

Phylogenetics

Brief introduction to Bayesian inference and MCMC

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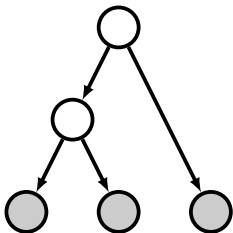
September 5, 2022

Analytical Paleobiology Workshop, Erlangen 2022

Part 4 objectives

Unbelievably brief introduction to:

- Bayesian inference
- MCMC



Bayes' theorem

$$P(\text{parameters} \mid \text{data}, \text{model}) =$$

$$\frac{P(\text{data} \mid \text{parameters}, \text{model}) P(\text{parameters} \mid \text{model})}{P(\text{data} \mid \text{model})}$$

Bayes' theorem

$$P(\text{parameters} \mid \text{data}, \text{model}) =$$

posterior

likelihood

priors

$$\frac{P(\text{data} \mid \text{parameters}, \text{model}) P(\text{parameters} \mid \text{model})}{P(\text{data} \mid \text{model})}$$

marginal probability of the data

Bayes' theorem

$P(\text{data} \mid \text{parameters, model}) \leftarrow$ the model used to calculate the **likelihood**.

$P(\text{parameters} \mid \text{model}) \leftarrow$ this represents our **prior knowledge** of the model parameters.

$P(\text{parameters} \mid \text{data, model}) \leftarrow$ the **posterior** reflects our combined knowledge based on the likelihood and the priors.

$P(\text{data} \mid \text{model}) \leftarrow$ the probability of the data integrated over all possible parameter values. Can be thought of as a normalising constant (i.e., ensuring the posterior sums to one). Worry less about this!

The output of a Bayesian phylogenetic analysis is a distribution of trees

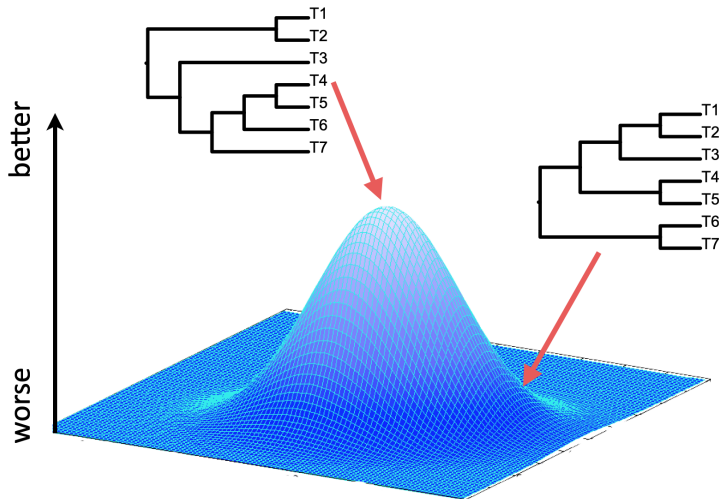


Image source: Tracy Heath

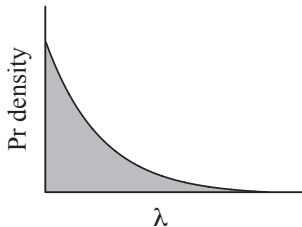
Introduction to MCMC

Probabilities versus probability densities

In phylogenetics, probabilities are not normally discrete (i.e. represented by a single value) and we're often dealing with a lot of uncertainty (esp. in the fossil record). Instead we typically work with **probability densities**.

See Paul Lewis's [archery prior](#) demo.

Probabilities versus probability densities



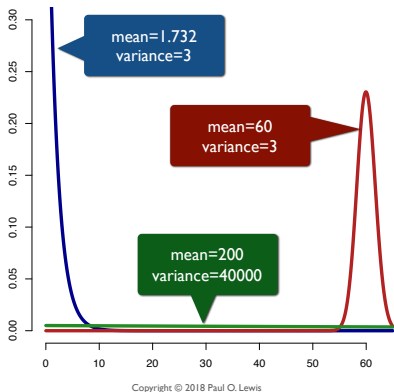
λ is drawn from an exponential distribution with mean δ

The x-axis represents the value of our parameter λ .

The y-axis does have a value but it is not so easily interpretable.

The distribution height reflects the relative probability of a given range of parameter values.

Probabilities versus probability densities



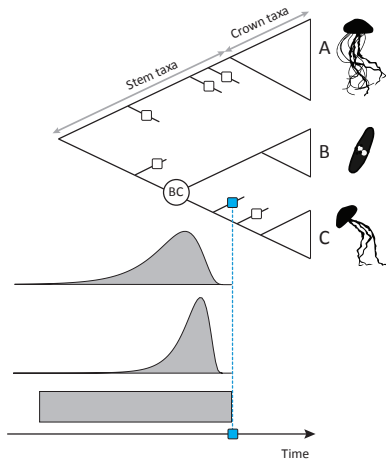
The x-axis represents the value of our parameter λ .

The y-axis does have a value but it is not so easily interpretable.

The distribution height reflects the relative probability of a given range of parameter values.

Variations of a gamma probability distribution.

Probabilities versus probability densities



Example calibration densities.

The x-axis represents the value of our parameter λ .

The y-axis does have a value but it is not so easily interpretable.

The distribution height reflects the relative probability of a given range of parameter values.

Why do we need Markov chain Monte Carlo?

Probability densities already introduce some complexity
→ Remember the posterior is not usually a point estimate (i.e. a single value) but a range of values.

The marginal probability of the data is also very tricky to calculate.

$P(\text{data} \mid \text{model})$

Calculating this requires taking into account all possible alternative parameter combinations (e.g. all possible trees).

This makes it challenging to calculate the posterior analytically (i.e. exactly).

What is Markov chain Monte Carlo (MCMC)?

A group of algorithms for approximating the posterior distribution (also known as samplers).

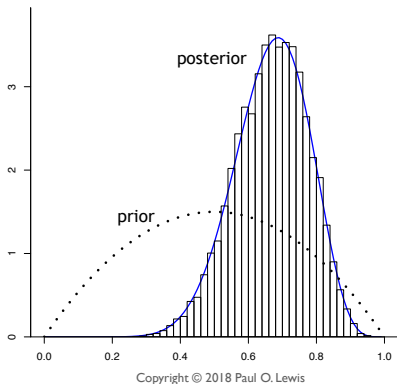
Markov chain means the progress of the algorithm doesn't depend on its past.

Monte Carlo (named for the casino in Monaco) methods estimate a distribution via random sampling.

We use this algorithm to visit different regions the parameter space. The number of times a given region is visited will be in proportion to its posterior probability.

Click [here](#) for a little bit of history.

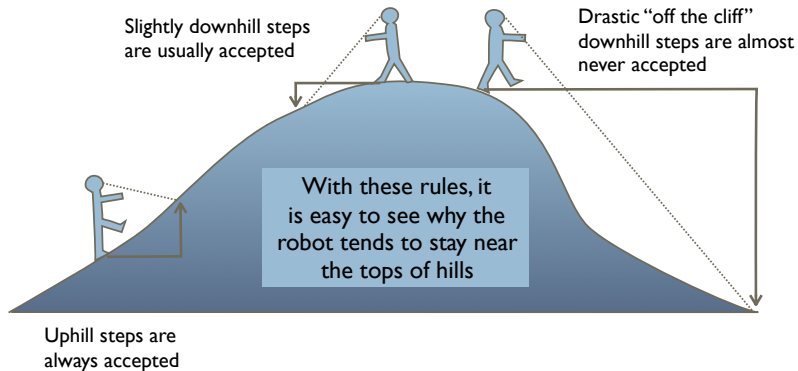
What is Markov chain Monte Carlo (MCMC)?



- The aim is to produce a *histogram* that provides a good approximation of the posterior.

Image source: Paul Lewis's [phyloseminar](#) lecture.

MCMC robot's rules



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Image source: Paul Lewis's [phyloseminar](#) lecture.

Actual rules (Metropolis algorithm)

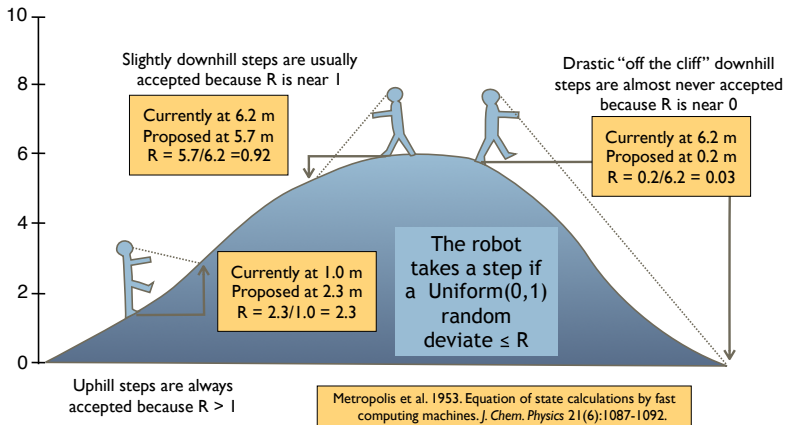


Image source: Paul Lewis's [phyloseminar](#) lecture.

The marginal likelihood is cancelled

When calculating the ratio (R) of posterior densities, the marginal probability of the data cancels.

$$\frac{p(\theta^* | D)}{p(\theta | D)} = \frac{\frac{p(D | \theta^*) p(\theta^*)}{p(D)}}{\frac{p(D | \theta) p(\theta)}{p(D)}} = \frac{p(D | \theta^*) p(\theta^*)}{p(D | \theta) p(\theta)}$$

Posterior
odds

Apply Bayes' rule to
both top and bottom

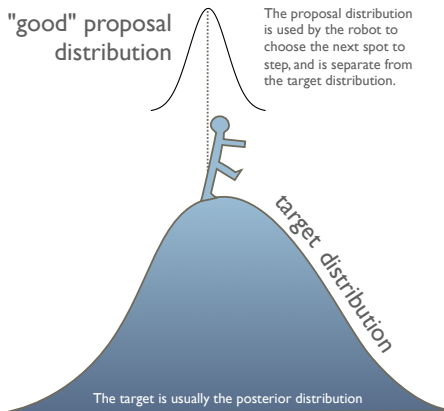
Likelihood
ratio

Prior
odds

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Image source: Paul Lewis's [phyloseminar](#) lecture.

MCMC robot

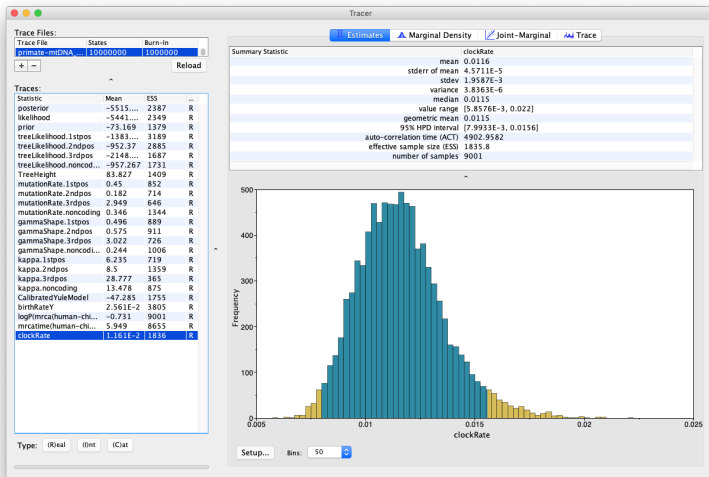


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See Paul Lewis's **MCMC robot** demo.

Summarising the posterior

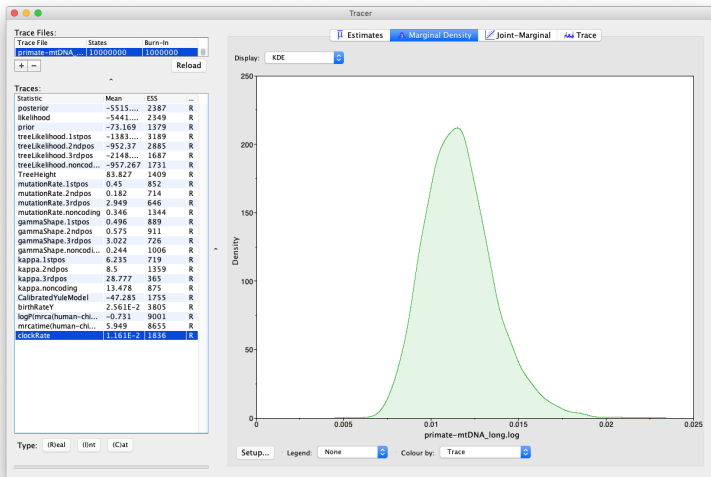
Tracer is an amazing program for exploring MCMC output.



Example MCMC output. Source: taming-the-beast.org.

Summarising the posterior

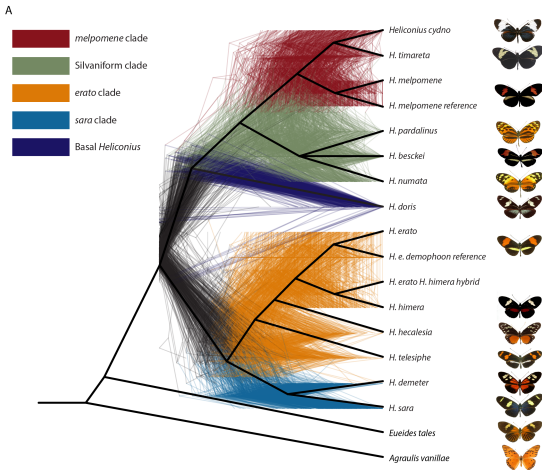
Tracer is an amazing program for exploring MCMC output.



Example MCMC output. Source: taming-the-beast.org.

Summarising the posterior

Summarising trees is much more challenging. Presenting a single summary tree can sometimes be misleading.



Edelman et al. (2019) *Science*.

Summarising the posterior

The **95% highest posterior density (HPD)**: the shortest interval that contains 95% of the posterior probability. The Bayesian equivalent of the 95% confidence interval.

Marginal posterior density: the probability of a parameter regardless of the value of the others, represented by the histogram.

Maximum clade credibility (MCC) tree: the tree in the posterior sample that has the highest posterior probability (i.e. clade support) across all nodes.

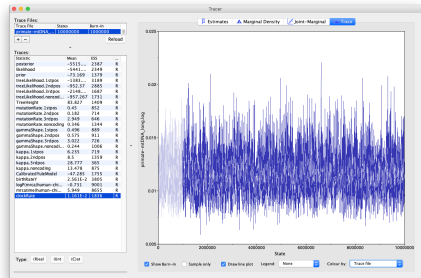
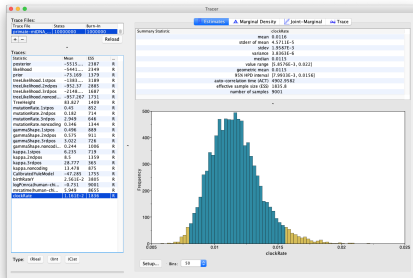
For more on issues associated with summary tree methods see O'Reilly & Donoghue (2018) *Sys Bio*.

Convergence

How do you know if you've run the chain long enough? → You don't! But there are some clues.

Convergence

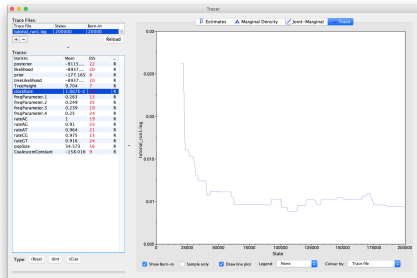
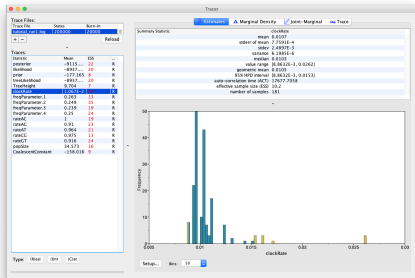
Good mixing.



Example MCMC output. Source: taming-the-beast.org.

Convergence

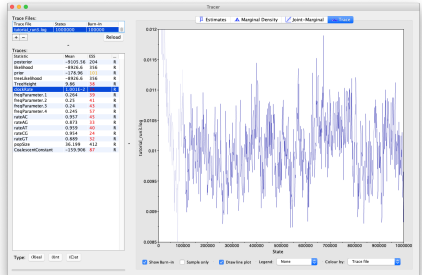
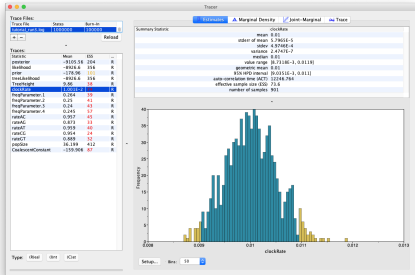
Poor mixing.



Example MCMC output. Source: taming-the-beast.org.

Convergence

Better mixing.



Revisit Paul Lewis's **MCMC** robot.

Bayesian inference provides a flexible and intuitive way to incorporate and represent uncertainty.

MCMC is an elegant algorithm trick to infer the posterior distribution.

It samples values directly from posterior in proportion to how probable they are, resulting in a histogram, which provides a good approximation of the posterior.

Suggested reading / listening

Short video: (3Blue3Brown) Bayes theorem

Short video: (PhyloMeth) Contrasting likelihood and Bayesian approaches.

Short reading: Huelsenbeck et al. (2001) Bayesian Inference of Phylogeny and Its Impact on Evolutionary Biology. *Science*.

Exercise