MCMC DIAGNOSIS FOR BASESIAN PHYLOGENETIC INFERENCE



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OUTLINE

Overview

Convergence and MCMC diagnosis

- tools and metrics for evaluating MCMC samples
- Tracer demo
- AWTY demo

break

Tutorial - Conor Meehan and Instructors

Phylogenetic reconstruction in MrBayes

- MCMC diagnostics in Tracer
- Partitioned phylogenetic inference in MrBayes



Andrey Markov

The Markov Chain



"An example of statistical investigation of the text Eugene Onegin concerning the connection of samples in chains."

23* January 1913

*Julian calendar



- Infinite MCMC samples will *converge* on the stationary/target distribution
- With a finite number of iterations, we can *never* be certain that our samples represent the underlying stationary distribution

Stationarity

The Markov chain reaches stationarity when the mean, variance, and autocorrelation structure do not change over time





MIXING

A chain has good "mixing time" if it rapidly samples the stationary distribution from an arbitrary starting state

A chain is said to mix poorly if it does not reach stationarity and if the samples are highly correlated



Burn-in

Burn-in refers to the common practice of discarding a percentage of initial states that were sampled before the chain reached stationarity.

This practice is not necessary for "adequately-long" chain lengths.



ASDSF

Average standard deviation of split frequencies

```
19929900 - (-96831.448) [-96812.848] (-96855.650) (-96850.506) * (-96814.997) ... - 0:18:41
19930000 - (-96826.655) [-96812.054] (-96853.963) (-96832.659) * [-96822.263] ... - 0:18:39
Average standard deviation of split frequencies: 0.002567
19930100 - (-96833.675) [-96806.706] (-96850.378) (-96842.572) * (-96824.515) ... - 0:18:38
19930200 - (-96827.767) [-96809.219] (-96838.541) (-96849.400) * (-96824.812) ... - 0:18:36
```

- Comparing the clade frequencies across multiple, independent runs
- ASDSF should approach 0.0 as the runs sample the same distribution
- MrBayes computes this statistic for multiple runs

ESS

The Effective Sample Sizes of the parameter values

This statistic gives you an idea of how independent your samples are and measures if you ran the chain sufficiently long

tmrca(N15)	0.363	18.109
tmrca(N16)	0.266	50.398
tmrca(N17)	0.136	55.039
tmrca(N18)	0.272	27.761
birthDeath.m	1.86	4212.589
birthDeath.rel	0.348	3205.636
ac	0.354	325.551
ag	1.037	199.392
at	0.37	374.979
cg	0.336	460.006
gt	0.314	367.218
frequencies1	0.248	187.687
frequencies2	0.254	243.874
frequencies3	0.247	224.262
frequencies4	0.251	198.998
alpha	0.918	803.829



http://tree.bio.ed.ac.uk/software/tracer/



AWTY

http://ceb.csit.fsu.edu/awty

