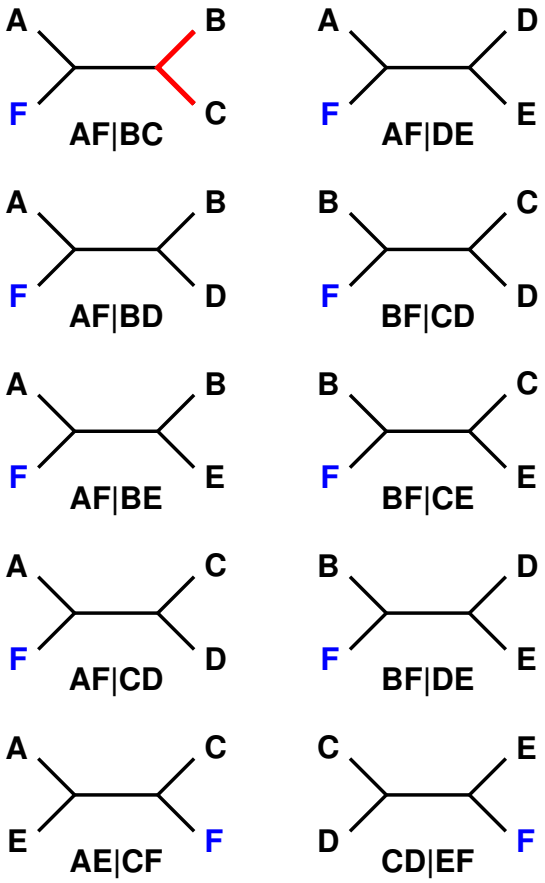

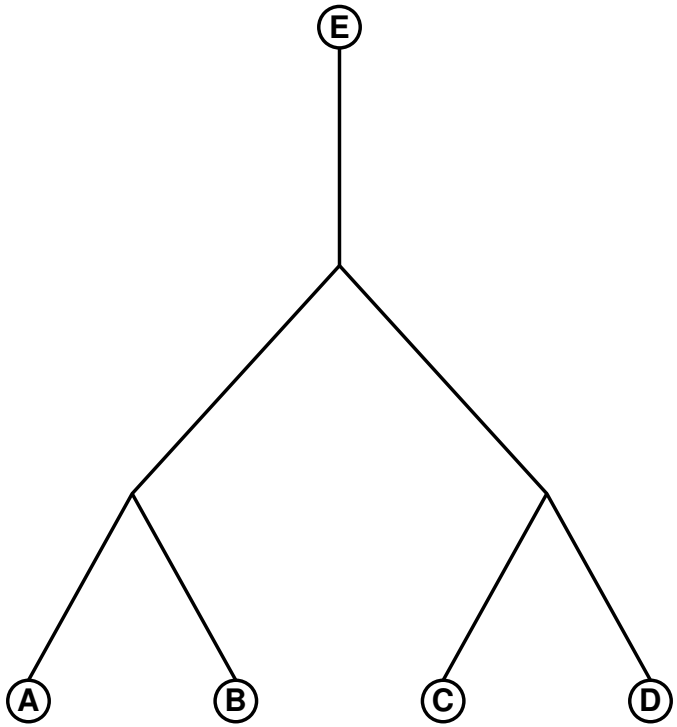

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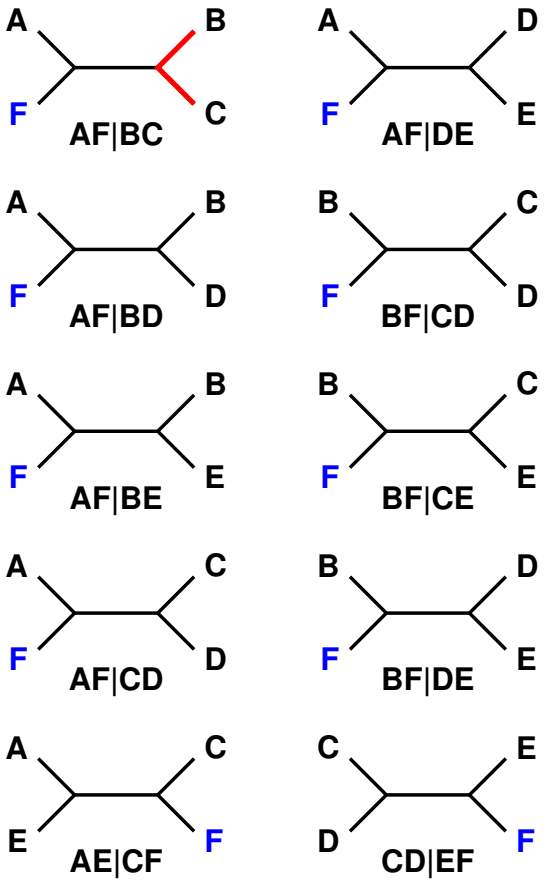

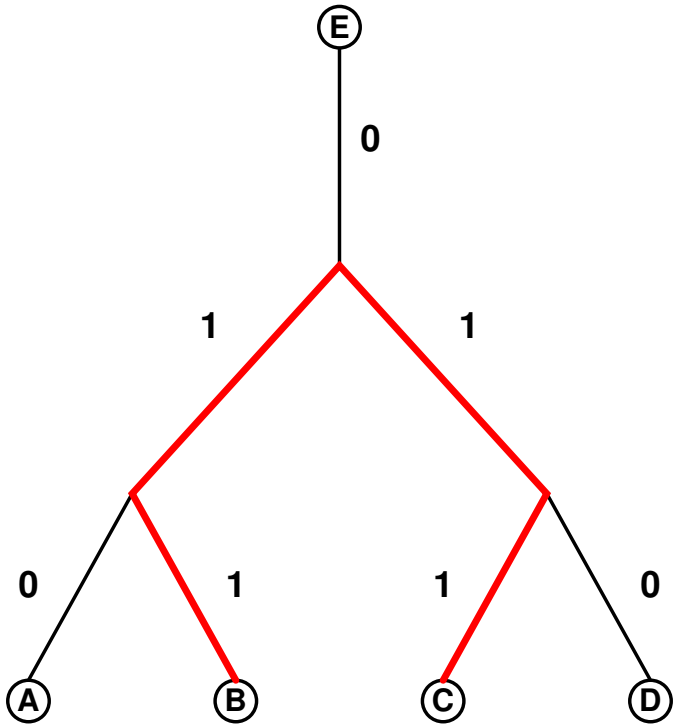

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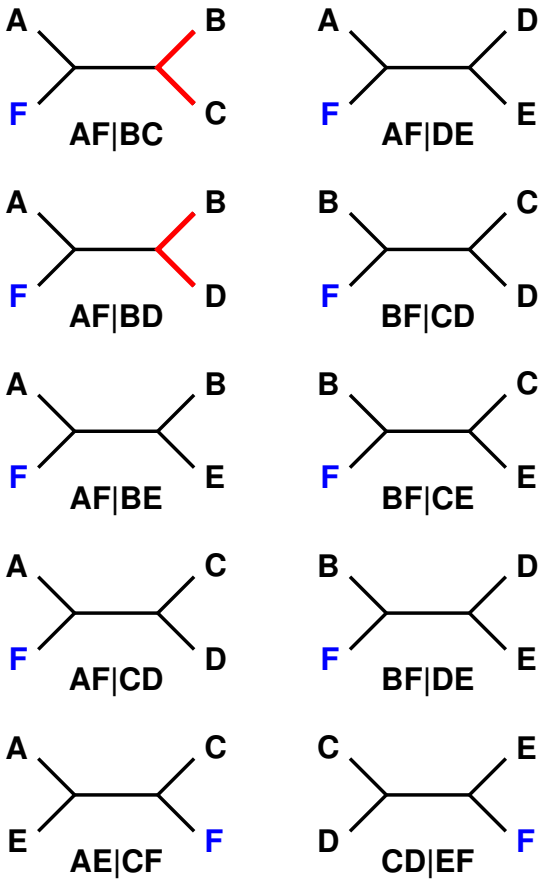

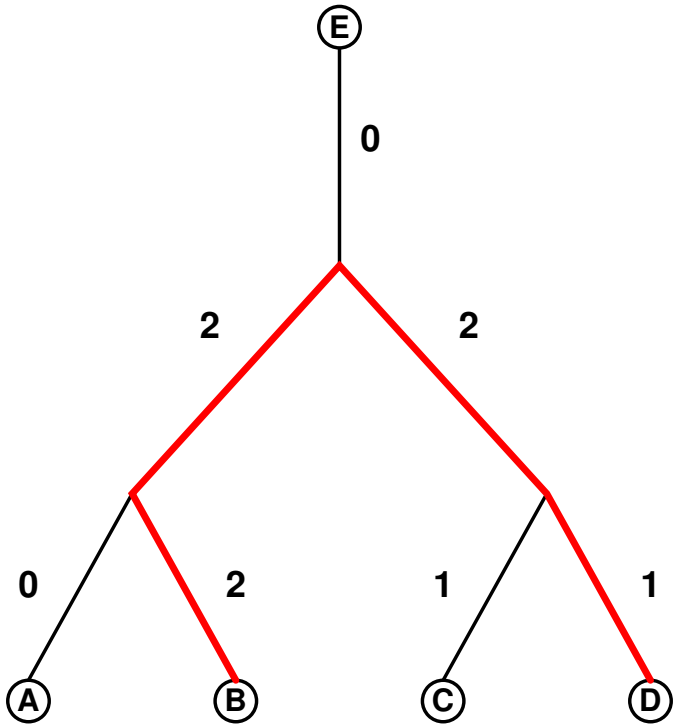

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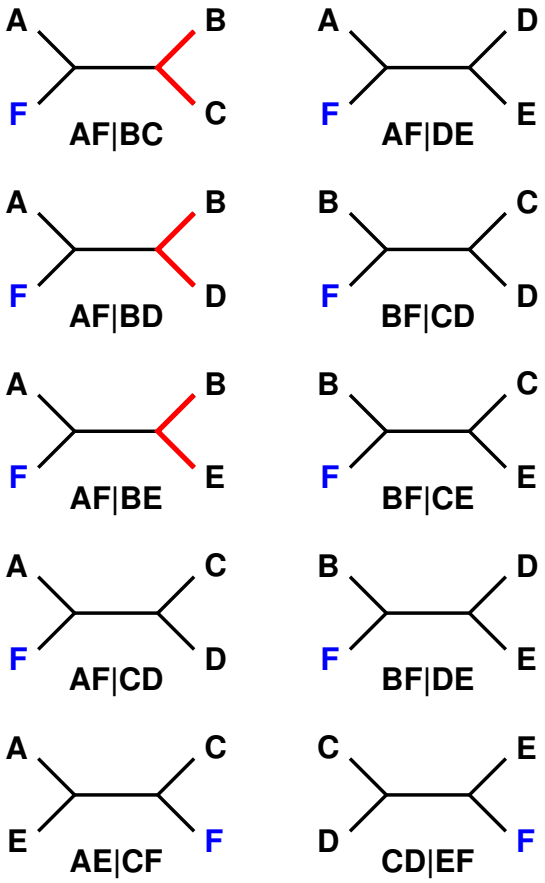

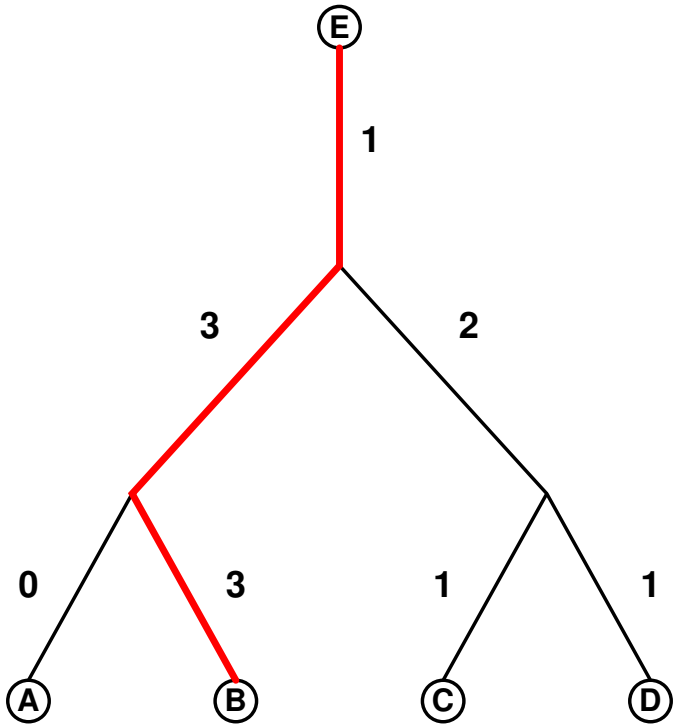

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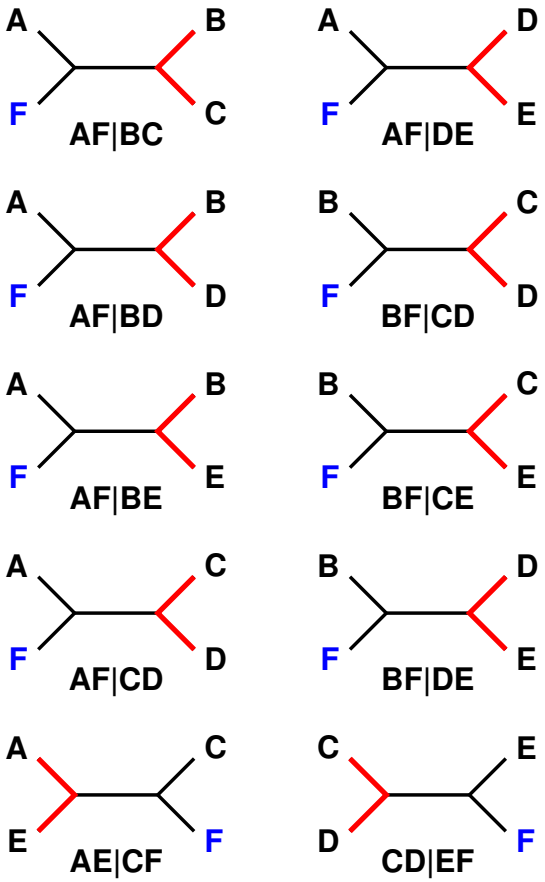

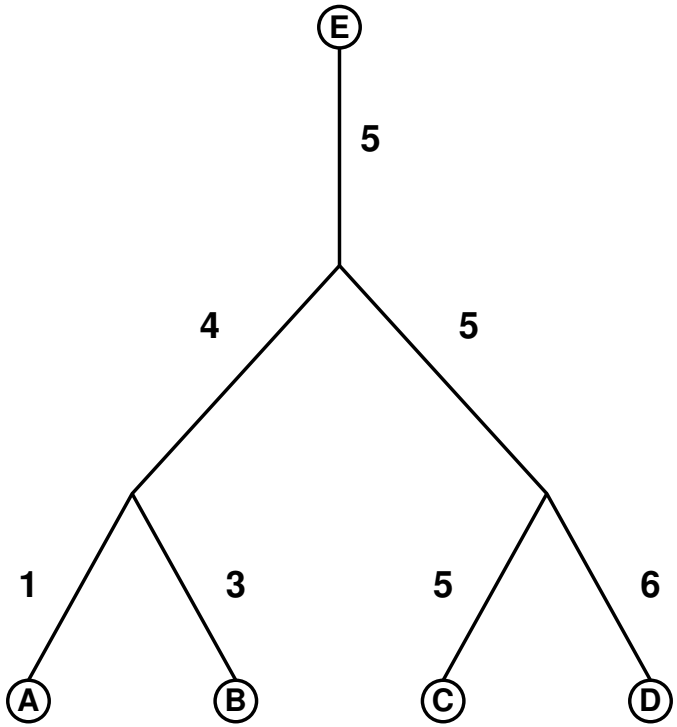

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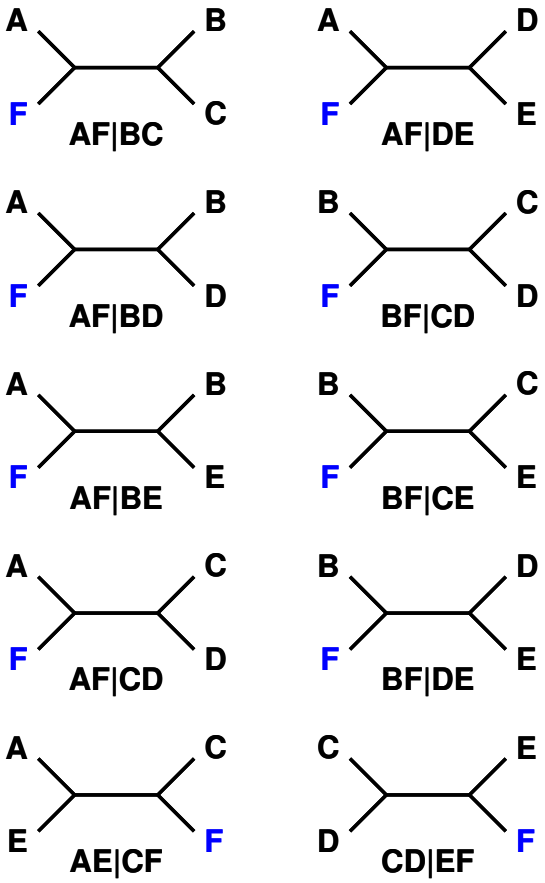
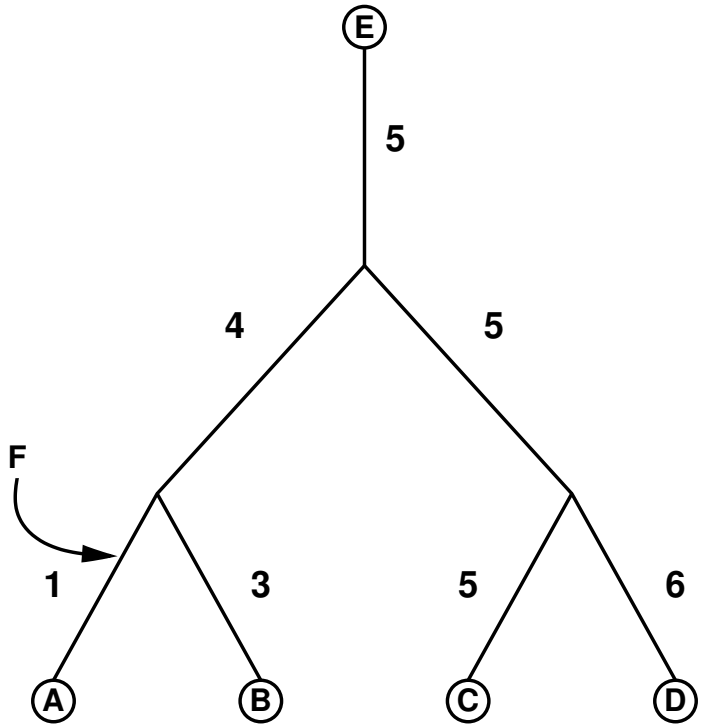
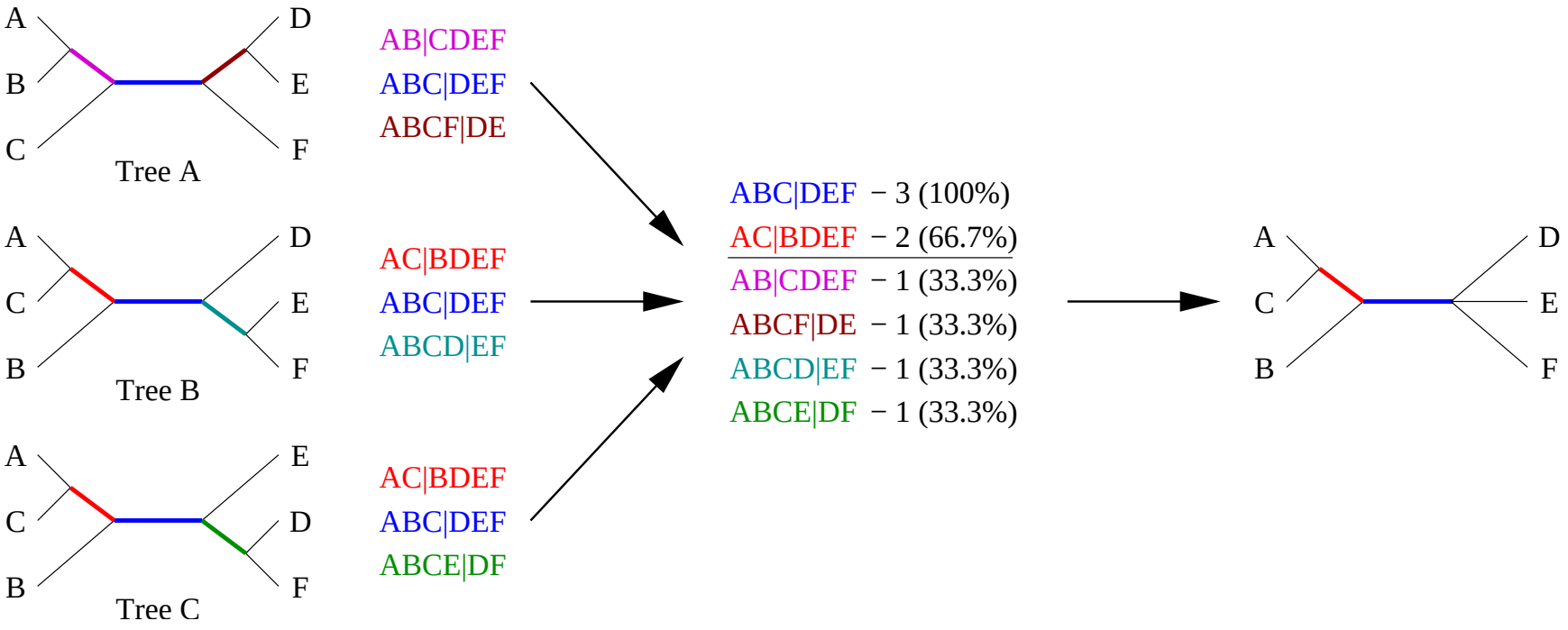




Consensus Step

From the collection of trees from the puzzling step we compute a majority consensus tree:



Speeding up TREE-PUZZLE

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- Parallel Computing

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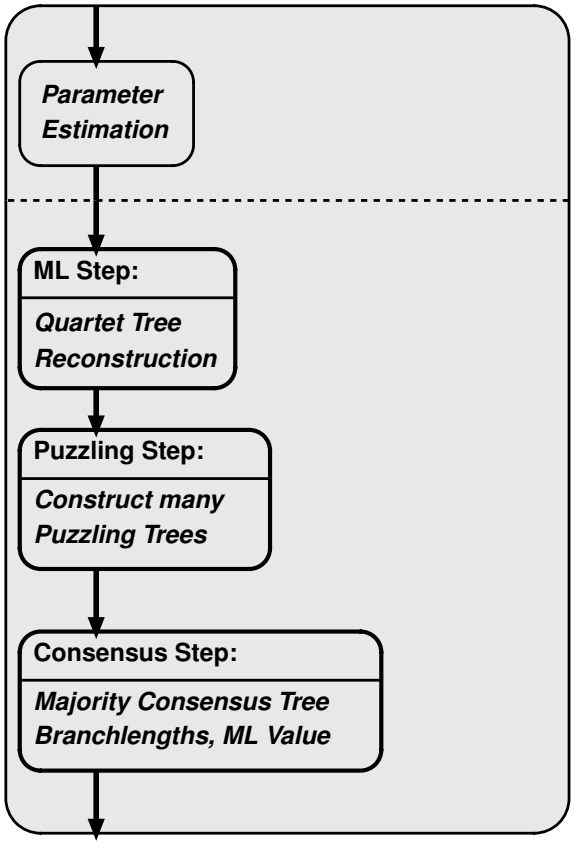
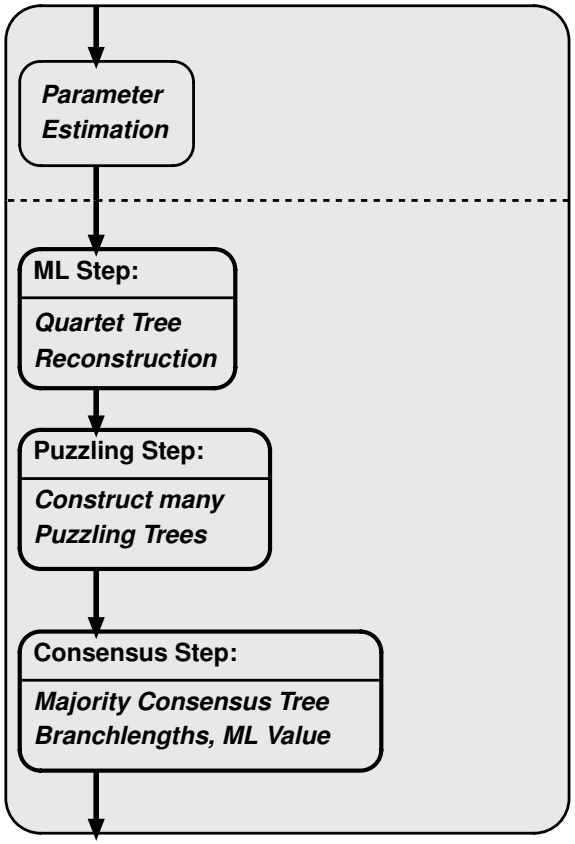


The *Quartet Puzzling* Algorithm

Runtime-Profile

64 sequences, 1000 bp, 11 h

- Parameters: 1.27 %
- ML Step: 43.15 %
- Puzzling Step: 55.53 %
- Consensus Step: 0.05 %



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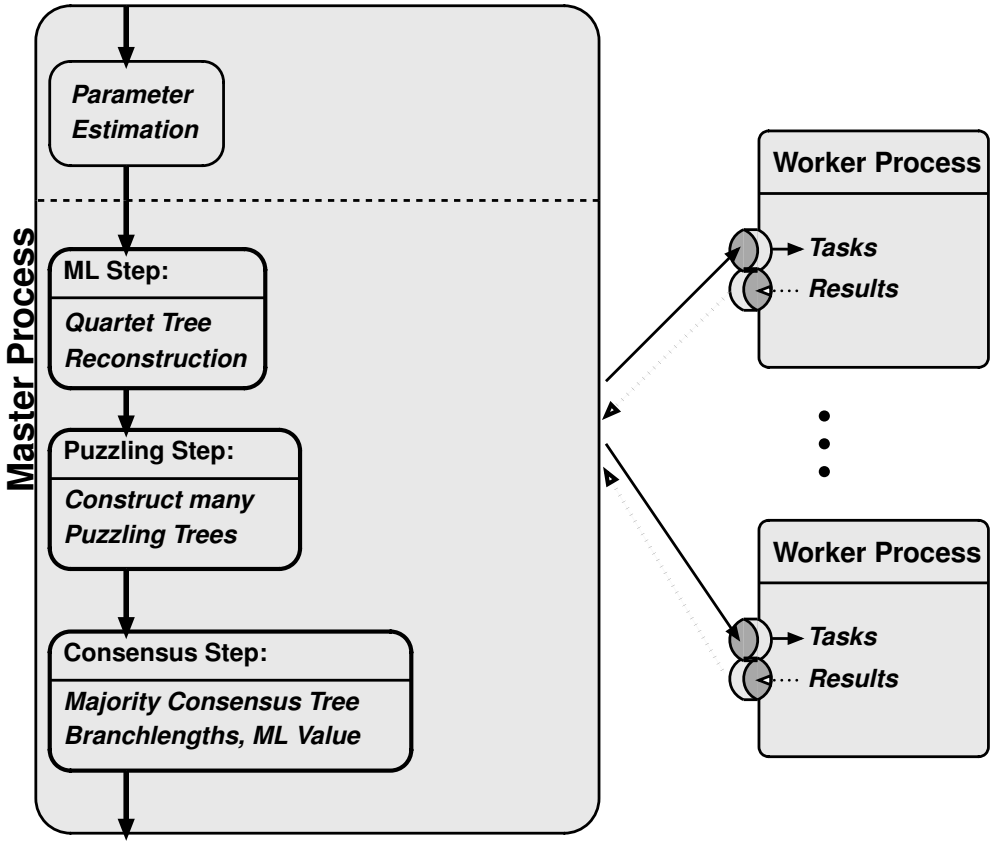

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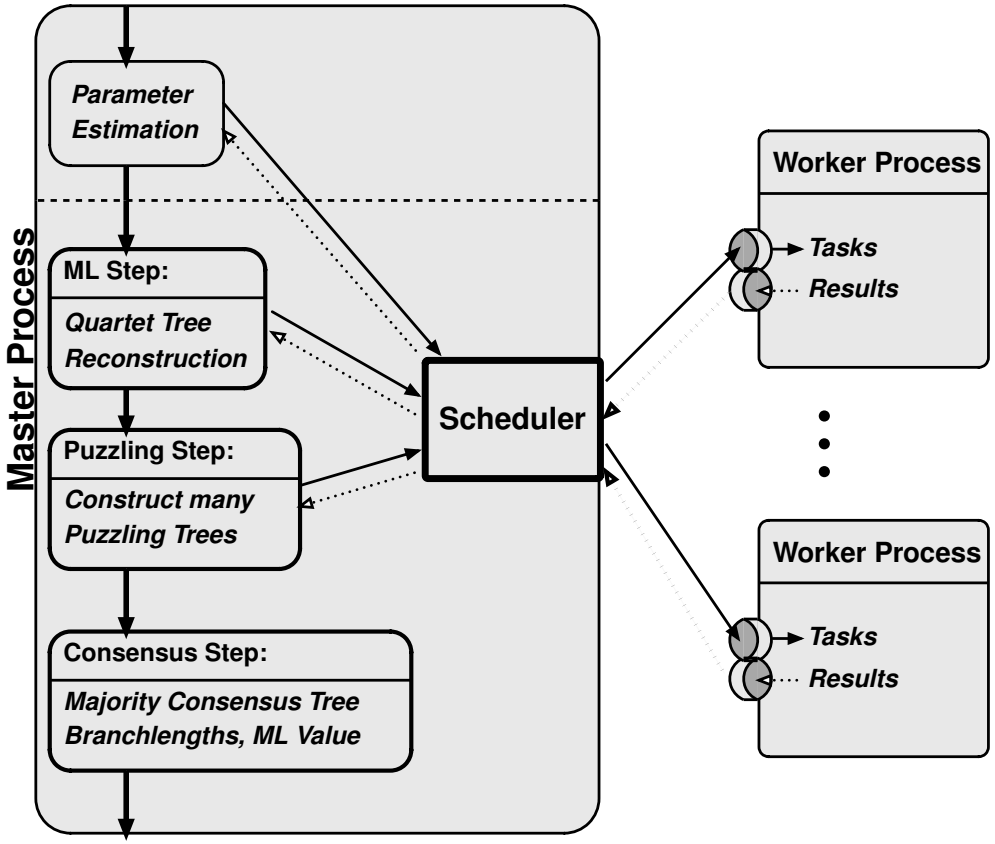

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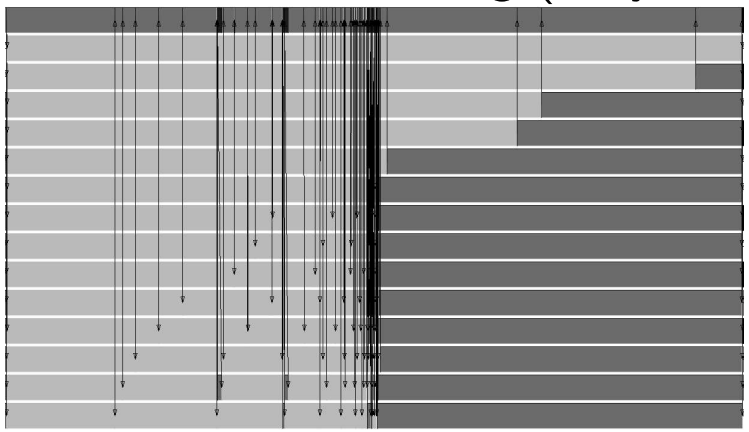

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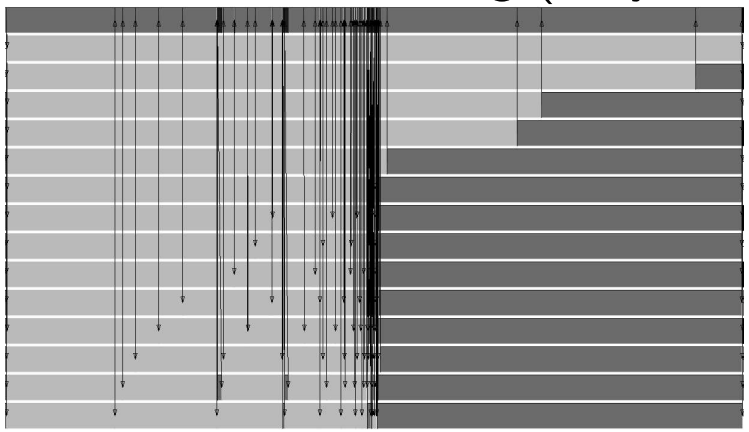
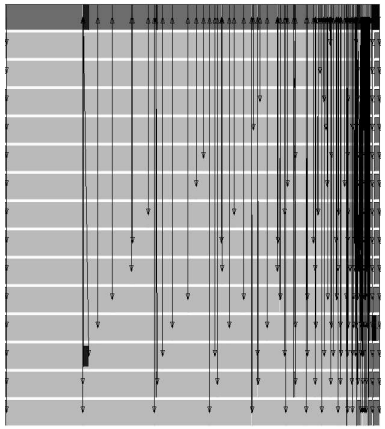
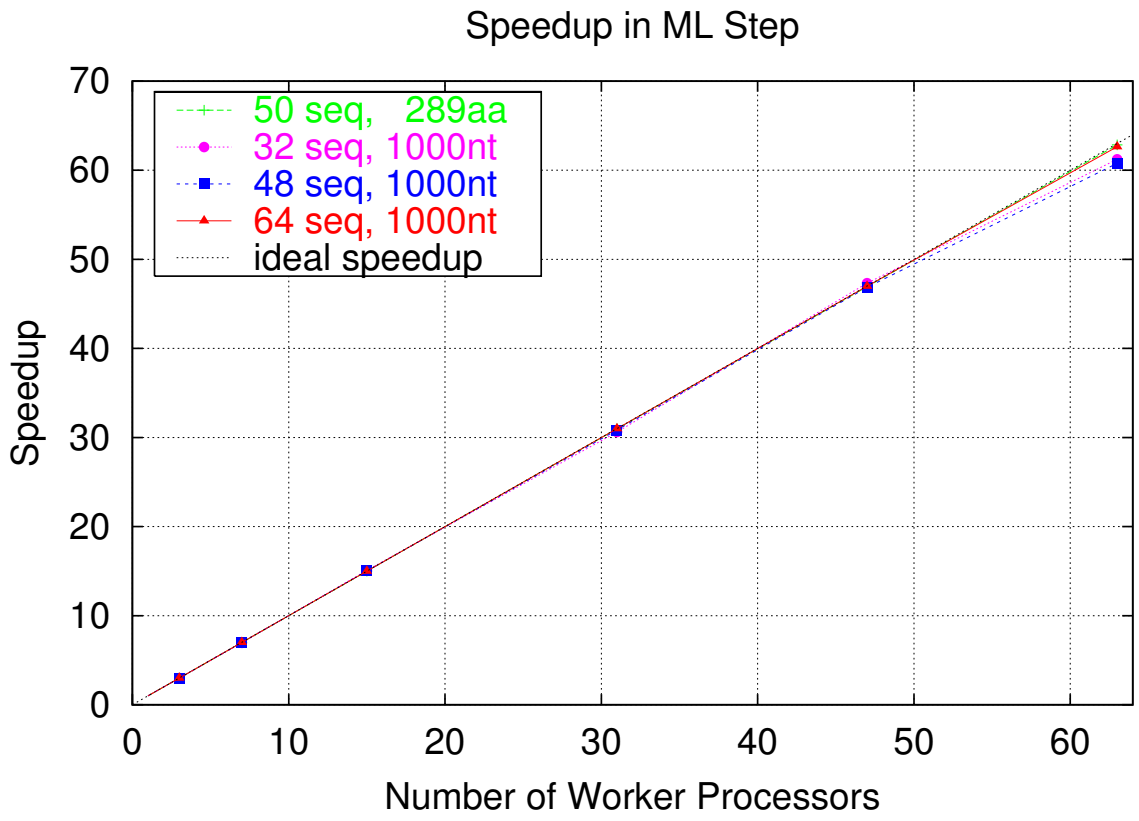


- Smooth Guided Self Scheduling (Schmidt et al., 2002)



Parallel ML Step



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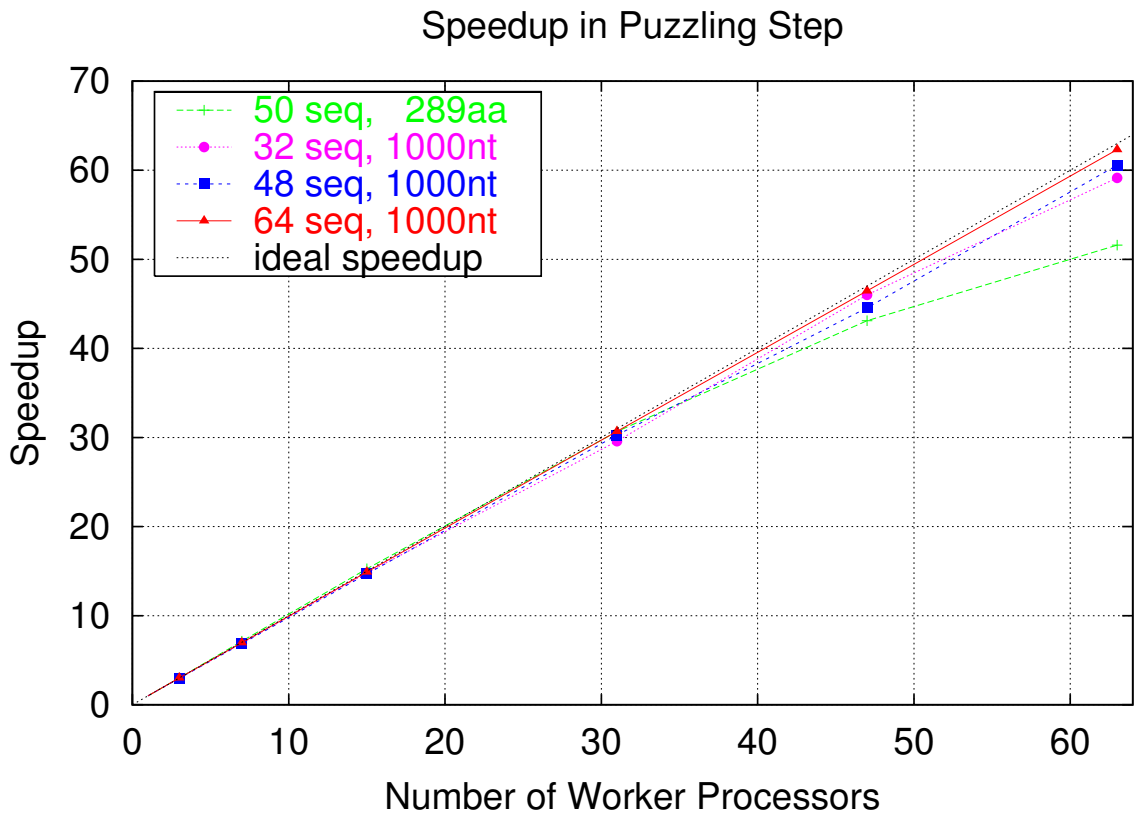
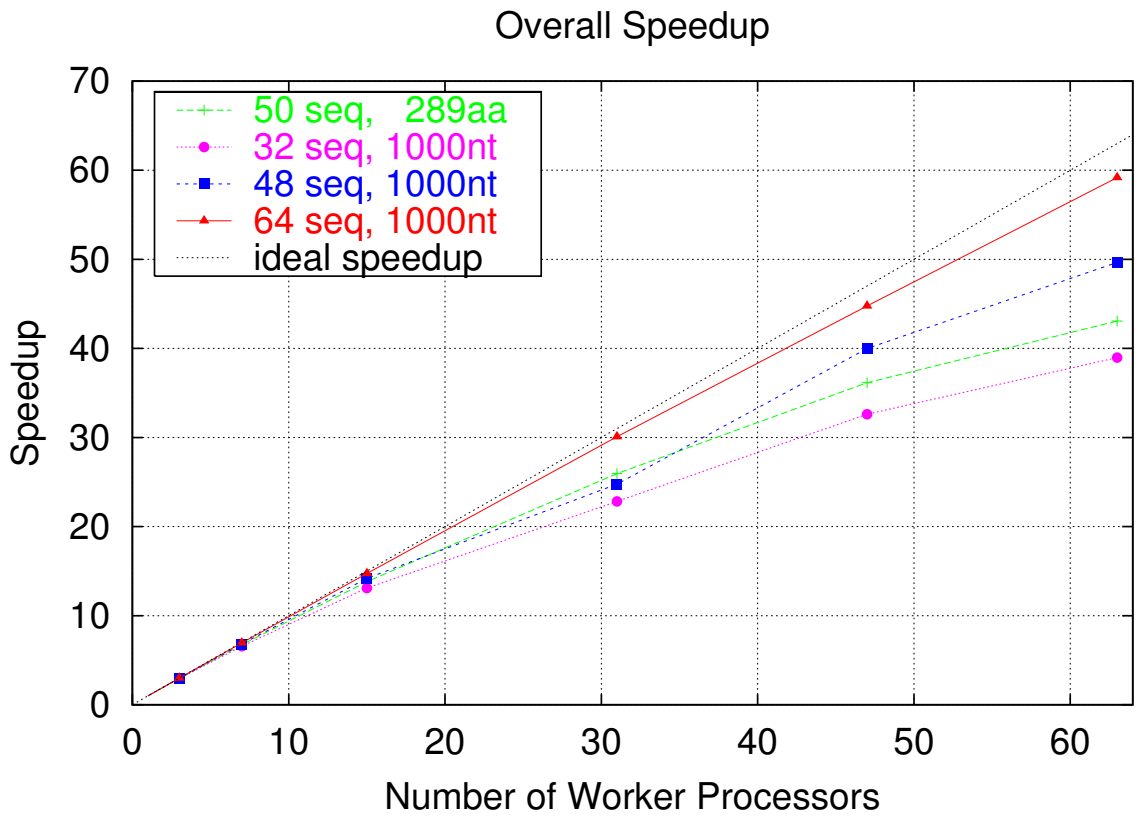


Parallel TREE-PUZZLE



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Dataset: 64 sequences, 1000 bp, rate heterogeneity

11 h (original algorithm)

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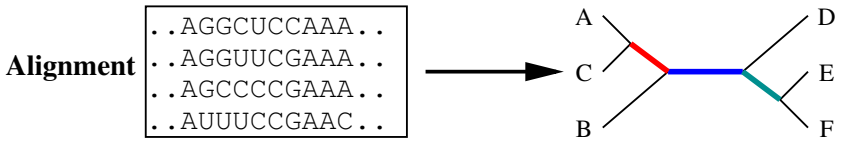
Confidence?

- TREE-PUZZLE produces support values in the consensus step.
- Bootstrap analysis.

Estimating Confidence: The Bootstrap



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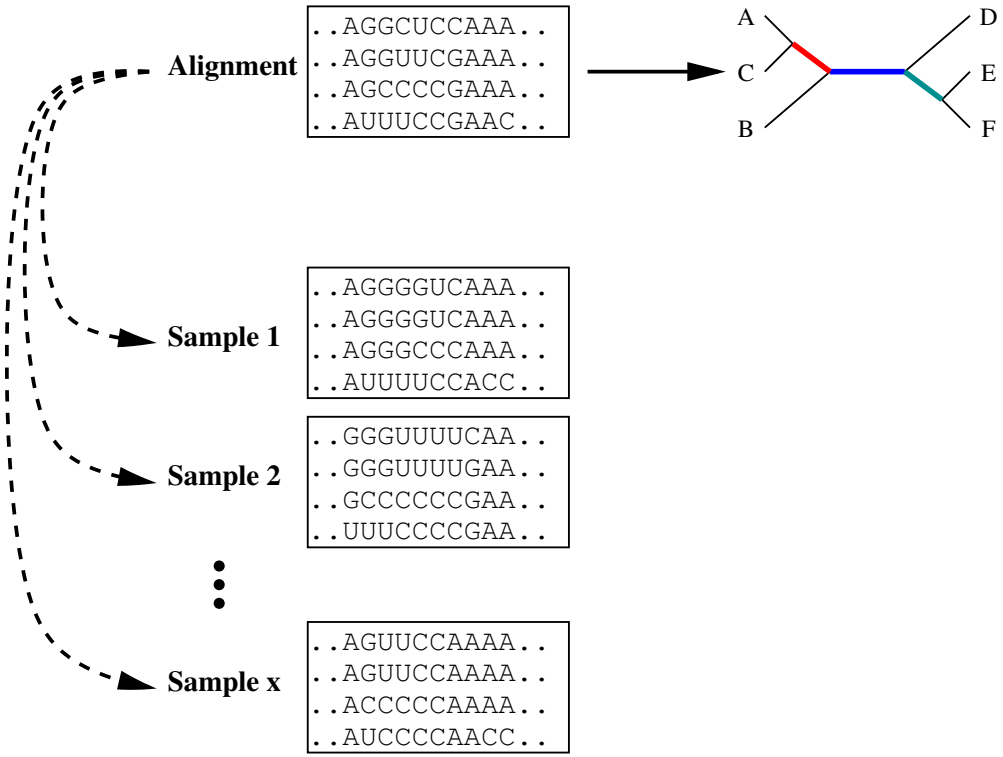

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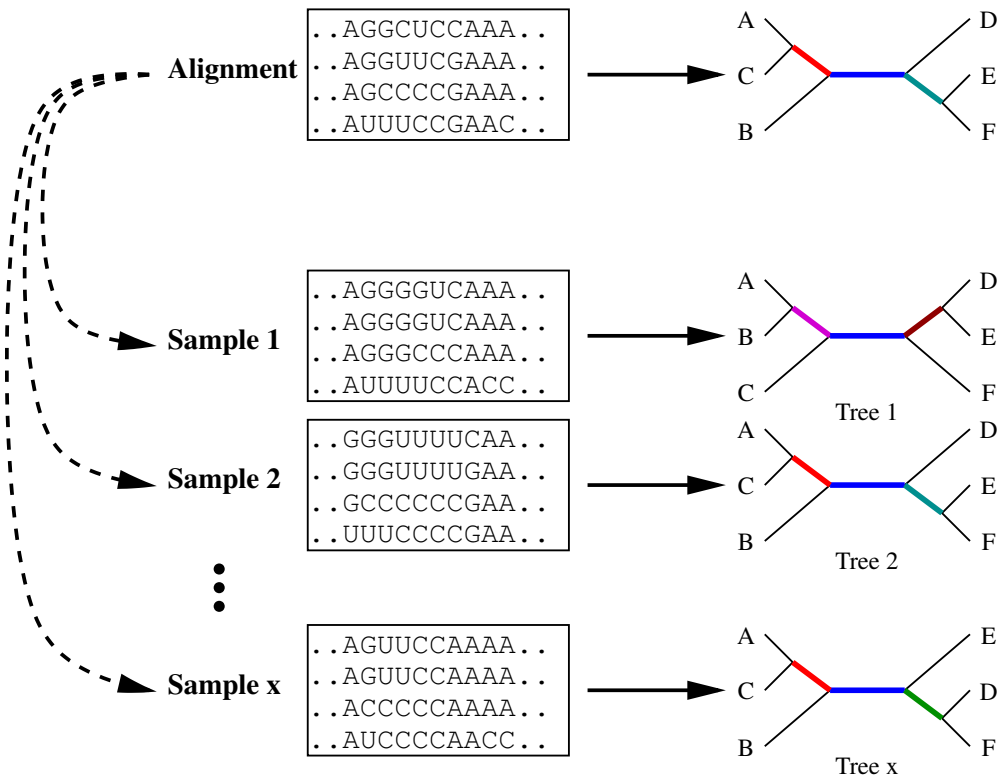
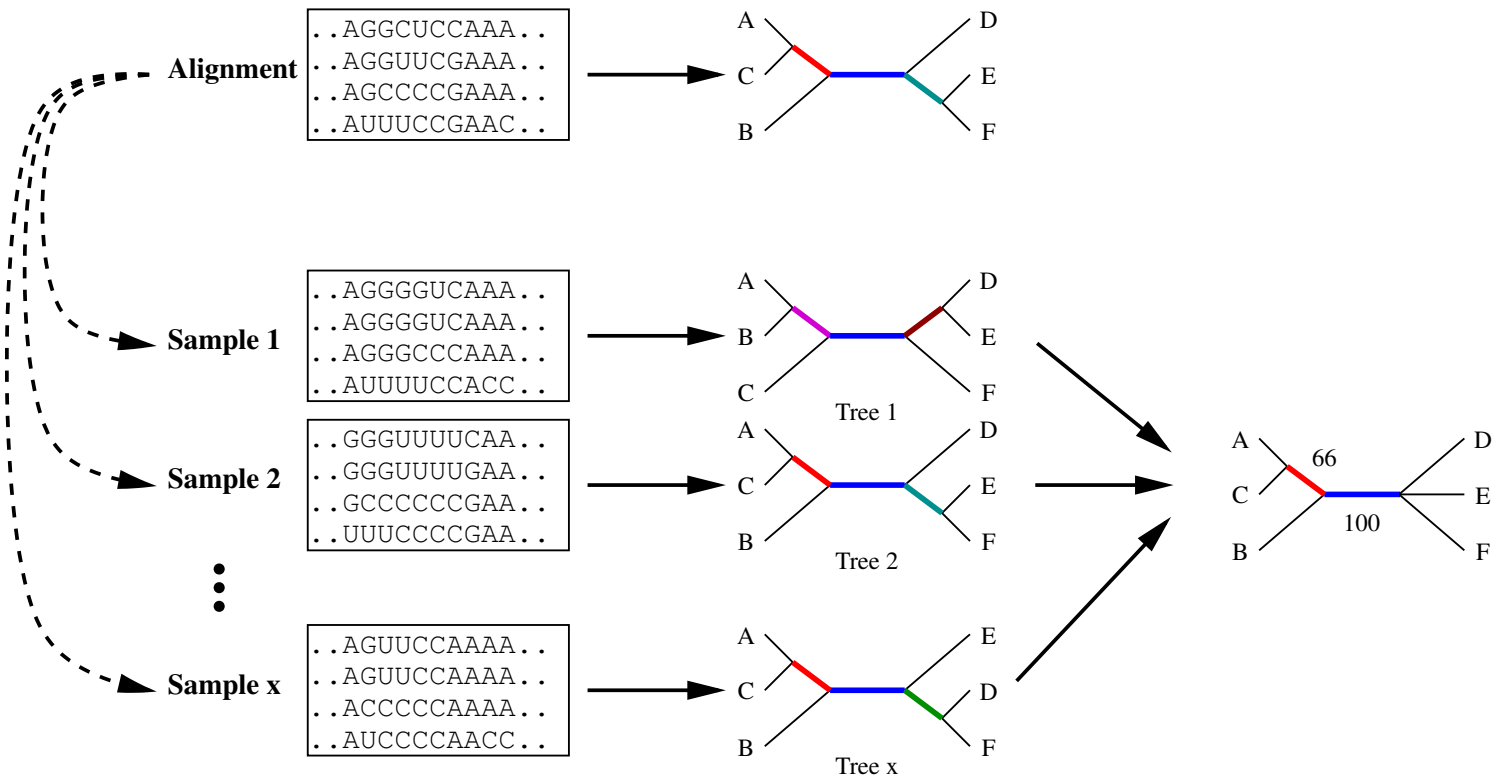
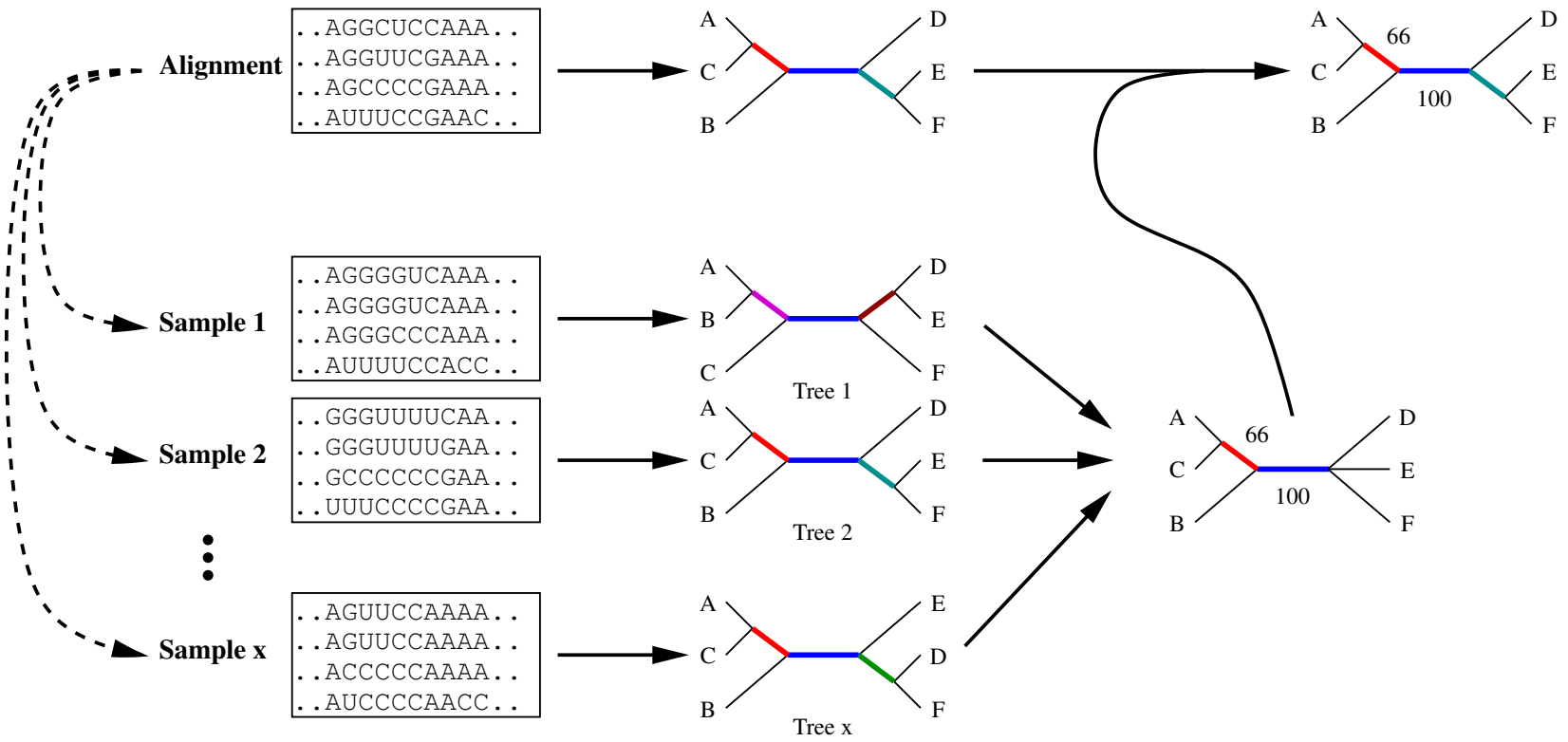


Estimating Confidence: The Bootstrap



Estimating Confidence: The Bootstrap



Obstacles in the analysis: numbers

- large numbers of possible trees:

$$B(n) = \prod_{k=3}^{n}(2k-5) = \frac{(2n-5)!}{2^{n-3}(n-3)!}$$

- Tree optimizations do examine many trees [NNI: $O(n)$, SPR: $O(n^2)$, TBR: $O(n^3)$]

- large numbers of iterations (IQPNNI), generations (MCMC) or samples (Bootstrap analysis, > 100).

- large numbers of $\binom{n}{4}$ quartets (quartet methods, concerning time and memory)

Hopes/wishes for discussion. . .

- efficient and applicable (distributed) algorithms
- (distributed) data structures (e.g. sparse arrays of quartets with a lot of missing data)
- ideas to improve the current algorithms, parallelizations, communication. . .
- new ideas for different new heuristics
- (parallel) optimization techniques
- ideas for (parallel) simultaneous branch length optimization (dependencies!)
- . . .
- maybe there is a good way for a more general distributed system usable for other problems in Bioinformatics.