

Generalizing Tree Probability Estimation via Bayesian Networks

Cheng Zhang and Frederick A. Matsen IV

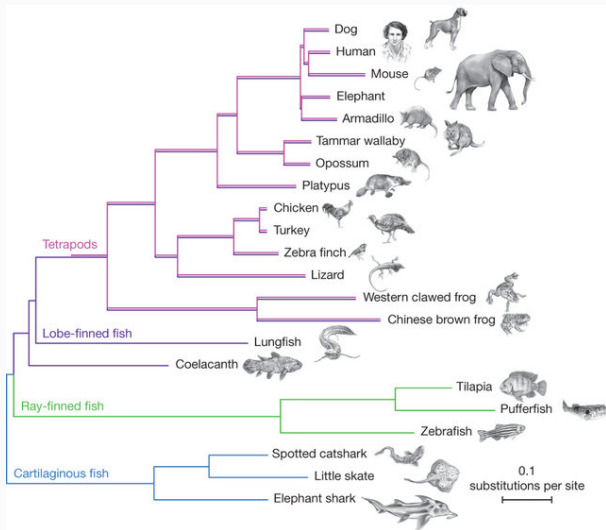
December 1, 2018

Fred Hutchinson Cancer Research Center, Seattle, WA



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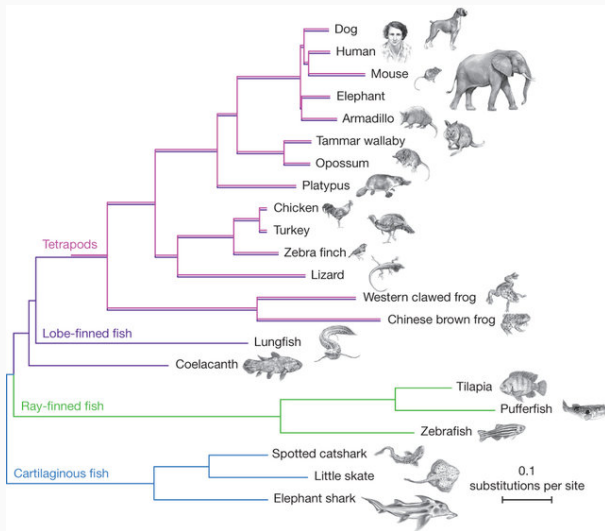
Phylogenetic Trees



Tree of life

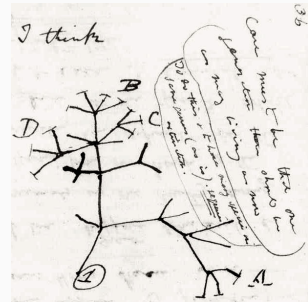
In Molecular Evolution, phylogenetic trees are used to model the evolutionary relationship among various biological species or other entities.

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In Molecular Evolution, **phylogenetic trees** are used to model the evolutionary relationship among various biological species or other entities.



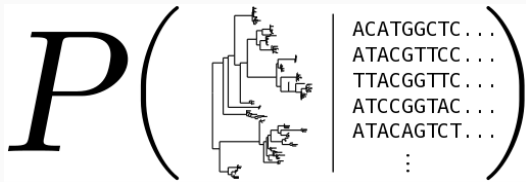
from Darwin's Notebook

Probability Estimation of Phylogenetic Trees

$$P \left(\begin{array}{c|c} \text{Phylogenetic Tree} & \begin{array}{l} \text{ACATGGCTC} \dots \\ \text{ATACGTTCC} \dots \\ \text{TTACGGTTC} \dots \\ \text{ATCCGGTAC} \dots \\ \text{ATACAGTCT} \dots \\ \vdots \end{array} \end{array} \right)$$

Markov chain Monte Carlo

Probability Estimation of Phylogenetic Trees

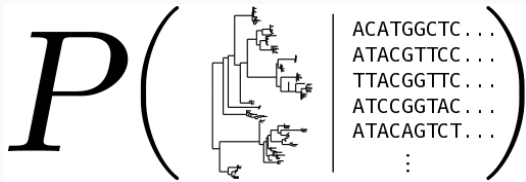


Markov chain Monte Carlo

Current approaches are unsatisfactory.

- Sample relative frequencies (SRF).
 - Do not generalize!
- Conditional clade distribution (CCD).
 - Not flexible enough for real data!

Probability Estimation of Phylogenetic Trees



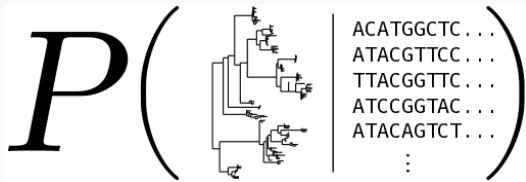
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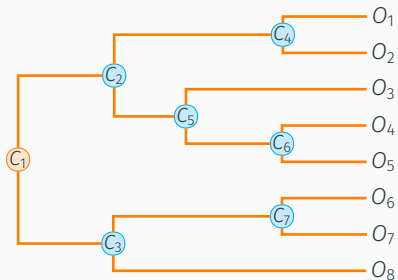
What is the best way to use MCMC samples?

Our Contribution: **Subsplit Bayesian Networks**. A general probability estimation framework for phylogenetic trees based on MCMC samples that

- generalizes to unsampled trees.
- provides accurate approximation for real data posteriors.

Key: harness the similarity of trees properly.

Problem Setup



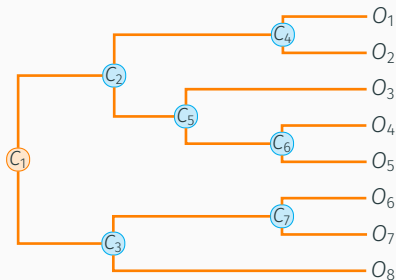
- Leaf label set $\mathcal{X} = \{O_1, \dots, O_N\}$, each label represents a species.
- A *clade* X is a nonempty subset of $\mathcal{X}$.

$$C_5 = \{O_3, O_4, O_5\}, \quad C_7 = \{O_6, O_7\}.$$

- *Clade Decomposition*

$$T_C = \{C_2, C_3, C_4, C_5, C_6, C_7\}$$

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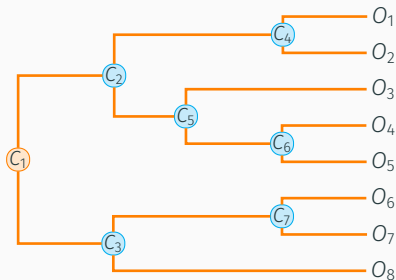
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A *subsplit* of a clade X is an ordered pair of disjoint subclades (Y, Z) such that $Y \cup Z = X$, $Y \succ Z$. Examples: $C_1 \rightarrow (C_2, C_3)$, $C_2 \rightarrow (C_4, C_5)$.

Subsplit Decomposition

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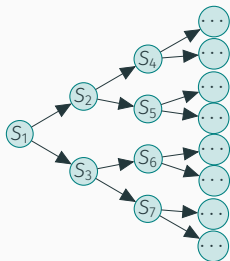
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$$p(T) = p(C_2, C_3)p(C_4, C_5|C_2, C_3)p(C_6|C_4, C_5)p(C_7|C_2, C_3)$$

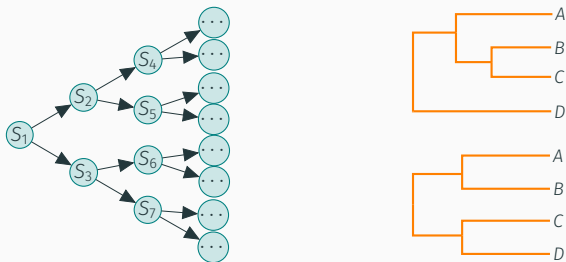
Subsplit Bayesian Networks



A **Subsplit Bayesian Network** on a leaf set $\mathcal{X}$ of size N is a Bayesian network

- nodes take on subsplit / singleton clade values.
- contains a full and complete binary tree.

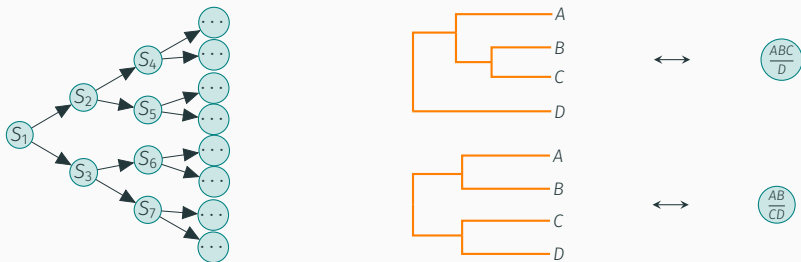
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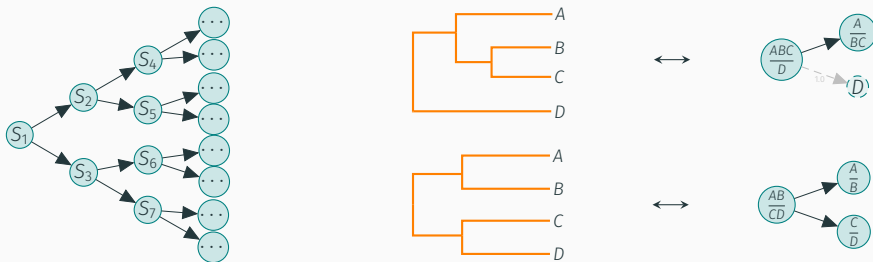
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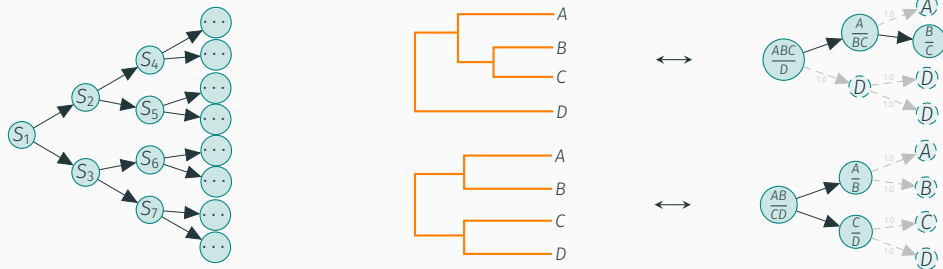
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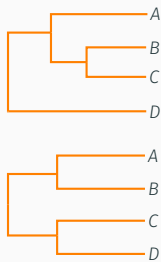
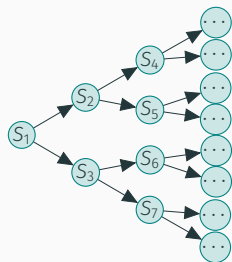
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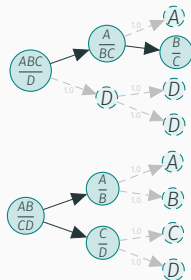
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$\longleftrightarrow$



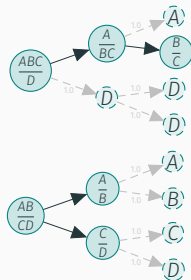
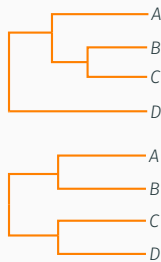
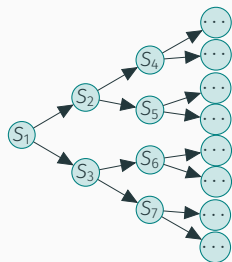
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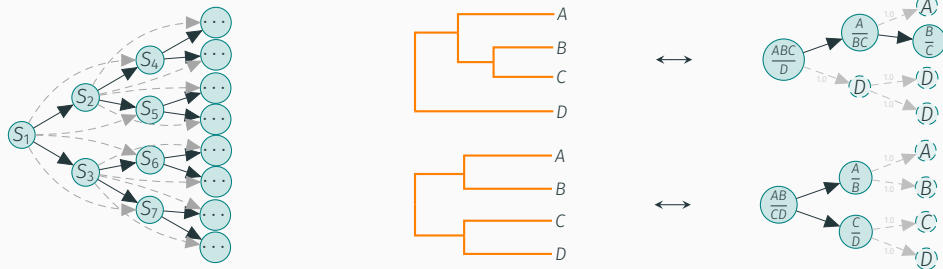
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SBN probability for rooted trees

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SBNs provide **valid probability distributions** and are **flexible**.

Rooted Trees

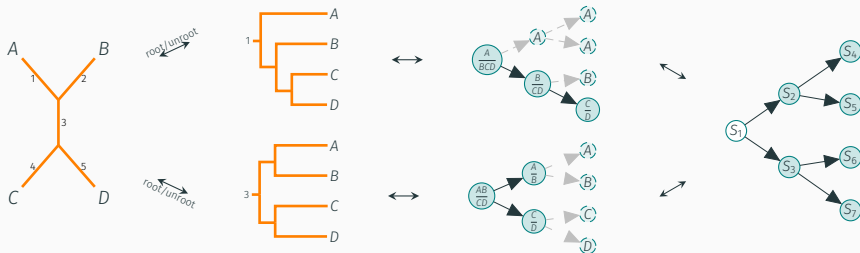
- maximum likelihood

Learning SBNs

Rooted Trees

- maximum likelihood

Unrooted Trees



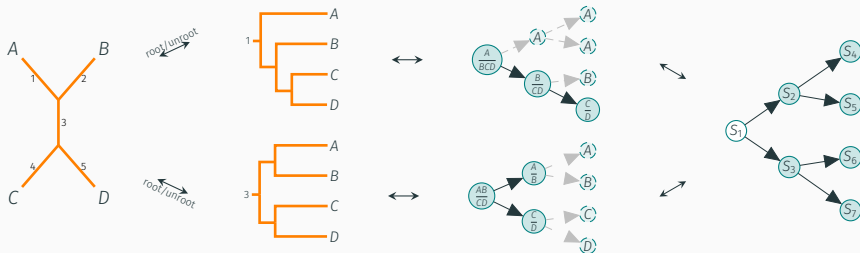
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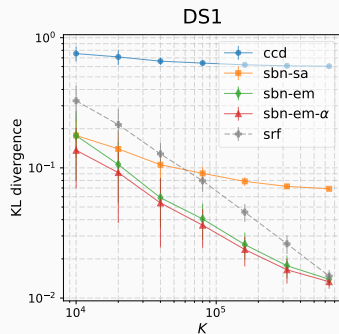
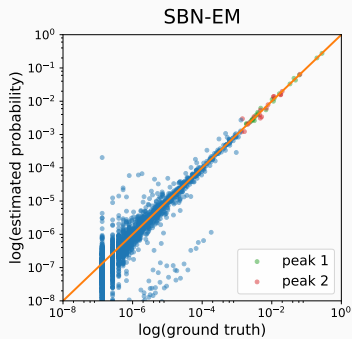
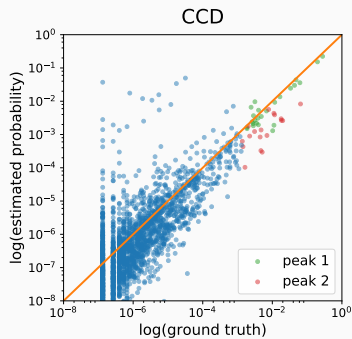
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Unrooted Trees

- Expectation Maximization
- simple averaging lower bound maximization
- incorporate regularization when necessary



Experiments



A real data set with multimodal posterior

Experiments

DATA SET	(#TAXA, #SITES)	TREE SPACE SIZE	SAMPLED TREES	KL DIVERGENCE TO GROUND TRUTH				
				SRF	CCD	SBN-SA	SBN-EM	SBN-EM- α
DS1	(27, 1949)	5.84×10^{32}	1228	0.0155	0.6027	0.0687	0.0136	0.0130
DS2	(29, 2520)	1.58×10^{35}	7	0.0122	0.0218	0.0218	0.0199	0.0128
DS3	(36, 1812)	4.89×10^{47}	43	0.3539	0.2074	0.1152	0.1243	0.0882
DS4	(41, 1137)	1.01×10^{57}	828	0.5322	0.1952	0.1021	0.0763	0.0637
DS5	(50, 378)	2.84×10^{74}	33752	11.5746	1.3272	0.8952	0.8599	0.8218
DS6	(50, 1133)	2.84×10^{74}	35407	10.0159	0.4526	0.2613	0.3016	0.2786
DS7	(59, 1824)	4.36×10^{92}	1125	1.2765	0.3292	0.2341	0.0483	0.0399
DS8	(64, 1008)	1.04×10^{103}	3067	2.1653	0.4149	0.2212	0.1415	0.1236

Poster # 123

- We proposed a general framework for tree probability estimation based on **subsplit Bayesian networks**.
- SBNs exploit the similarity among trees to provide **flexible** probability estimators that **generalize** to unsampled trees.
- Future work
 - extends to general trees
 - structure learning of SBNs
 - deeper investigation on the effect of parameter sharing
 - applications in other probabilistic learning problems in tree spaces (e.g., MCMC transition kernel design and variational inference)