Generalizing Tree Probability Estimation via Bayesian Networks

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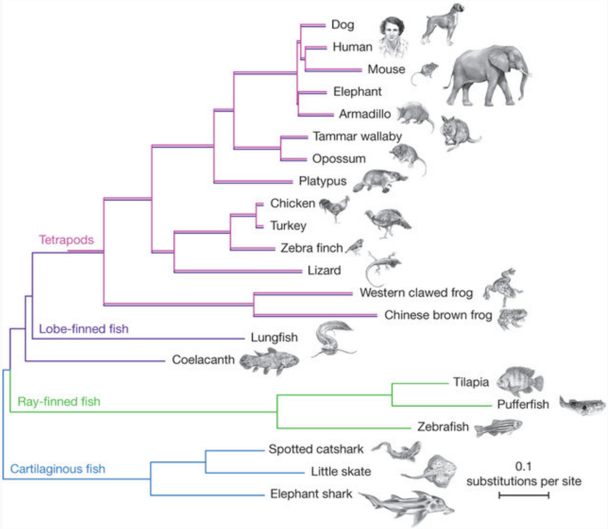
December 1, 2018

Fred Hutchinson Cancer Research Center, Seattle, WA

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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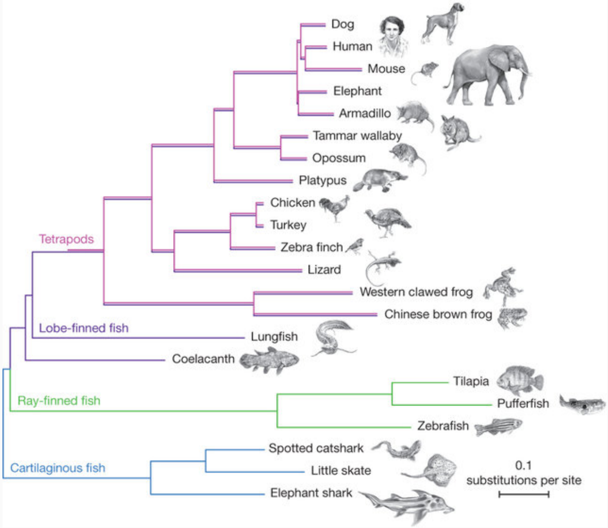

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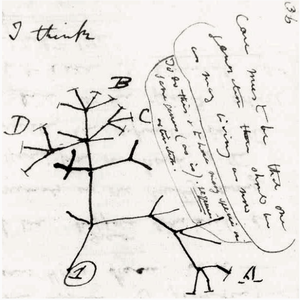
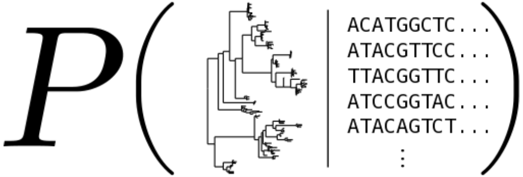

36
I think
B
C
D
1
A
Case must be that one generation then should be as many living as now.
To do this & to have many species in same genus (as is) requires extinction.

from Darwin's Notebook

Probability Estimation of Phylogenetic Trees



Markov chain Monte Carlo

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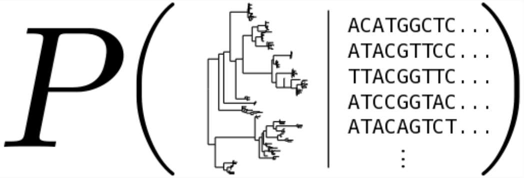

Markov chain Monte Carlo

Current approaches are unsatisfactory.

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

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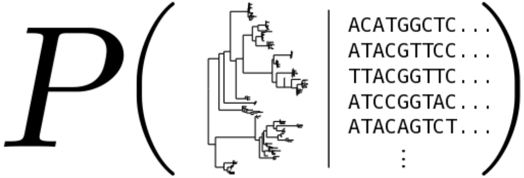

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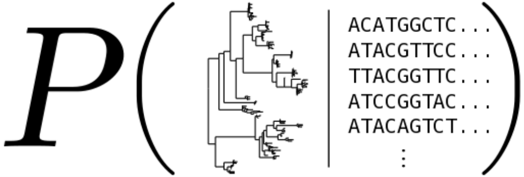

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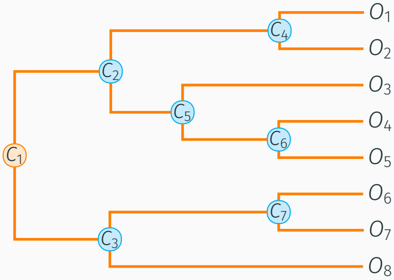
Our Contribution: Subsplit Bayesian Networks. A general probability estimation framework for phylogenetic trees based on MCMC samples that

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

Key: harness the similarity of trees properly.

Problem Setup



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

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

- *Clade Decomposition*

$$T_{\mathcal{C}} = \{C_2, C_3, C_4, C_5, C_6, C_7\}$$

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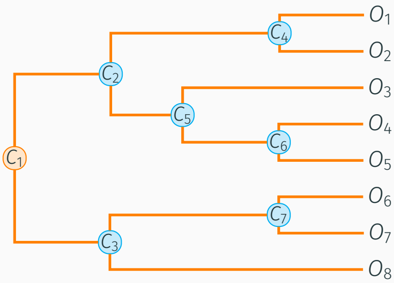

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A *subsplit* of a clade X is an ordered pair of disjoint subclades (Y, Z) such that $Y \cup Z = X, \ Y \succ Z$. Examples: $C_1 \to (C_2, C_3), \ C_2 \to (C_4, C_5)$.

Subsplit Decomposition

$$T_{\mathcal{S}} = \{(C_2, C_3), (C_4, C_5), (\{O_3\}, C_6), (C_7, \{O_8\})\}$$

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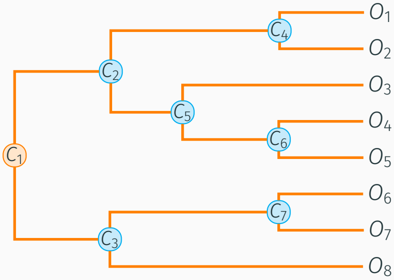

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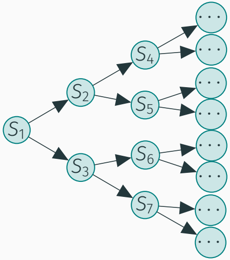
$$p(T) = p(C_2, C_3)p(C_4, C_5|C_2, C_3)p(C_6|C_4, C_5)p(C_7|C_2, C_3)$$

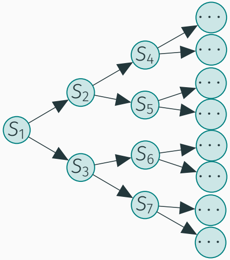
Subsplit Bayesian Networks

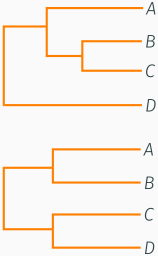


A **Subsplit Bayesian Network** on a leaf set $\mathcal{X}$ of size N is a Bayesian network

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

Subsplit Bayesian Networks





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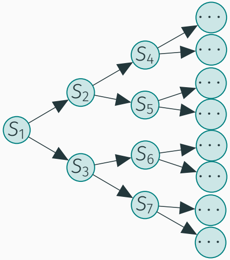

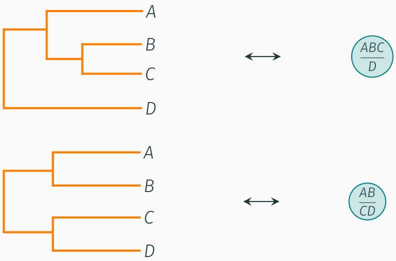

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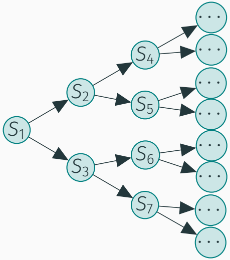

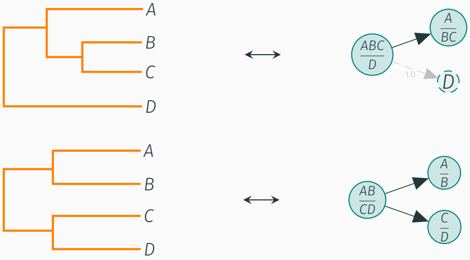

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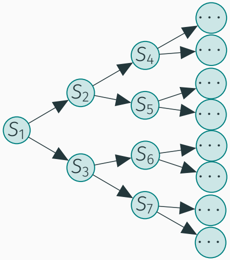

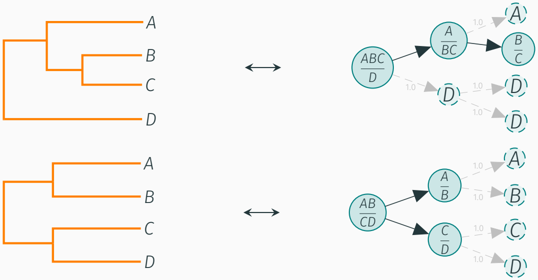

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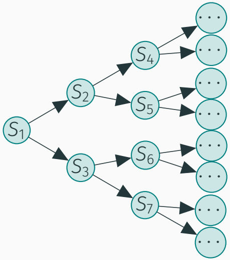

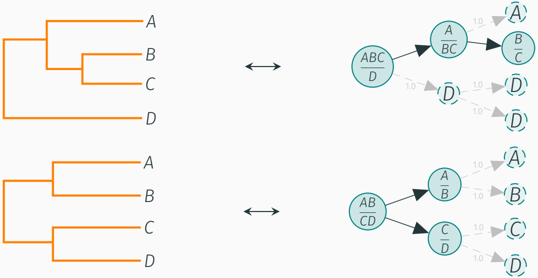

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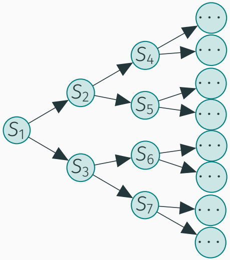
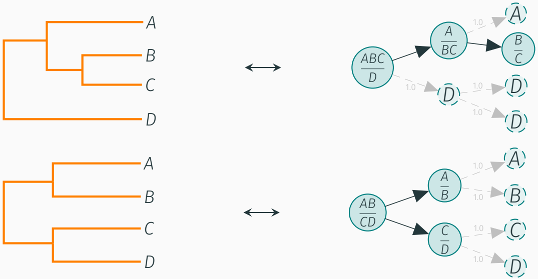
SBN probability for rooted trees

$$p_{\mathrm{sbn}}(T) = p(S_1)\prod_{i>1} p(S_i|S_{\pi_i})$$

Subsplit Bayesian Networks





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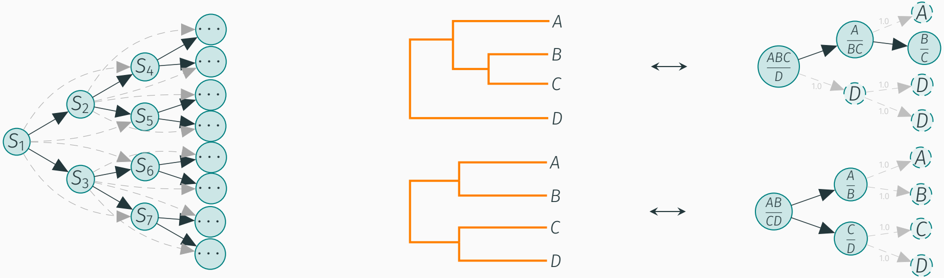

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SBN probability for rooted trees

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SBNs provide valid probability distributions and are flexible.

Learning SBNs

Rooted Trees

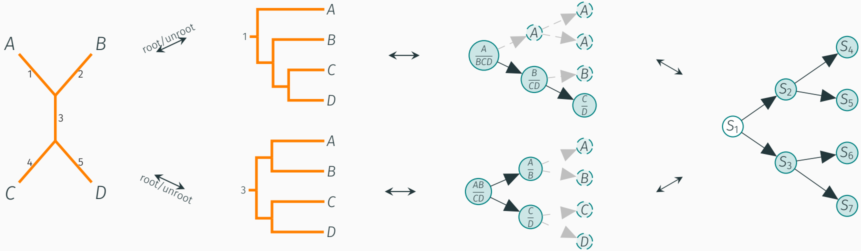
- maximum likelihood

Learning SBNs

Rooted Trees

- maximum likelihood

Unrooted Trees



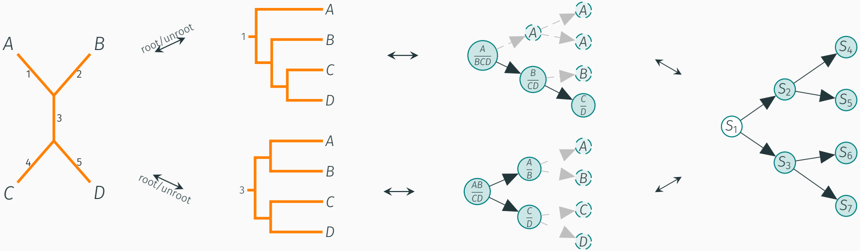
Learning SBNs

Rooted Trees

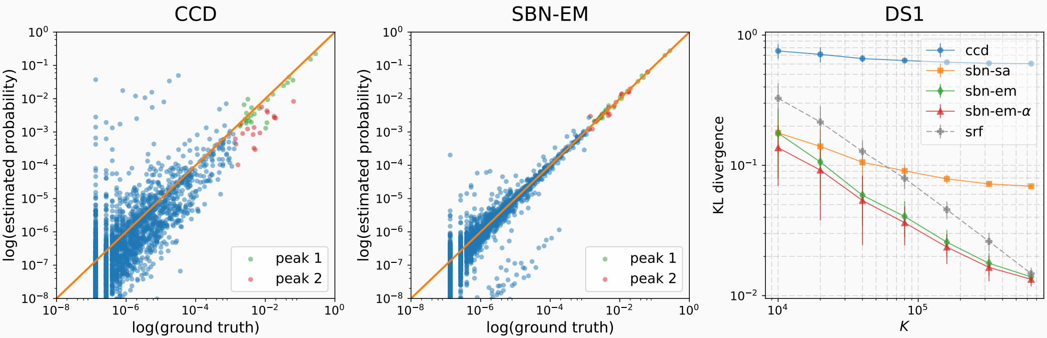
- maximum likelihood

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**

Summary

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)