Bayesian Inference of Phylogenetic Trees

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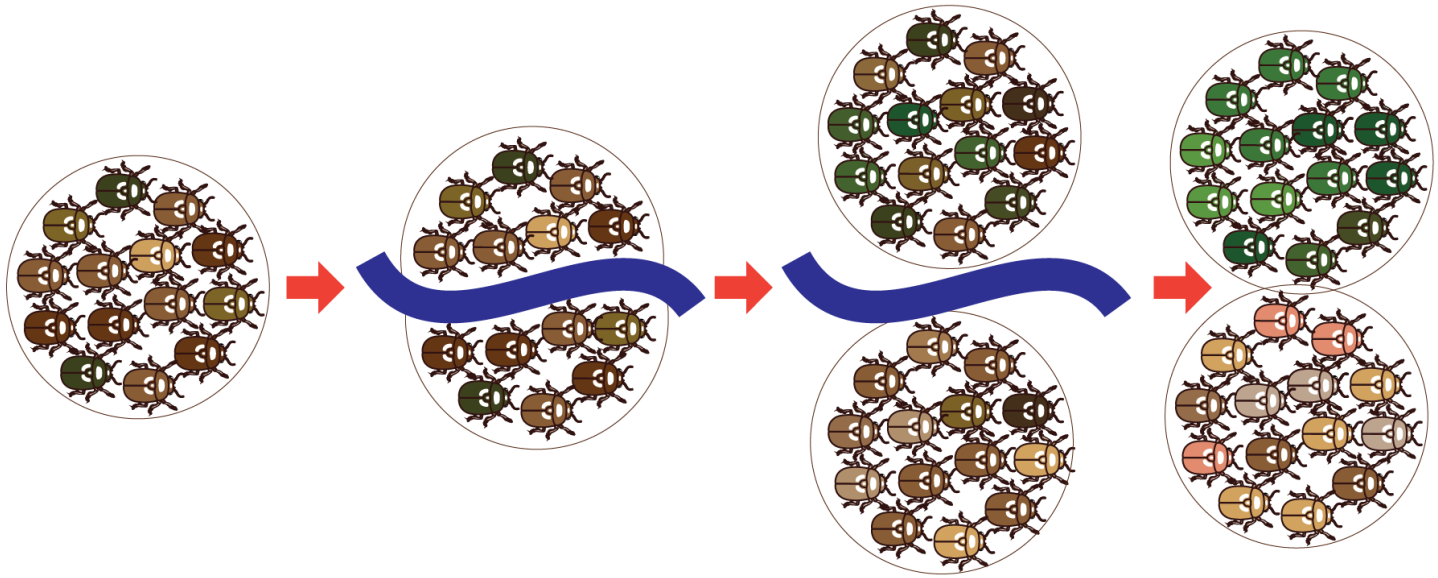
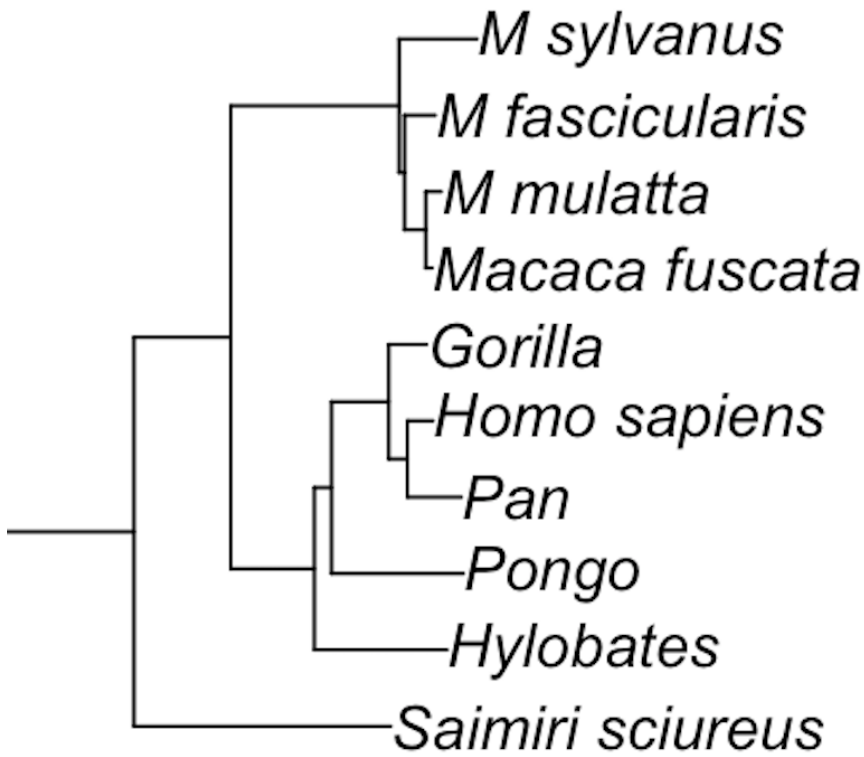
Speciation

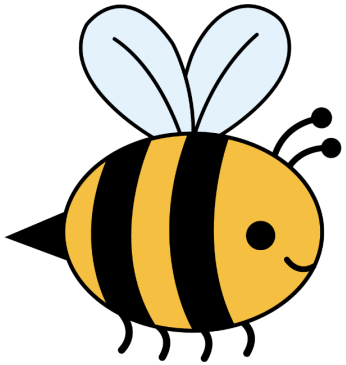


Phylogenetic Trees



Example Species

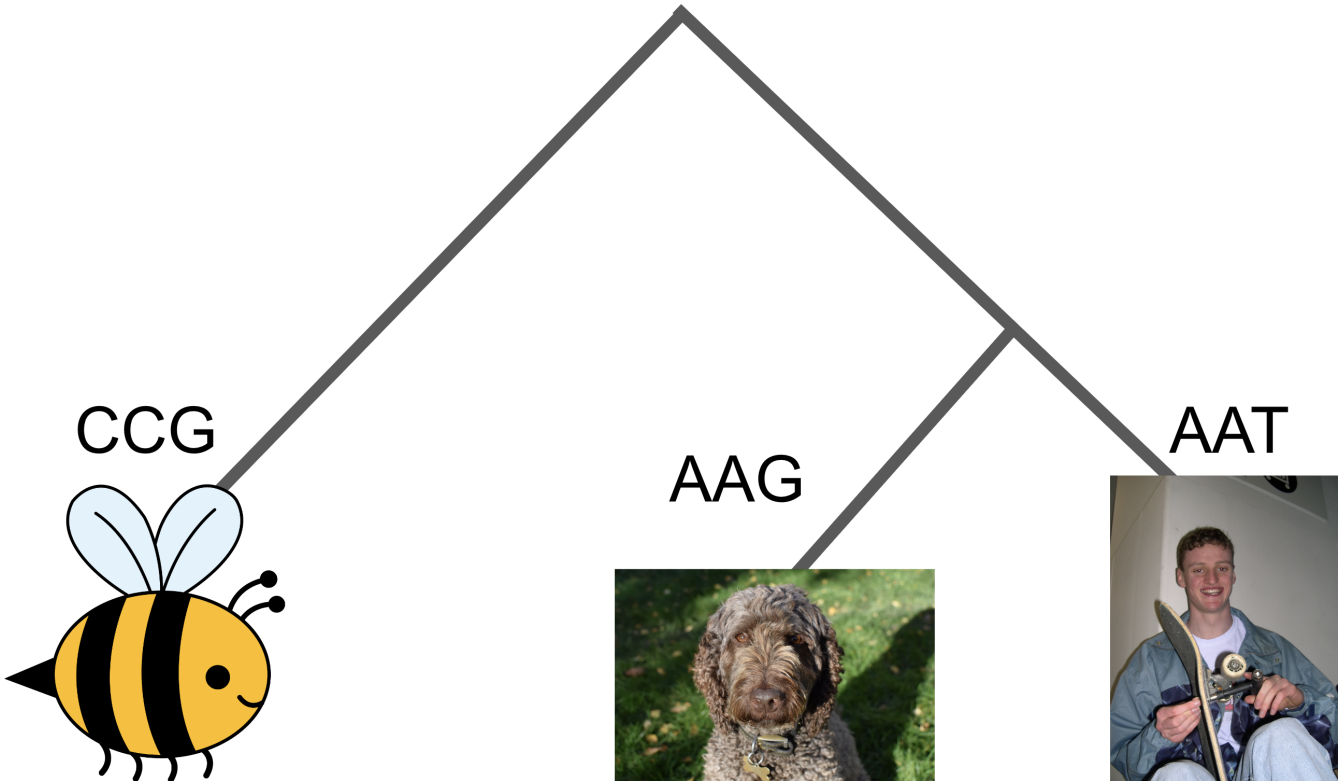
AAG



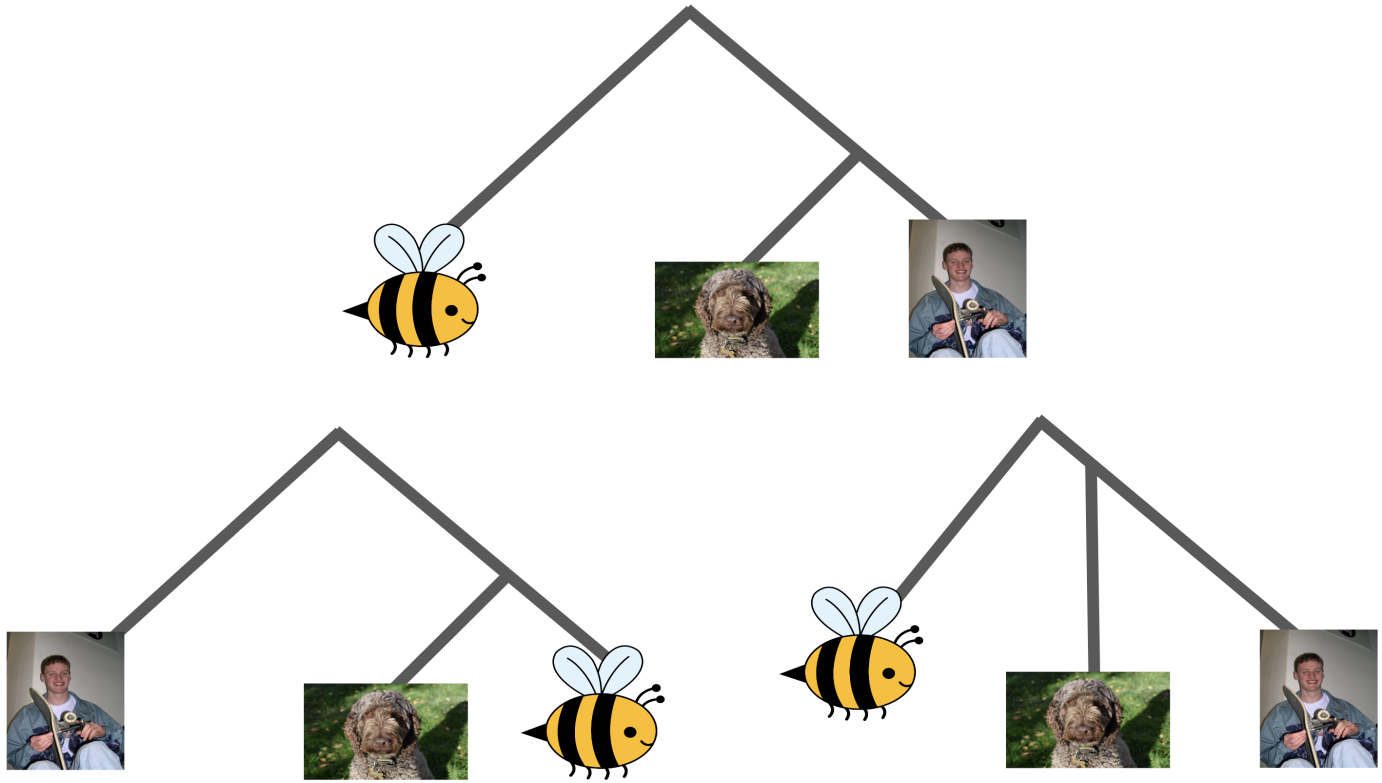
CCG

AAT

Example Phylogenetic Tree

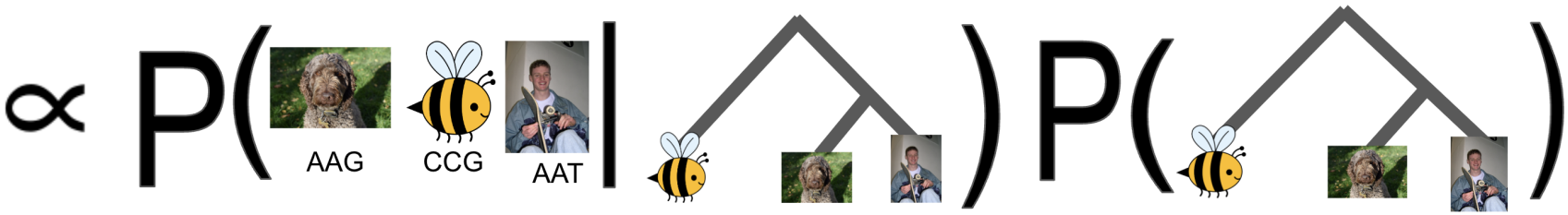


Example Phylogenetic Trees

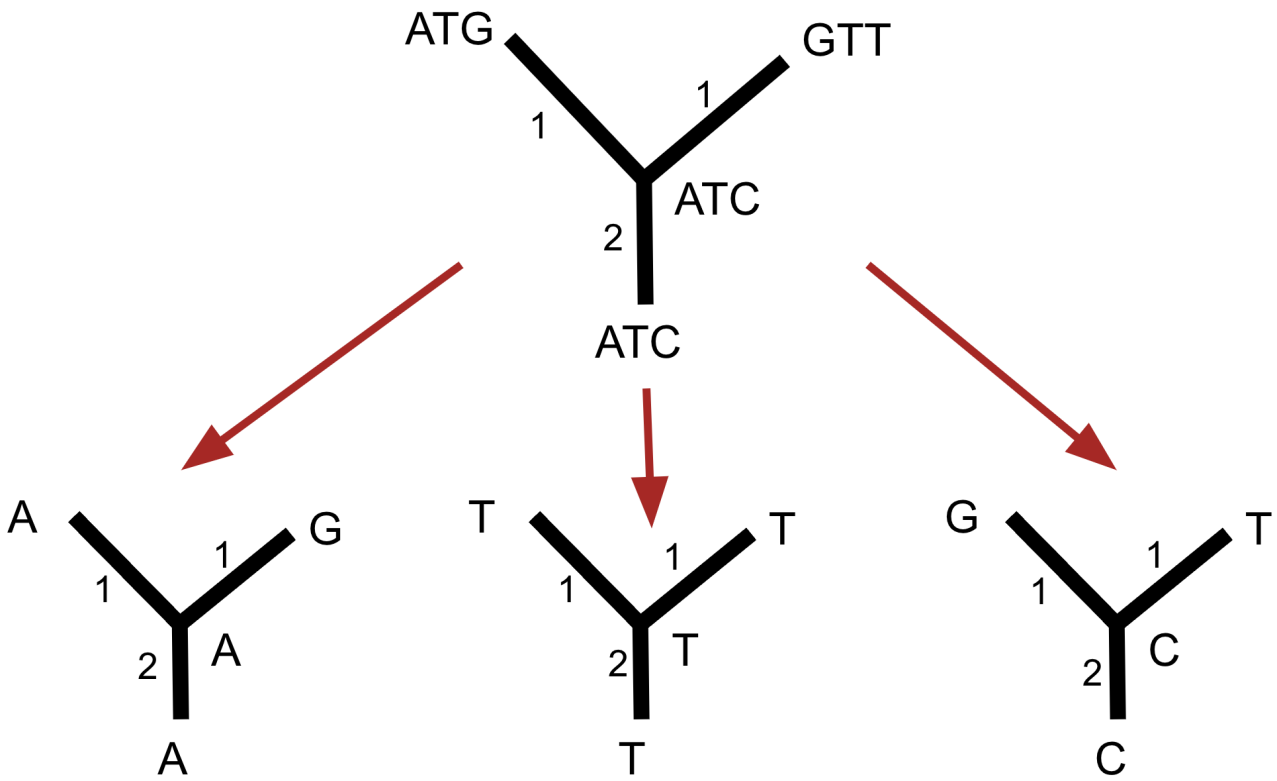


Target distribution

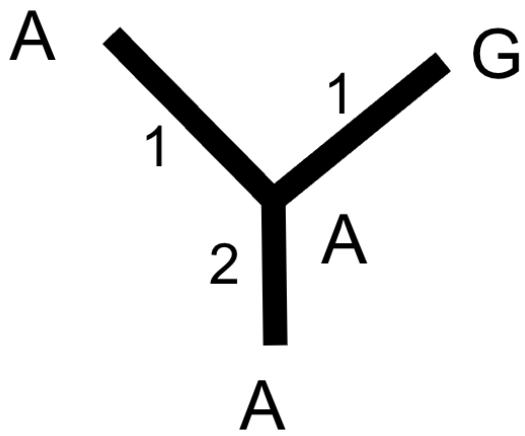
Target distribution



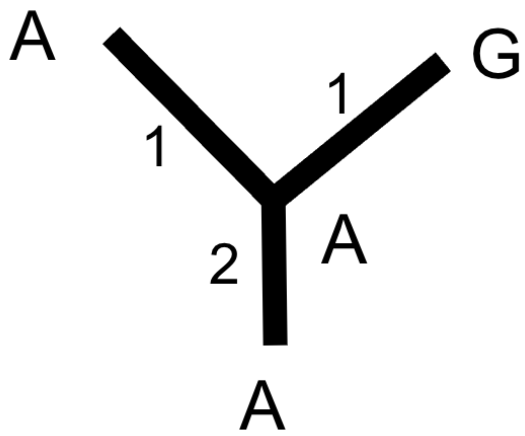
Independence Assumptions



Independence Assumptions



Independence Assumptions



$$\mathbf{P}_{AA}(1) \times \mathbf{P}_{AA}(2) \times \mathbf{P}_{AG}(1)$$

Transition Probabilities

$$P(t) = \begin{pmatrix} p_{\mathrm{AA}}(t) & p_{\mathrm{AG}}(t) & p_{\mathrm{AC}}(t) & p_{\mathrm{AT}}(t) \\ p_{\mathrm{GA}}(t) & p_{\mathrm{GG}}(t) & p_{\mathrm{GC}}(t) & p_{\mathrm{GT}}(t) \\ p_{\mathrm{CA}}(t) & p_{\mathrm{CG}}(t) & p_{\mathrm{CC}}(t) & p_{\mathrm{CT}}(t) \\ p_{\mathrm{TA}}(t) & p_{\mathrm{TG}}(t) & p_{\mathrm{TC}}(t) & p_{\mathrm{TT}}(t) \end{pmatrix}$$

Jukes and Cantor 1969

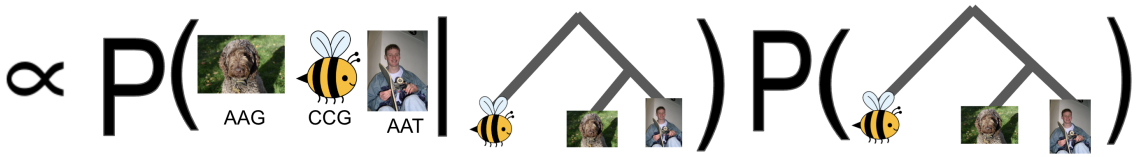
- Symmetrical rates
- Underlying base frequencies equal
- $P_{ii}(t) = \frac{1}{4} + \frac{3}{4}e^{-t}$
- $P_{ij}(t) = \frac{1}{4} - \frac{1}{4}e^{-t}, \quad i \neq j$

GTR Model, Tavaré 1986

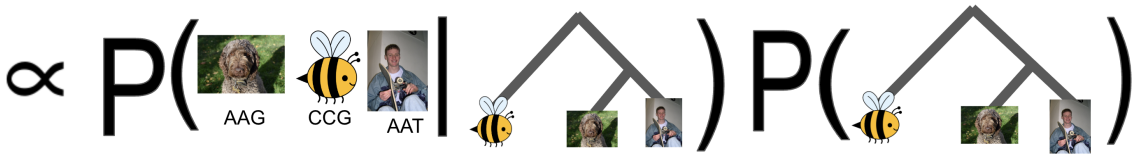
- Time-reversible
- Variable rate parameters $\alpha, \beta, \gamma, \delta, \epsilon, \eta$
- Underlying base frequencies π_i variable

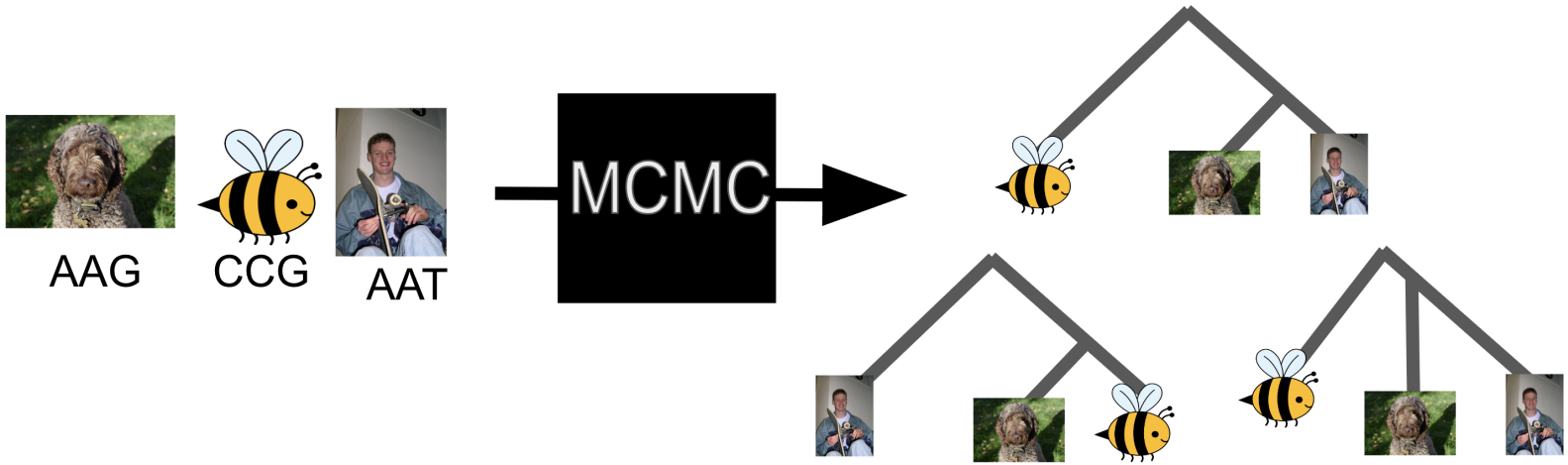
$$Q = \begin{pmatrix} * & \alpha\pi_G & \beta\pi_C & \gamma\pi_T \\ \alpha\pi_A & * & \delta\pi_C & \epsilon\pi_T \\ \beta\pi_A & \delta\pi_G & * & \eta\pi_T \\ \gamma\pi_A & \epsilon\pi_G & \eta\pi_C & * \end{pmatrix}$$

Markov chain Monte Carlo

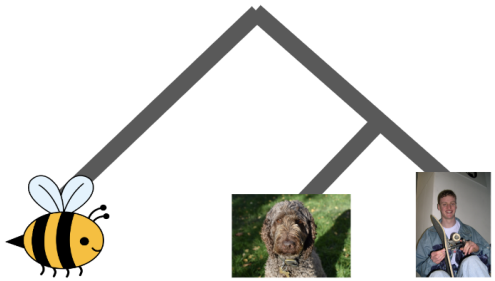
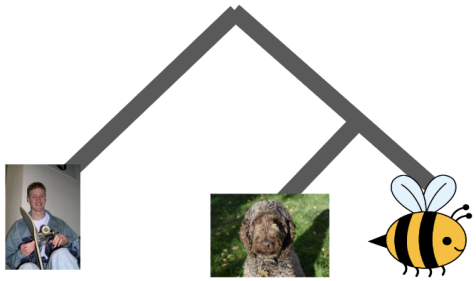


Markov chain Monte Carlo





Summary Statistics

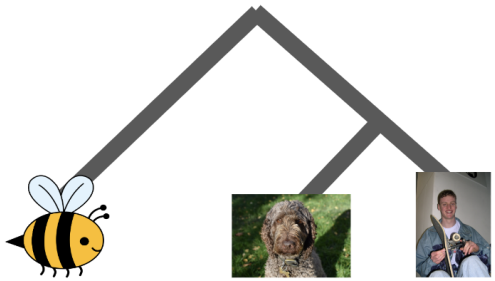
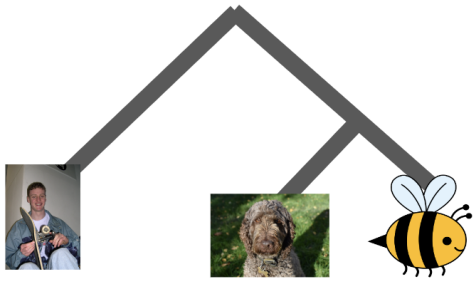
Topology	Proportion
	66.7%
	33.3%

Method

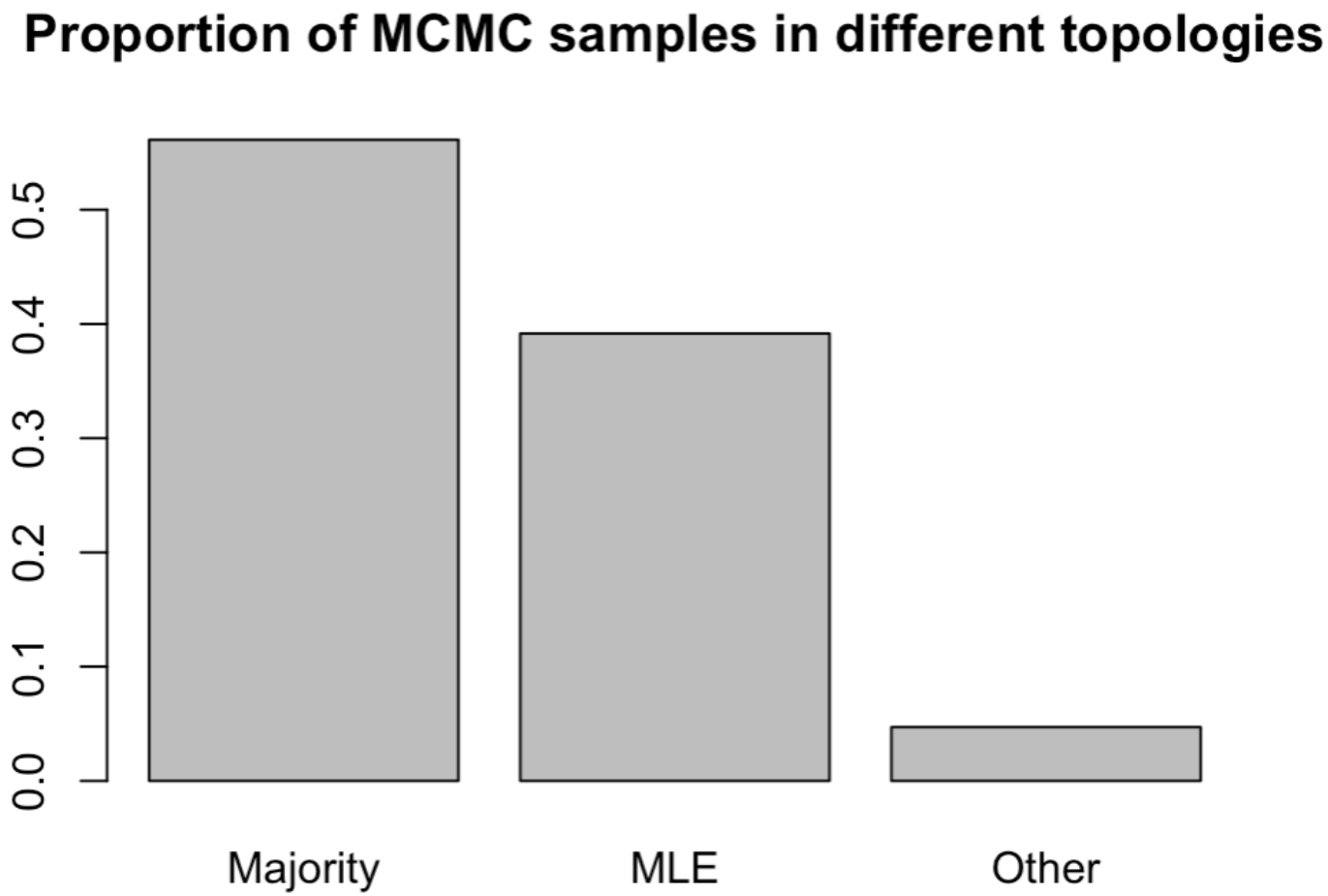
We analysed over 600 different genes. For each gene, we:

- Computed the tree which maximises the likelihood (the MLE) using IQ-TREE2 [1].
- Ran Markov chain Monte Carlo to sample thousands of trees from the posterior distribution using MrBayes 3 [2]. We then computed summary statistics of our samples.
- Explored relationship between MLE structure and our MCMC summary statistics.

Summary Statistics

Topology	Proportion
	66.7%
	33.3%

Gene 262 Topology Proportions



MLE not in Majority Topology

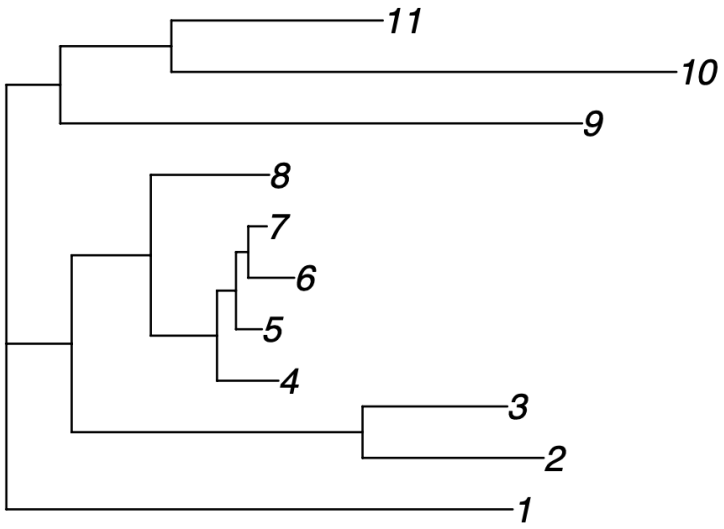


Figure: MLE Tree

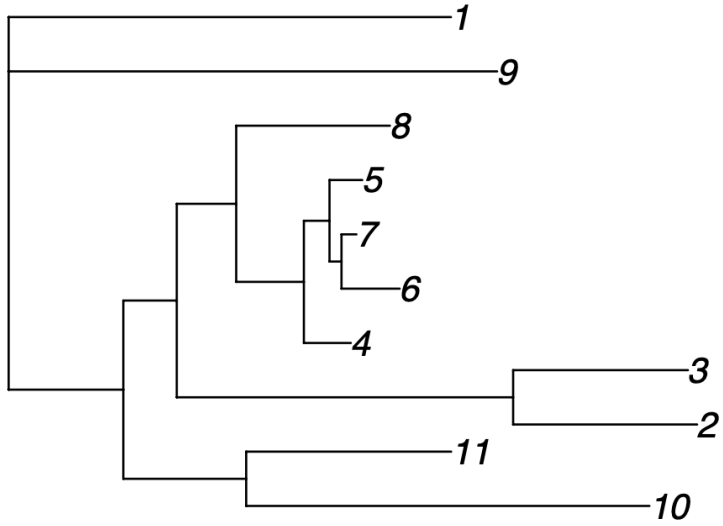
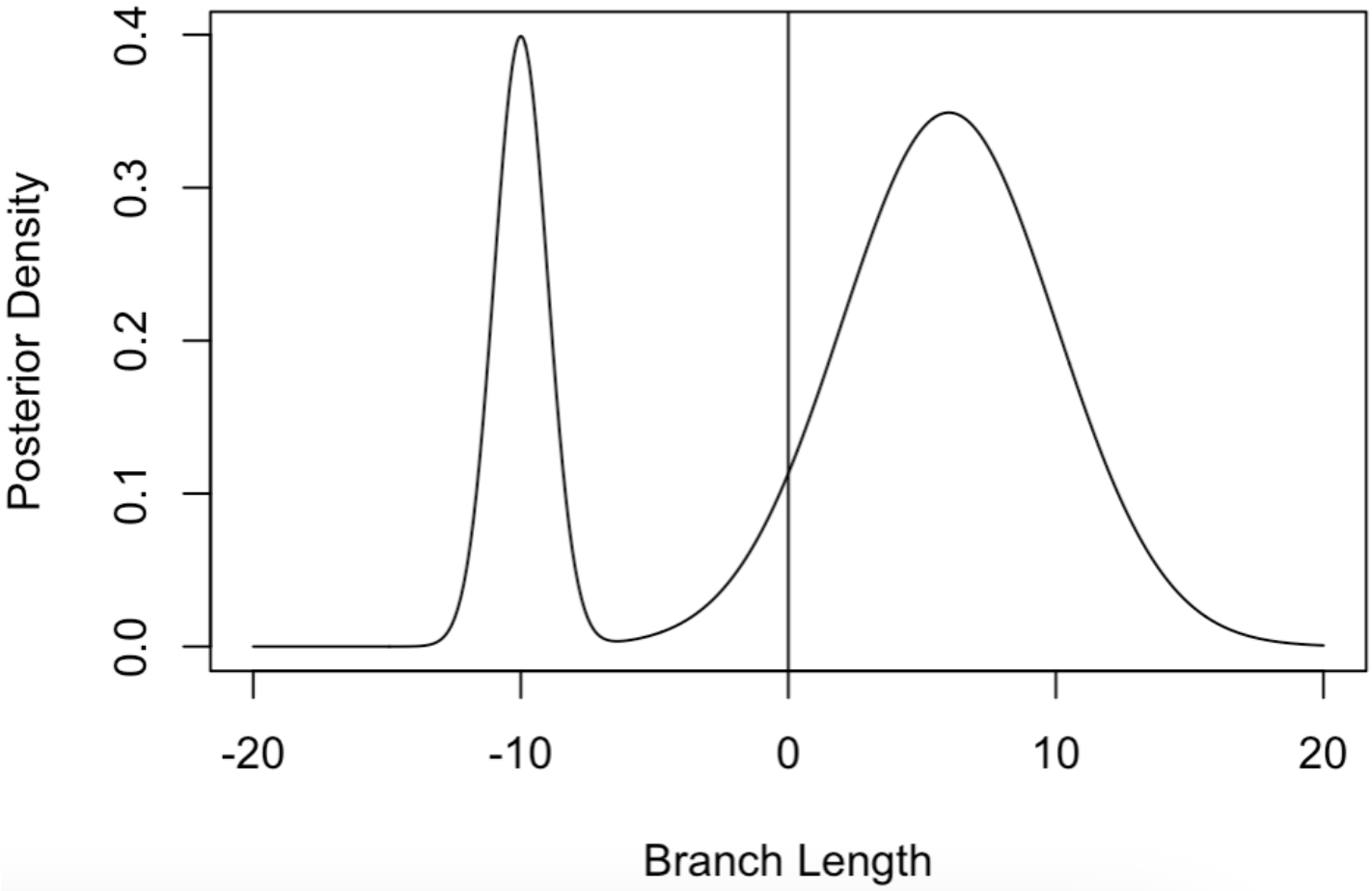
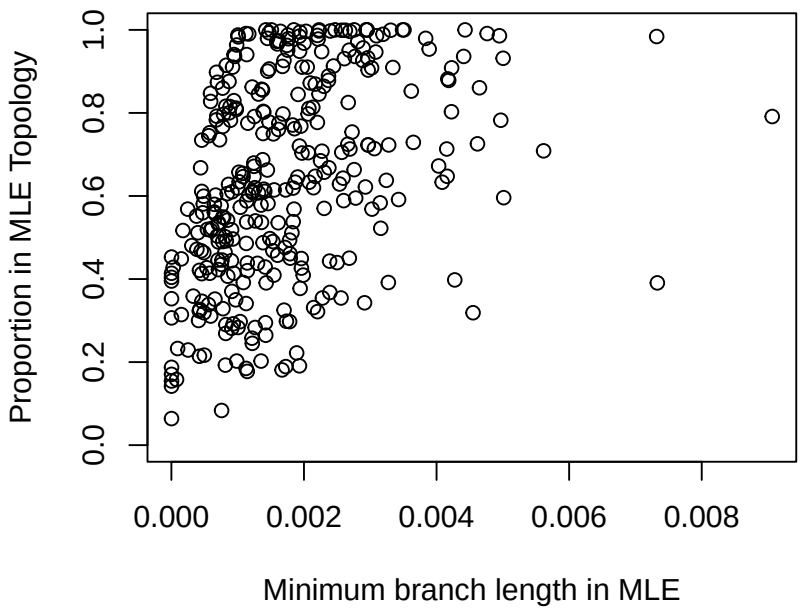


Figure: Tree in MCMC majority topology

Future Work



Correlation between MLE and samples



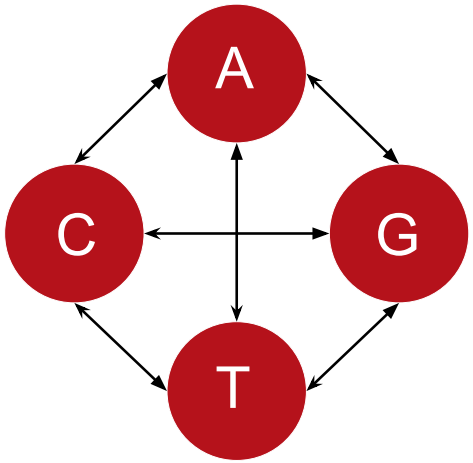
References

[1] Bui Quang Minh, Heiko A Schmidt, Olga Chernomor, Dominik Schrempf, Michael D Woodhams, Arndt von Haeseler, and Robert Lanfear. IQ-TREE 2: New models and efficient methods for phylogenetic inference in the genomic era. 2020.

[2] Fredrik Ronquist and John P. Huelsenbeck. MrBayes 3: Bayesian phylogenetic inference under mixed models. 2003.

Transition Rates

$$Q = \begin{pmatrix} -\mu_A & \mu_{AG} & \mu_{AC} & \mu_{AT} \\ \mu_{GA} & -\mu_G & \mu_{GC} & \mu_{GT} \\ \mu_{CA} & \mu_{CG} & -\mu_C & \mu_{CT} \\ \mu_{TA} & \mu_{TG} & \mu_{TC} & -\mu_T \end{pmatrix}$$



Continuous Time Markov Chains

$$P'(t) = P(t)Q$$

$$P(0) = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$$

Continuous Time Markov Chains

$$P'(t) = P(t)Q$$

$$P(0) = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$$

$$P(t) = \exp(Qt) = \sum_{n=0}^{\infty} Q^n \frac{t^n}{n!}$$