MCMC Diagnosis

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Stationary distribution of MCMC I

- Stationary distribution of MCMC is the key, and the ergodicity means that

$$\sum_{i=1}^{N} \theta_i / N \xrightarrow{p} \mathbb{E}[\theta]$$

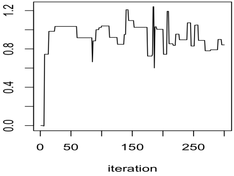
as $N \to \infty$ where $\{\theta_i\}_{i=1}^{N}$ is the MCMC samples.

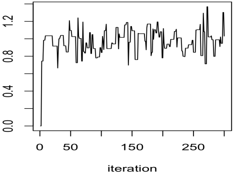
Stationary distribution of MCMC II

- In practice we can have the following issues:
  1. How long do we need to run the Markov Chain to approximate the posterior distribution?
  2. Mixing is a concept from the ergodicity, which means the moving around the full distribution. Fast mixing indicates the fast convergence to the posteriors.

Stationary distribution of MCMC III

- Examples of slow mixing and fast mixing





Brief Sketch of Diagnosis I

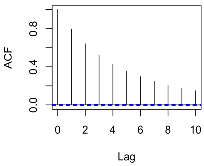
- Basic tools is the trace plot. Also the reason of ergodicity is the weak correlation between chain.

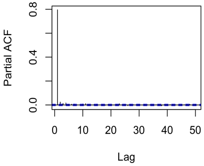
$$\frac{\sum_i \mathrm{Var}(X_i)}{\sum_{i \neq j} \mathrm{Cov}(X_i, X_j)} = O(1).$$

- This implies that the correlation within chain is the key points to show the speed of convergence. Note that the iid samples have the ratio of 0.

Brief Sketch of Diagnosis II

- Simple measure: ACF (auto correlation function) and PACF (partial auto correlation plot)
- Example (ACF and PACF)





Mathematical Aspects I

- When we have the following notations:

$$\hat{g}_{MC} = \frac{1}{N}\sum_i g(\theta^{(i)}) \text{ MC mean}$$
$$\hat{g}_{MCMC} = \frac{1}{N}\sum_i g(\theta^{(i)}) \text{ MCMC mean}$$

- Here, the distribution and the stationary distribution are same.

Mathematical Aspects II

- Then we have the following:

$$\begin{aligned}\text{Var}(\hat{g}_{MCMC}) &= \text{Var}(\hat{g}_{MC}) + \sum_{i \neq j} \mathbb{E}\Big[\left(g(\theta^{(i)}) - \mathbb{E}[g(\theta^{(i)})]\right) \\ &\quad \times \left(g(\theta^{(j)}) - \mathbb{E}[g(\theta^{(j)})]\right)\Big]\end{aligned}$$

  - The second term depends on the autocorrelation of samples within the Markov chain.

Mathematical Aspects III

- Often positive so MCMC variance is larger than MC variance.
- Often positive so MCMC variance is larger than MC variance, and high correlation is an indicator of poor mixing.
- Effective sample size: how times samples are required for the equivalent to the variance of iid mean.

$$s_{eff} = \frac{\mathrm{Var}(\hat{g}_{MCMC})}{\mathrm{Var}(\hat{g}_{MC})}$$

Mathematical Aspects IV

- When we know the ρ_k of the lag k autocorrelation, we have

$$S_{eff} = \frac{S}{1 + 2\sum_k \rho_k}$$

where S is the length of Markov chain (sample size).

Measures to be studied I

- Geweke (1992)
  1. Test for equality of the means of the first and last part of a Markov chain (by default the first 10% and the last 50%).
  2. If the samples are drawn from the stationary distribution, the Geweke's statistic has an asymptotically standard normal distribution.

Measures to be studied II

- Gelman and Rubin (1992): using $m > 1$ chains
  1. Use different starting values.
  2. The chains have ”forgotten” their initial values, and the output from all chains should be indistinguishable.

Measures to be studied III

3. Based on a comparison of within-chain and between-chain variances:

$$R = \frac{\frac{L-1}{L}W + \frac{1}{L}B}{W}$$

where $B : L \times$ variance between chains, W : average over variances of chains, and L is the length of chain.

Measures to be studied IV

- Heidelberg-Welch (1981)
    1. After discarding the first 10%, 20%, of the chain until either the null hypothesis is accepted, or 50% of the chain has been discarded.
    2. The test is for the stationary distribution.
    3. The halfwidth test calculates half the width of the $(1`\alpha)\%$ credible interval around the mean.
    4. If the ratio of the halfwidth and the mean is lower than some ϵ, then the chain passes the test. Otherwise, the chain must be run out longer.

Measures to be studied V

- Raftery-Lewis (1992): burn-in and iterations
  1. Select a posterior quantile of interest q.
  2. Select an acceptable tolerance r for this quantile
  3. Select a probability s, which is the desired probability of being within $(q-r, q+r)$.
  4. Run a "pilot" sampler to generate a Markov chain of minimum length given by rounding up $nmin = \left[\Phi^{-1}\left(\frac{s+1}{2}\frac{\sqrt{q(1-q)}}{r}\right)\right]^2$
  5. Compare the required number of burin-in and iteration with $nmim$. (Inflation factor)

Measures to be studied VI

- Example of Geweke

```
library(coda)
rs = geweke.diag(x, frac1=0.1, frac2=0.5)
2*(1-pnorm(abs(unlist(rs[[1]]))))
 var1
0.6886054
```

- First 10% and the last 50%, the p-value if greater than 0.05 (not rejection of stationarity).

Measures to be studied VII

- Example of Heidelberg-Welch

```
heidel.diag(x, eps=0.1, pvalue=0.05)
Stationarity start     p-value
     test          iteration
[,1] passed        1          0.768
     Halfwidth Mean Halfwidth
     test
[,1] passed    1.92 0.00467
```

- The first step is passes with high p-value greater than 0.05, and the second step is passes with a small halfwidth less than 0.1.

Measures to be studied VIII

- Example of Raftery-Lewis

```
raftery.diag(x, q=0.025, r=0.005, s=0.95, converge.eps=0.001
Quantile (q) = 0.025
Accuracy (r) = +/- 0.005
Probability (s) = 0.95
 Burn-in  Total Lower bound  Dependence
 (M)      (N)   (Nmin)       factor (I)
 8        8515  3746         2.27
```

- The 25% quantile $\pm$ 0.005 with prob. 0.95 requires the 8 burn-in and 8515 samples compare to $nmin$=3746, IF 2.27.

Measures to be studied IX

- Example of Gelman-Rubin

```
library(Bolstad2) ; theta0 = c(0,1) ; theta1 = c(3,2)
p = 0.6 ;  candidate = c(0, 3)
v1 = normMixMH(theta0, theta1, p, candidate, steps = 200)
v2 = normMixMH(theta0, theta1, p, candidate, steps = 200)
v3 = normMixMH(theta0, theta1, p, candidate, steps = 200)
v4 = normMixMH(theta0, theta1, p, candidate, steps = 200)
theta = cbind(v1,v2,v3,v4) ;
GelmanRubin(theta)
1.00077577156633
```

Model Selection I

- Amon various metrics, we consider three.
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- Bayes factor

$$\frac{\int p_k(y \mid \theta_k)\pi(\theta_k)d\theta_k}{\int p_l(y \mid \theta_l)\pi(\theta_l)d\theta_l}$$

Model Selection II

- DIC (Deviance Information Criteria)

$$-2\log p(y \mid \hat{\theta}) + 2p_d$$

where $\hat{\theta}$ is Bayes estimator and

$$p_d = 2\left(\log p(y \mid \hat{\theta}) - \mathbb{E}_{post}[\log p(y \mid \theta)]\right).$$

- Key idea is to assess the uncertainty of posteriors by p_d. Pratical in various models, and comparison possible with difference models.

Model Selection III

- It is assumed that the specified parametric family of probability distributions that generate future observations encompasses the true model. Overfitted properties are observed.

Model Selection IV

- Pseudo-marginal likelihood (LPML): (psuedo) predictive distribution is the measure.

$$\text{LPML}_m = \sum_{i=1}^{m} \log p(y_i \mid y^{-i}, \text{Data})$$

where

$$p(y_i \mid y^{-i}, \text{Data}) \approx \left(\frac{1}{S} \frac{1}{p(y_i \mid \theta_s)} \right)^{-1}$$

and θ_s are posterior samples.