MCMC Diagnostics

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Learning goals

Be able to assess whether Markov chains have converged in distribution to the target distribution.

- trace/history plots
- BGR diagnostic

Regarding correlation in samples simulated by MCMC,

- be able to quantify correlation
- know how to deal with correlation by thinning
- know how long we should run our chains to obtain reasonably accurate estimates of the posterior

MCMC Diagnostics

As we have seen, there are two main concerns with the use of MCMC methods for posterior inference: $\theta^{(1)}, \theta^{(2)}, \dots \theta^{(n)}$ as $n \to \infty$ $\theta \sim p(\theta|x)$.

- Has our chain converged in distribution to the posterior (target distribution)?
- Correlation in samples simulated by MCMC can cause inefficiencies in simulations. sample is not independent.

Let's learn about methods - both informal (graphical/visual checks) and formal - for assessing each of the above concerns.

Has our chain converged in distribution to the posterior (target distribution)?

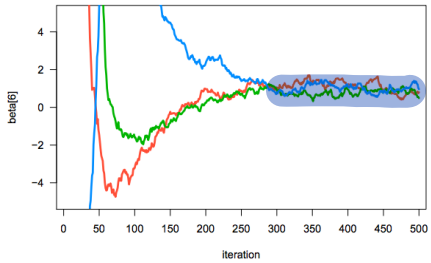
Most approaches for detecting convergence, both formal and informal, rest on the idea of

- running multiple Markov chains with overdispersed initial values and
- observing whether they come together and start to behave similarly (if they do, we can pool samples from each chain).

'Overdispersed' means 'more variable than the target distribution (i.e., posterior distribution)'.

Trace/history plot

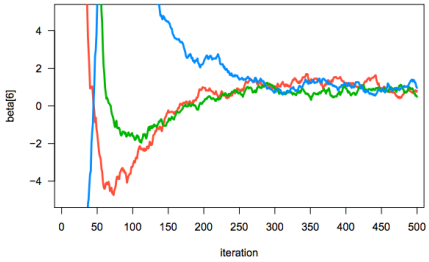
$\theta^{(i)}$



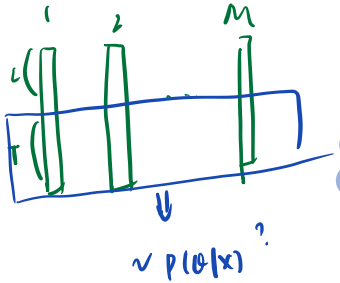
Burn-in

To diminish the effect of initial values, we generally discard some iterations at the beginning of each Markov chain.

The practice of discarding early iterations in each Markov chain is referred to as 'burn-in'; depending on the context, different burn-in fractions can be appropriate.



Brooks-Gelman-Rubin (BGR) diagnostic



Although looking at trace/history plots is certainly useful, it is also desirable to obtain an objective, quantifiable measure of convergence.

Numerous methods exist, although we will focus on the measure originally proposed in Gelman and Rubin (1992).

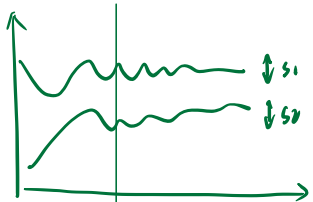
Suppose that we have run M independent chains, each of length $L + T$. We wish to decide if the last T observations look stationary (i.e., converged in distribution to target distribution)?
The diagnostic works best if the M initial values are widely separated.

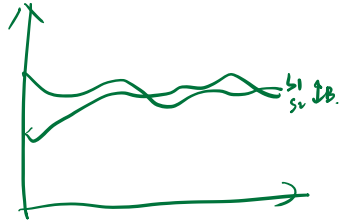
overdispersed initial value

Brooks-Gelman-Rubin (BGR) diagnostic

The basic idea of the estimator is as follows (the actual estimator makes a number of modifications to account for degrees of freedom):

- Let B denote the standard deviation of the pooled sample of all MT iterations (the between-chain variability).
- Let W denote the average of the M within-chain standard deviations from each chain (the within-chain variability).
- Put $\hat{R} = B/W$ then if $\hat{R} < 1.05$ then we accept the last T observations of each chain as stationary.
- Collect the MT samples from all the chains together and treat them as a sample from the target distribution.





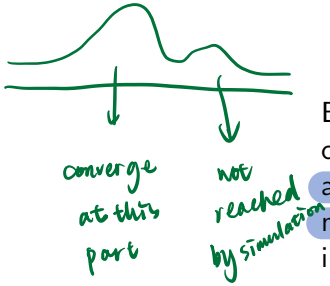
Note that if $\hat{R} >> 1$, this is clear evidence that the chains have not converged, and as $T \to \infty$, $\hat{R} \to 1$.

Has our chain converged in distribution to the posterior (target distribution)?

- trace/history plots.
- $\hat{R} < 1.05$

Our chain has not converged!?

- Increase the length of chain.
- Add efficient proposal methods.



Even if Markov chain appears to converge and has passed the test of convergence, it still may actually be far from convergence if important areas of the target distribution were not captured by initial values and are not easily reachable by the simulation algorithm. Choose overdispersed initial values!!

Correlation in samples simulated by MCMC can cause inefficiencies in simulations.

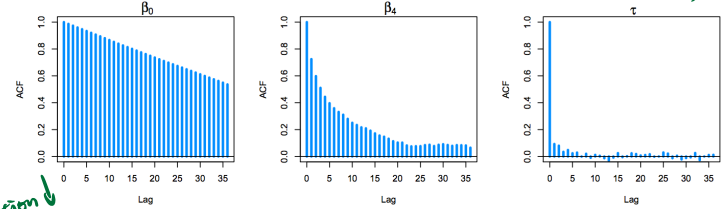
Compared to 4000 independent samples, 4000 correlated samples contain less information about the posterior.

- Quantify correlation?
- How to deal with correlation?
- How long should we run our chains to obtain reasonably accurate estimates of the posterior?

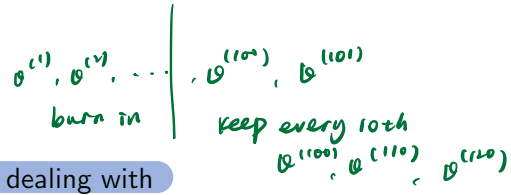
Quantify correlation

The autocorrelation between two states s and t of a Markov chain is defined, simply, as the correlation between $\theta^{(s)}$ and $\theta^{(t)}$.

If the chain is stationary, in the sense that its mean and variance are not changing with time, then the correlation between $\theta^{(t)}$ and $\theta^{(t+k)}$ does not depend on t; this is known as the lag-k autocorrelation.



How to deal with correlation? Thinning



A somewhat crude, yet reasonably effective, method dealing with autocorrelation is to only keep every kth simulated sample from each Markov chain and discard the rest; this is known as thinning the chain.

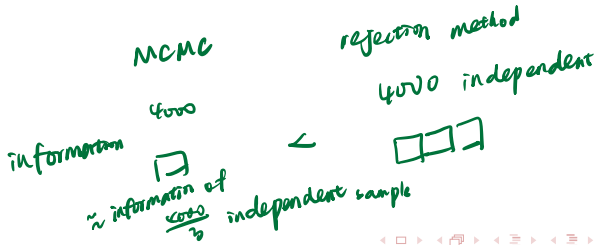
- The advantages of thinning are (a) simplicity and (b) a reduction in memory usage.
- The disadvantage is that we are clearly throwing away information.

How long should we run our chains to obtain reasonably accurate estimates of the posterior?

Effective Sample Size (ESS) for a parameter is the sample size of an independent sample giving the same amount information about the posterior as the correlated MCMC sample.

ESS can be estimated by $\frac{n}{1+2\sum_{i=1}^{\infty}\rho_i} \approx n\frac{1-\rho_1}{1+\rho_1}$, where ρ_i is the lag i autocorrelation. Read Diagnostics_additional.pdf to see the derivation.

ESS $>$ 4,000



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