BEAST2 tree (space) tools
Convergence + Means

ASM and CCD

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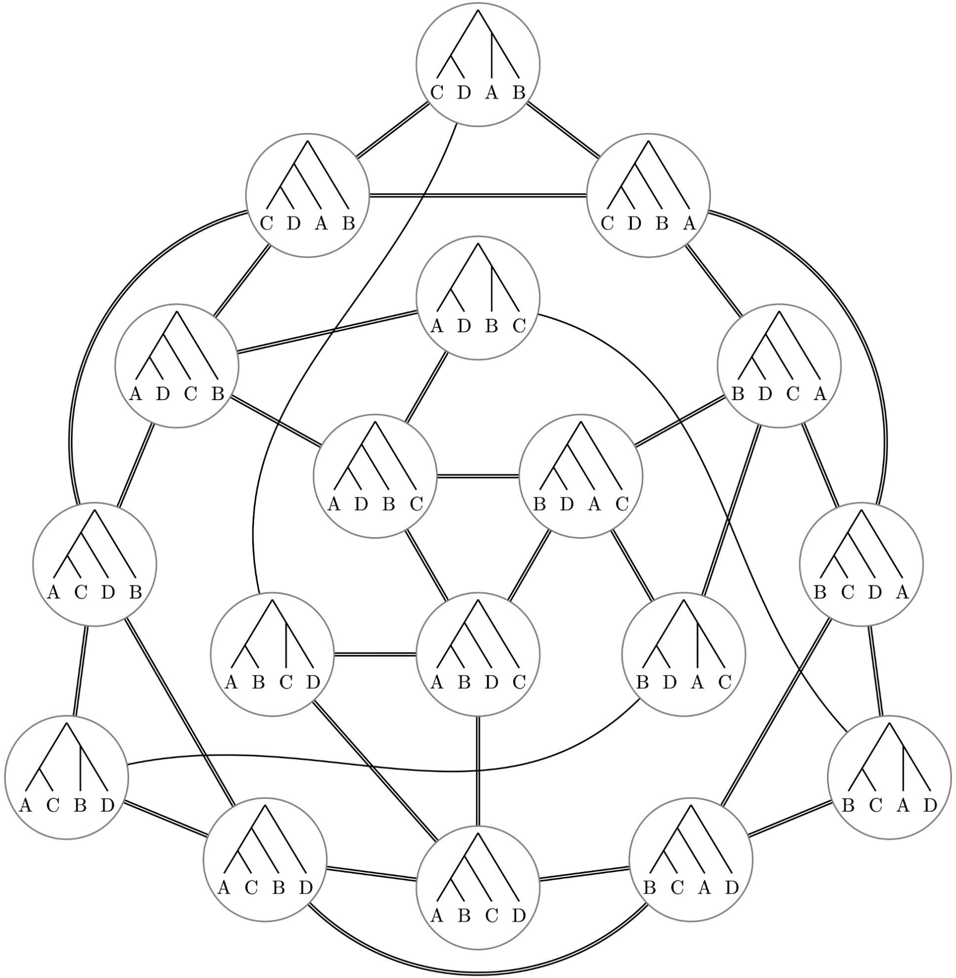
RNNI space with 4 taxa

- Rank moves – single edges
- NNI moves – double edges



Convergence of Markov chain Monte Carlo

- In theory MCMC converges to the target distribution asymptotically
- Consider: convergence = indistinguishable samples form independent runs
- Phylogenetics rule of thumb for effective sample size (ESS):
  - ESS < 100 is bad
  - ESS > 100 is okay
  - ESS > 200 is converged
  - !NOTE: ESS is only for continuous parameter traces

→ No one is checking the trees!

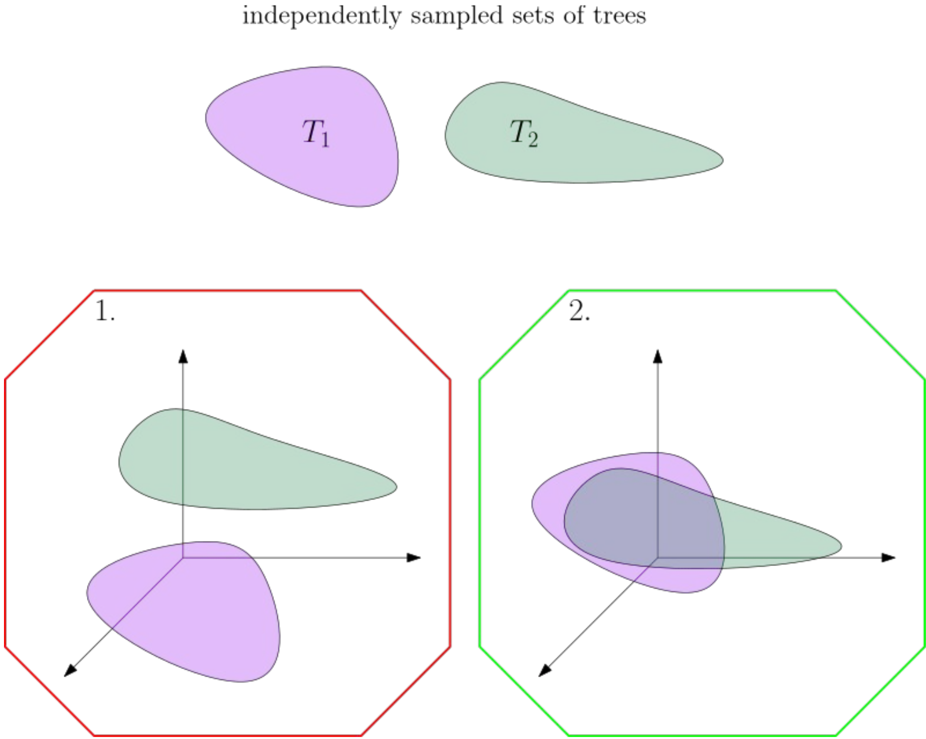
The ASM package automates best practises and adds tree space based diagnosis

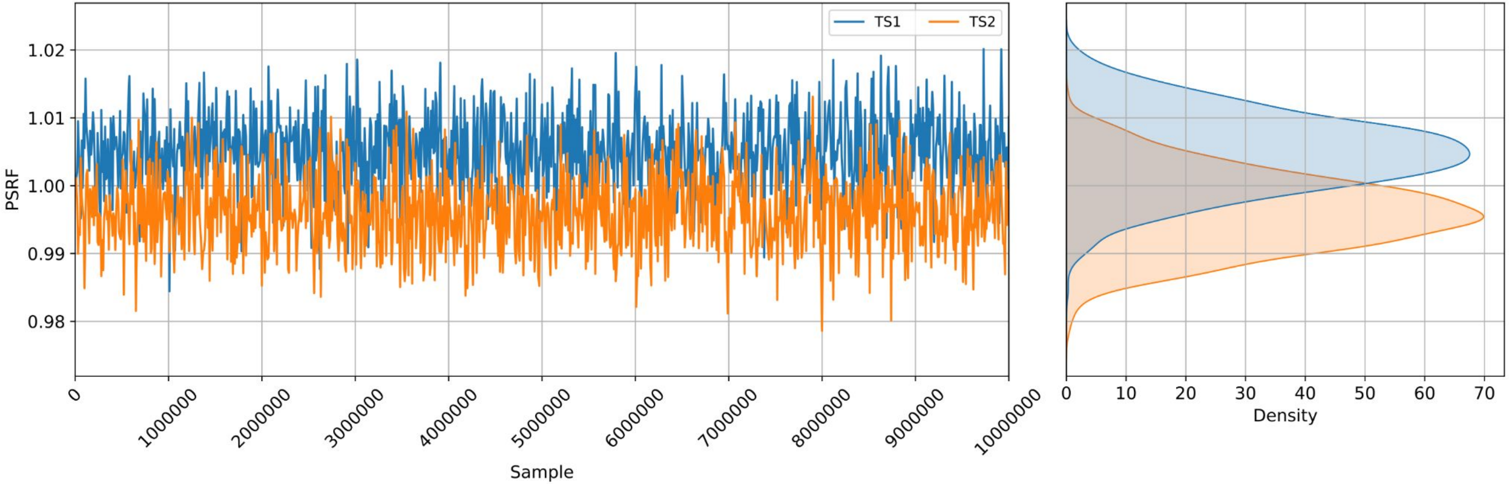
Use the RNNI space to define a convergence diagnostic:

$$\mathbf{Var}(t)_{\mathcal{T}} = \frac{\Sigma_{t_i \in \mathcal{T}} d(t_i, t)^2}{|\mathcal{T}|}.$$

$$\mathbf{PSRF}(t; \mathcal{T}_1, \mathcal{T}_2) = \sqrt{\frac{\mathbf{Var}(t)_{\mathcal{T}_2}}{\mathbf{Var}(t)_{\mathcal{T}_1}}}, t \in \mathcal{T}_1$$

$$\mathbf{GR}(t_i^1; \mathcal{T}_1, \mathcal{T}_2) = \frac{1}{i} \sum_{s=1}^{i} \mathbf{PSRF}(t_s; \mathcal{T}_1, \mathcal{T}_2)$$

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TS2
PSRF
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1.01
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Sample
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10000000
Density
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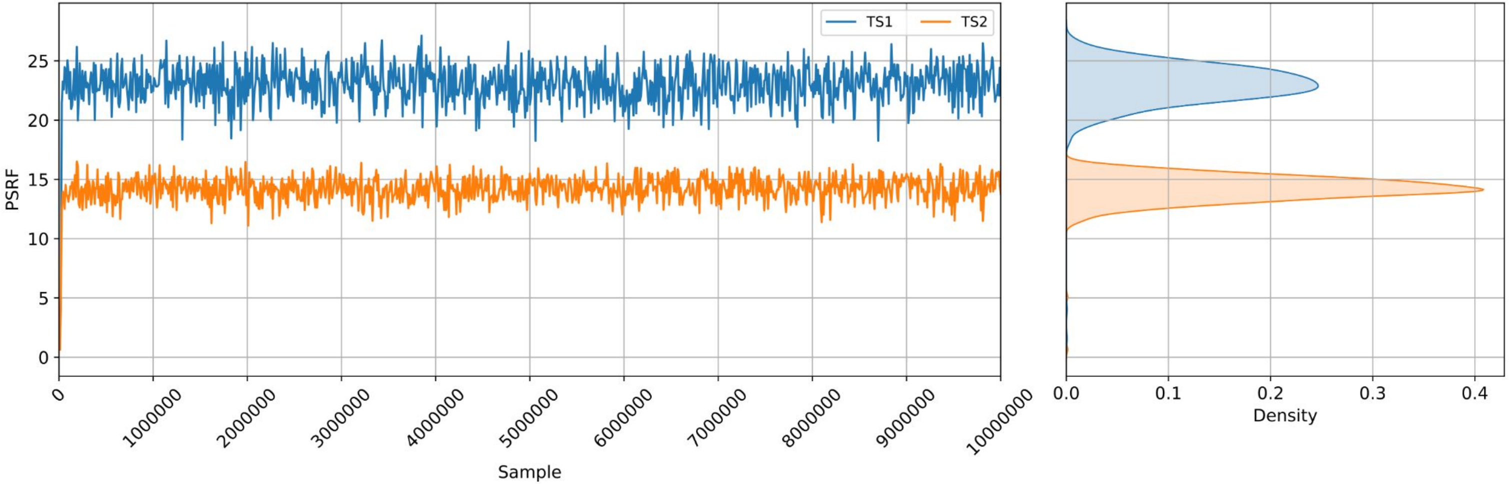
10
20
30
40
50
60
70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TS2
PSRF
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20
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10
5
0
Sample
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1000000
2000000
3000000
4000000
5000000
6000000
7000000
8000000
9000000
10000000
Density
0.0
0.1
0.2
0.3
0.4

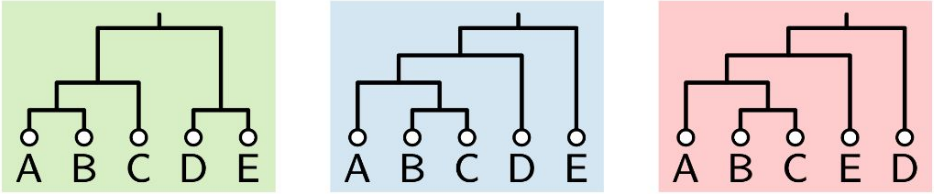
Summary/Consensus/Mean tree

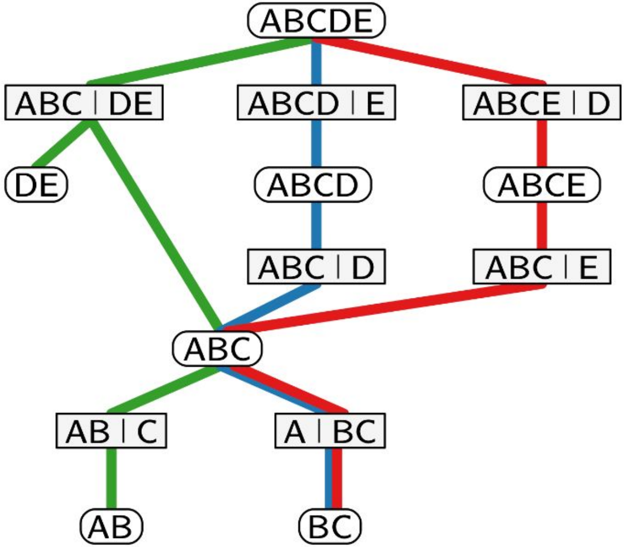
- Trees are now only topologies
- Tractable tree distribution:
  - A simple example would be a MCMC sample
  - Here we use: Conditional clade distributions (CCDs)
- We want an accurate representation of the posterior
- Use a MCMC sample to generate a CCD

CCD graph & CCD1

- Based on observed clade splits

sampled trees





CCD graph & CCD1

- Based on observed clade splits

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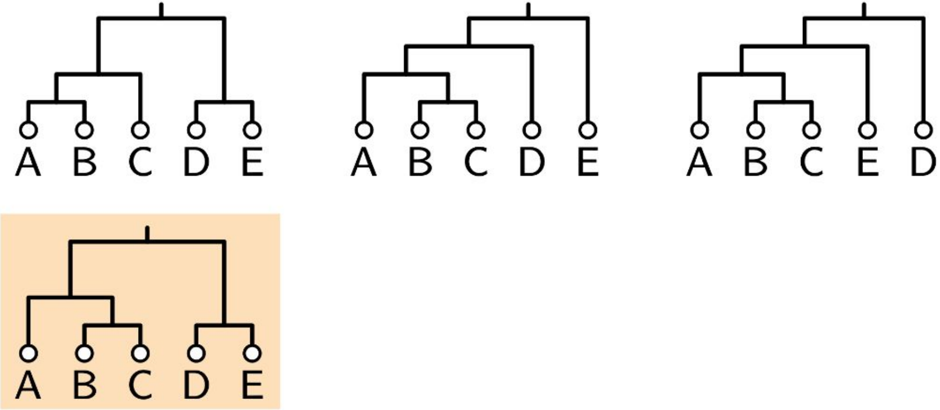
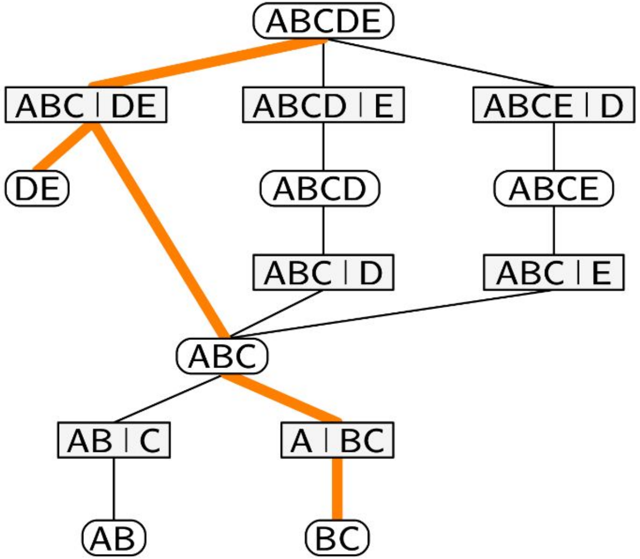



ABCDE

ABC | DE
ABCD | E
ABCE | D

DE
ABCD
ABCE

ABC | D
ABC | E

ABC

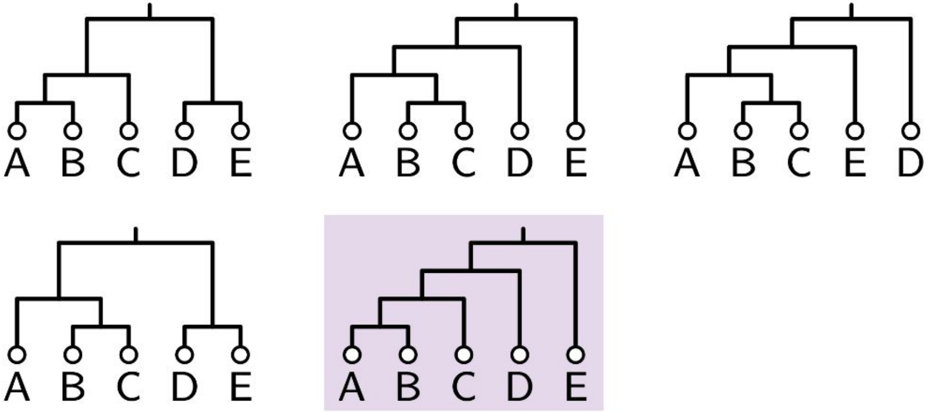
AB | C
A | BC

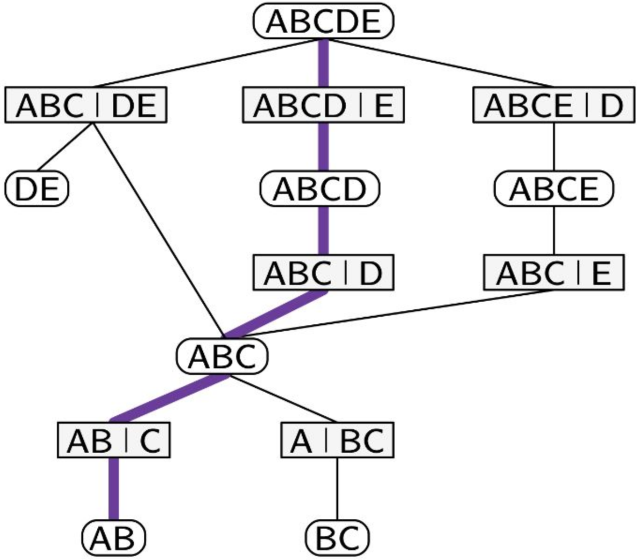
AB
BC

CCD graph & CCD1

- Based on observed clade splits

sampled trees





CCD graph & CCD1

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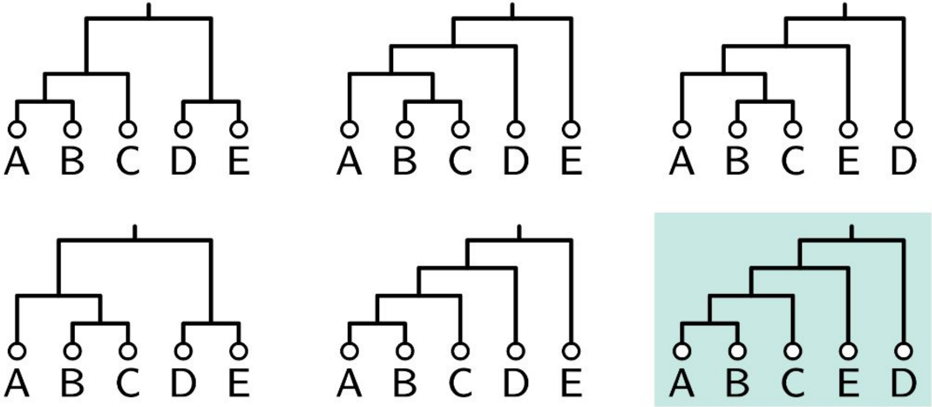
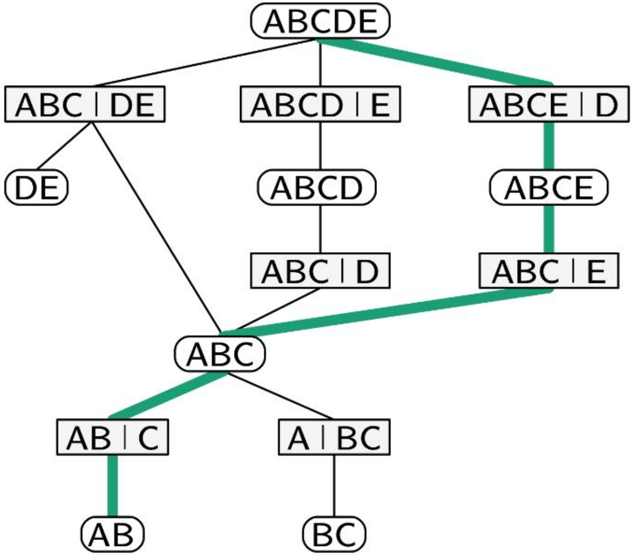
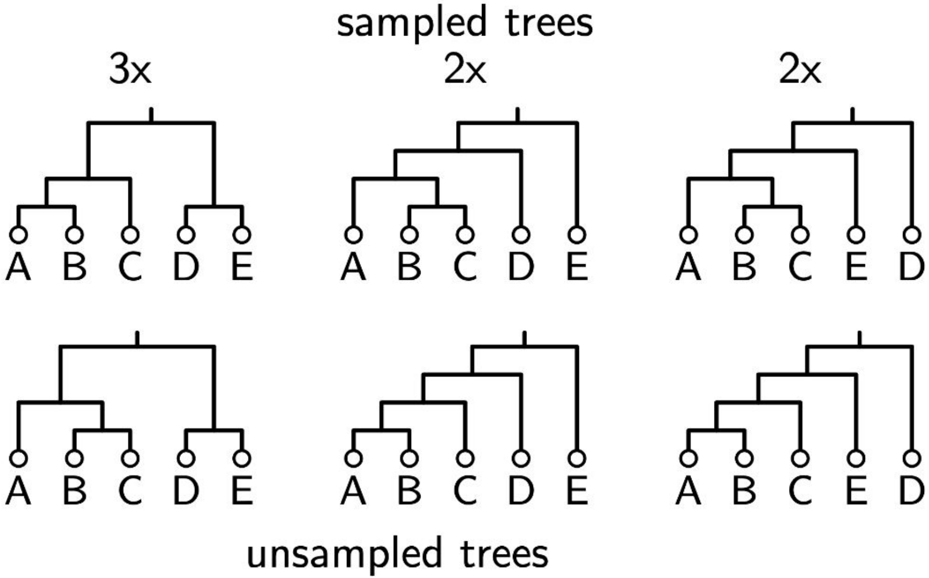
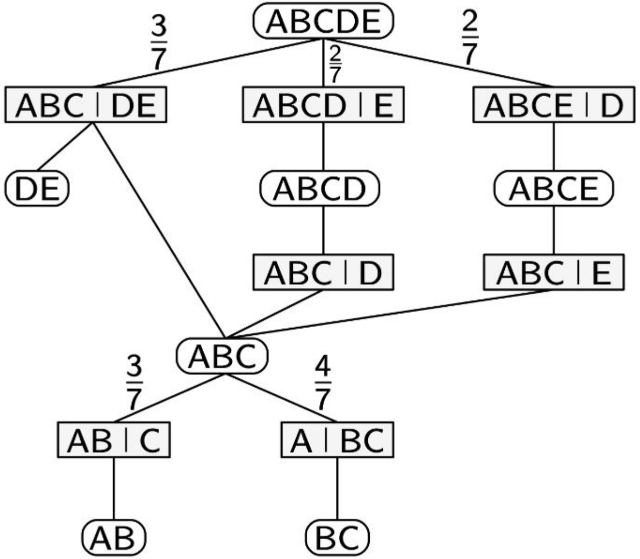




CCD graph & CCD1

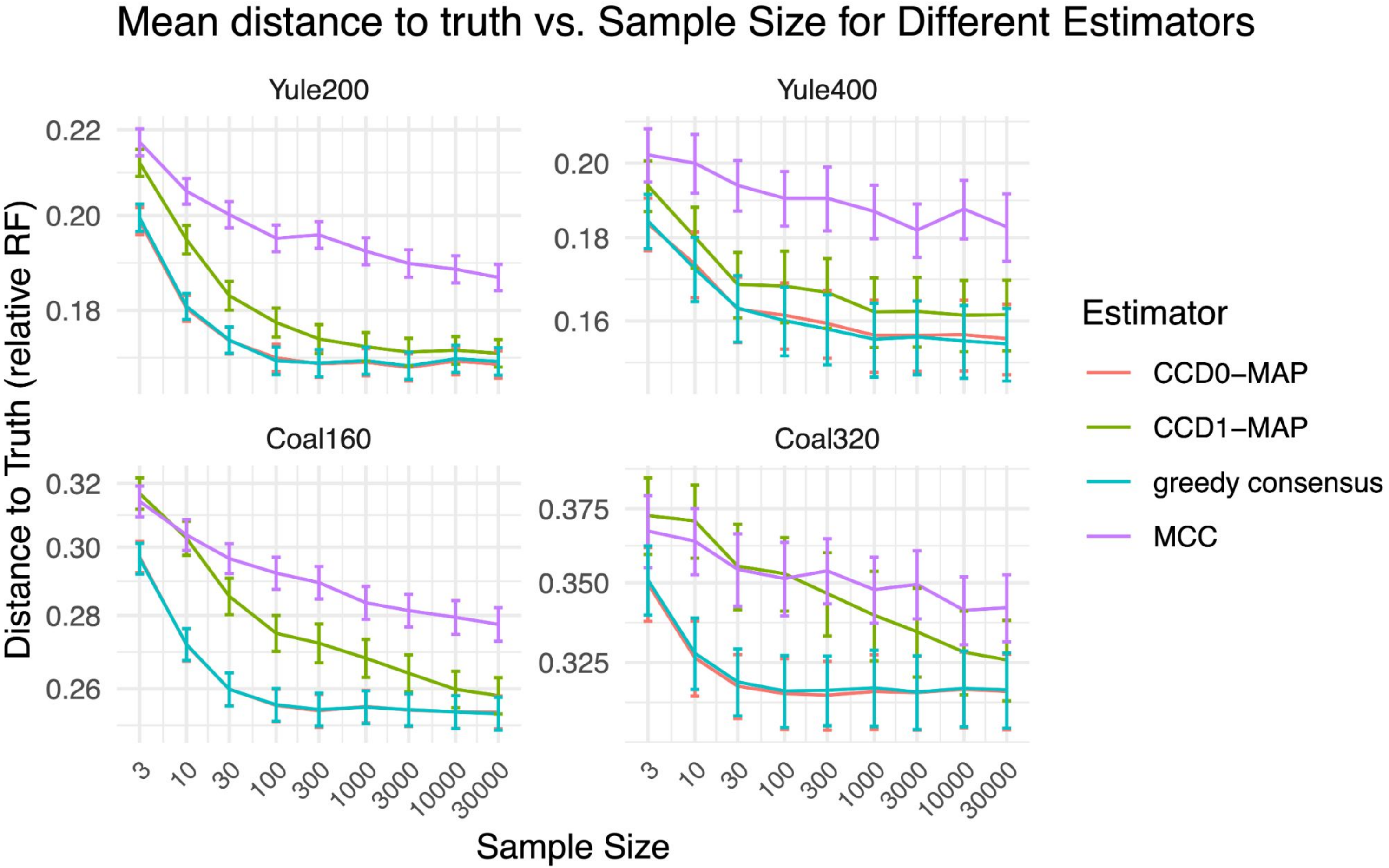
- Based on observed clade splits



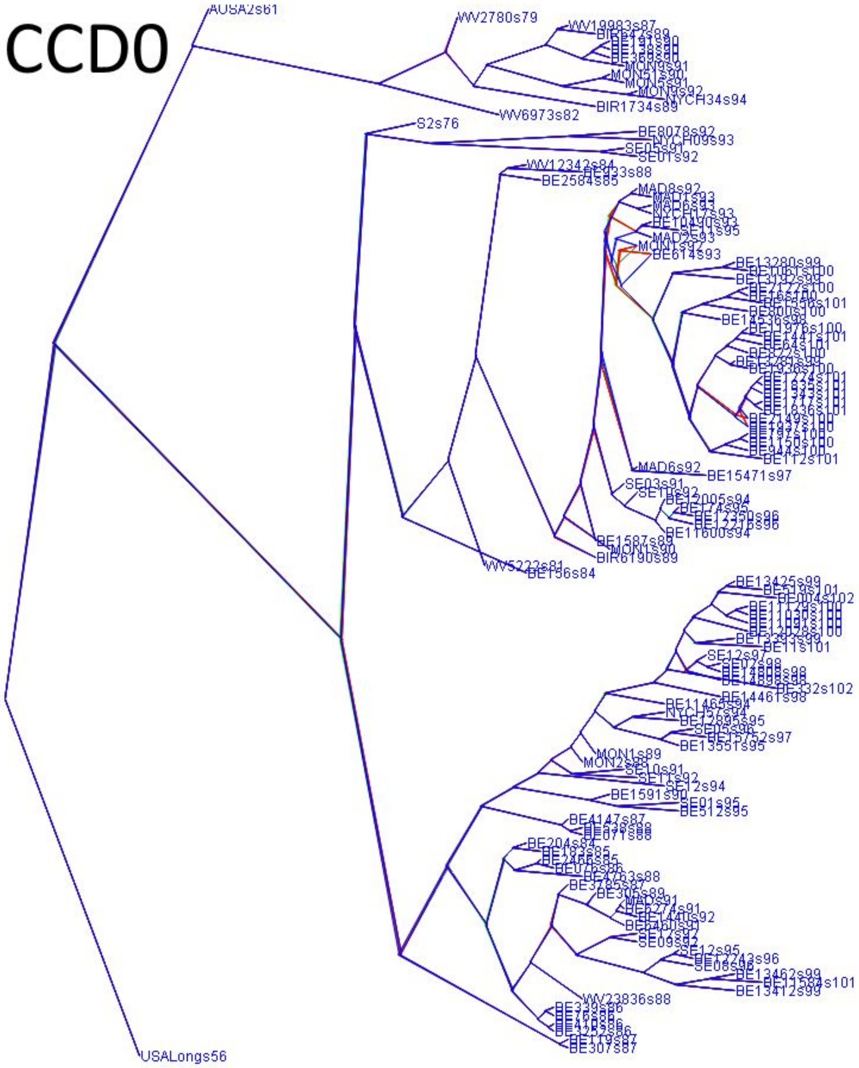


- Tree probabilities . . .

Accuracy of CCD MAP trees



CCD0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WV19983s87
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MON9s92
NYCH34s94
BIR1734s89
WV6973s82
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BE8078s92
NYCH09s93
SE05s91
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WV12342s84
BE933s88
BE2584s85
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MAD1s93
MAD2s93
MON1s92
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BE12005s94
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BE1587s89
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SE09s92
SE12s95
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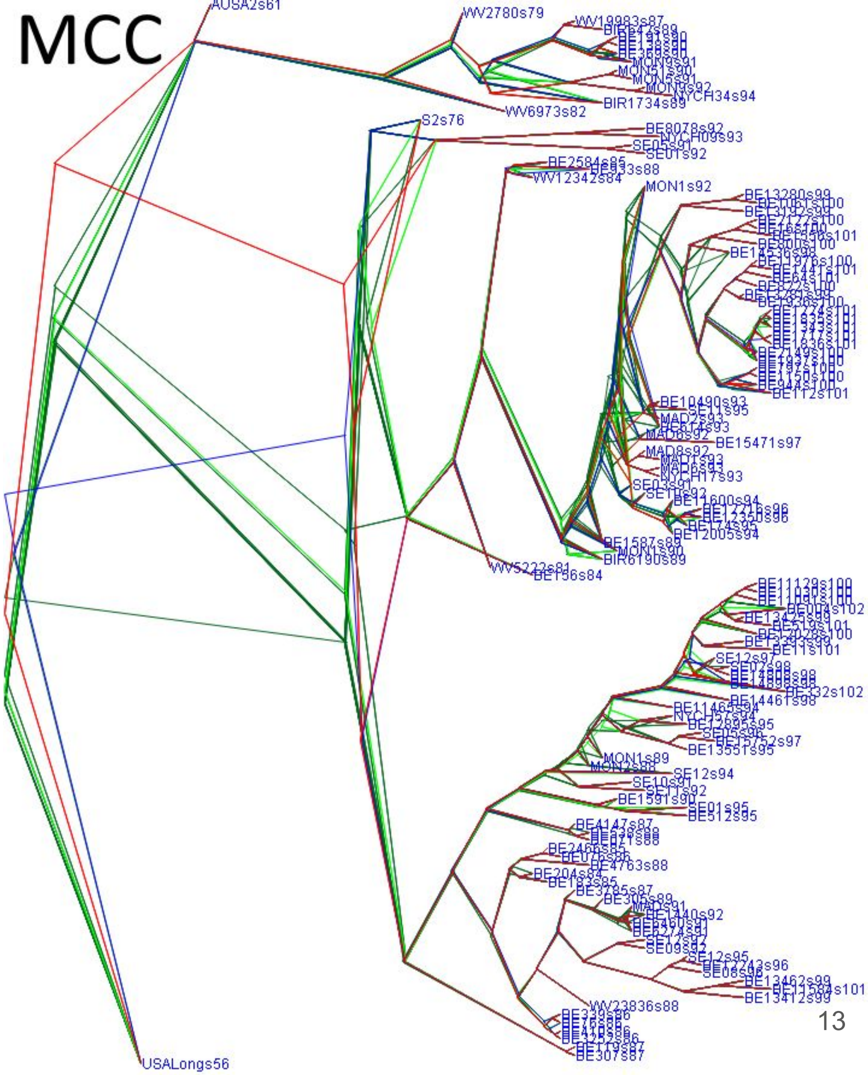
BE339s86
BE307s87
USALongs56

MCC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BE11584s101
BE13412s99
WV23836s88
BE339s86
BE307s87
USALongs56

- Check trees for convergence!
- Don’t use the MCC tree!

Thank you!

ASM package

"An automated convergence diagnostic for phylogenetic MCMC analyses." *IEEE/ACM Transactions on Computational Biology and Bioinformatics* (2024)

CCD package

"Accurate Bayesian phylogenetic point estimation using a tree distribution parameterized by clade probabilities." *PLOS Computational Biology (2025)*