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Bayesian Statistics and Data Analysis
Lecture 5

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Thanks to Aki Vehtari, Aalto University

It's all about expectations

$$E_{p(\theta|y)}[f(\theta)] = \int f(\theta) p(\theta|y) d\theta,$$

$$\text{where} \quad p(\theta|y) = \frac{p(y|\theta)p(\theta)}{\int p(y|\theta)p(\theta)d\theta}$$

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- Monte Carlo recap
- Markov Chain Monte Carlo (MCMC)
  - Gibbs sampling
  - Metropolis-Hastings
- Diagnostics
  - Warm-up
  - Convegernce
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  - S_{eff}, MCSE, and autocorrelation

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- Monte Carlo methods which can sample from $p(\theta^{(s)}|y)$ using only $q(\theta^{(s)}|y)$

$$E_{p(\theta|y)}[f(\theta)] \approx \frac{1}{S}\sum_{s=1}^{S} f(\theta^{(s)})$$

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  - Inverse CDF works for 1D

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  - Laplace, Variational*, EP* (Ch 4, 13*, next course)

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- Goal in MCMC: Construct a transition distribution with $p(\theta|y)$ as the stationary distribution

Markov chain Monte Carlo (MCMC)

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  - \+ central limit theorem holds for expectations
  - \- draws are dependent
  - \- construction of efficient Markov chains is not always easy

Markov chain Monte Carlo (MCMC)

- Set of random variables $\theta_1, \theta_2, \ldots$, so that with all values of t, θ_t depends only on the previous $\theta_{(t-1)}$

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- Chain has to be initialized with some starting point θ_0
- Transition distribution $T_t(\theta_t|\theta_{t-1})$ (may depend on t)
- Choose a transition distribution so the stationary distribution of the Markov chain is $p(\theta|y)$

Gibbs sampling

- Alternate sampling from conditional distributions
- Basic algorithm, for $j \in \{1, ..., J\}$

$$\text{sample } \theta_{j,t} \text{ from} \quad p(\theta_j | \theta_{-j,t-1}, y),$$
$$\text{where} \quad \theta_{j,t-1} = (\theta_{1,J}, \ldots, \theta_{j-1,t}, \theta_{j+1,t-1}, \ldots, \theta_{t-1,J})$$

- Will converge (in total variation) to $p(\theta|y)$ as $T \to \infty$

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- Related to the (stochastic) EM algorithm

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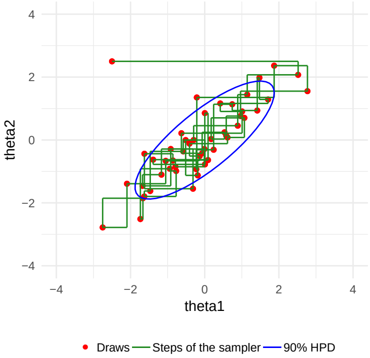

demo

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- Slow if parameters are highly dependent in the posterior...

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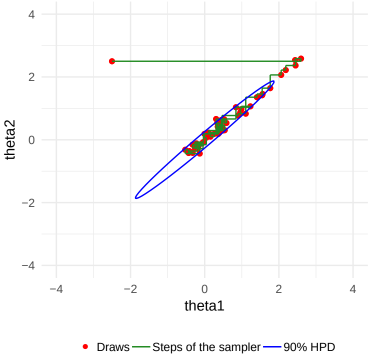

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Sampling conditional vs joint

- How about sampling θ jointly?
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- How about sampling θ jointly?
  - e.g. it is easy to sample from multivariate normal
- Can we use that to form a Markov chain?

The Metropolis algorithm

- Algorithm
  1. starting point θ^0
  2. $t = 1, 2, \dots$
     (a) pick a proposal θ^* from a proposal distribution $J_t(\theta^* | \theta_{t-1})$.
     Proposal distribution has to be symmetric, i.e. $J_t(\theta_a | \theta_b) = J_t(\theta_b | \theta_a)$, for all θ_a, θ_b

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     $$\theta_t = \begin{cases} \theta^* & \text{with probability } \min(r, 1) \\ \theta_{t-1} & \text{otherwise} \end{cases}$$

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     ie, if $p(\theta^*|y) > p(\theta_{t-1}|y)$ accept the proposal always and otherwise accept the proposal with probability r

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- step c is executed by generating a random number from $\mathcal{U}(0, 1)$
- $p(\theta^*|y)$ and $p(\theta_{t-1}|y)$ have the same normalization terms, and thus instead of $p(\cdot|y)$, unnormalized $q(\cdot|y)$ can be used, as the normalization terms cancel out!

Metropolis algorithm

- Example: one bivariate observation (y_1, y_2)
  - bivariate normal distribution with unknown mean and known covariance

$$\begin{pmatrix}\theta_1\\ \theta_2\end{pmatrix} \Bigg| \, y \sim \mathcal{N}\left(\begin{pmatrix}y_1\\ y_2\end{pmatrix}, \begin{pmatrix}1 & \rho\\ \rho & 1\end{pmatrix}\right)$$

  - proposal distribution $J_t(\theta^*|\theta_{t-1}) = \mathcal{N}(\theta^*|\theta_{t-1}, \sigma_p^2)$

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- Theoretically
  1. Prove that simulated series is a Markov chain which has unique stationary distribution
  2. Prove that this stationary distribution is the desired target distribution

Why Metropolis algorithm works

1. Prove that simulated series is a Markov chain which has unique stationary distribution
   a) irreducible

   b) aperiodic

   c) recurrent / not transient

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      = probability to return to a state i is 1 as $T \to \infty$
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     which is the same as the probability of transition from θ_a to θ_b, since we have required that $J_t(\cdot|\cdot)$ is symmetric
   - since their joint distribution is symmetric, θ_t and θ_{t-1} have the same marginal distributions, and so $p(\theta|y)$ is the stationary distribution of the Markov chain of θ

Metropolis-Hastings algorithm

- Generalization of Metropolis algorithm for non-symmetric proposal distributions
  - acceptance ratio includes ratio of proposal distributions

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  - acceptance ratio includes ratio of proposal distributions

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Metropolis-Hastings algorithm

- Ideal proposal distribution is the distribution itself
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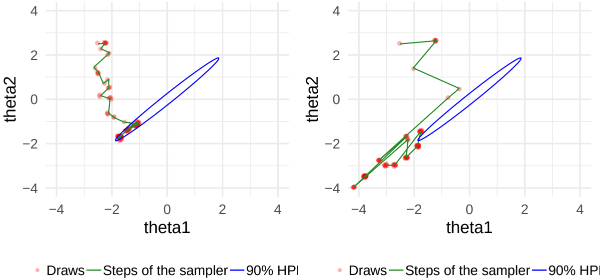
  demo
- Generic rule for rejection rate is 60-90%

Gibbs sampling as a special case

- Specific case of Metropolis-Hastings algorithm
  - single updated (or blocked)
  - proposal distribution is the conditional distribution
    $\rightarrow$ proposal and target distributions are same
    $\rightarrow$ acceptance probability is 1

Metropolis

- Usually doesn't scale well to high dimensions
  - if the shape doesn't match the whole distribution, the efficiency drops



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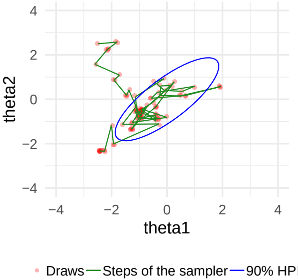

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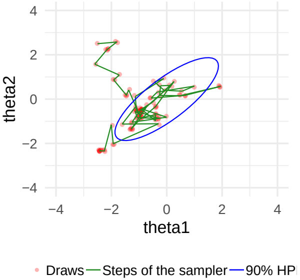

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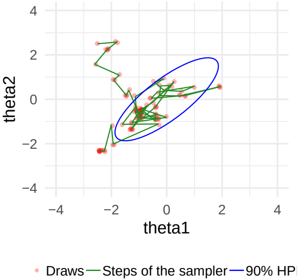


- Warm-up = remove draws from the beginning of the chain
  - warm-up may include also phase for adapting algorithm parameters
- Convergence diagnostics
  - Do we get samples from the target distribution?

MCMC draws are dependent

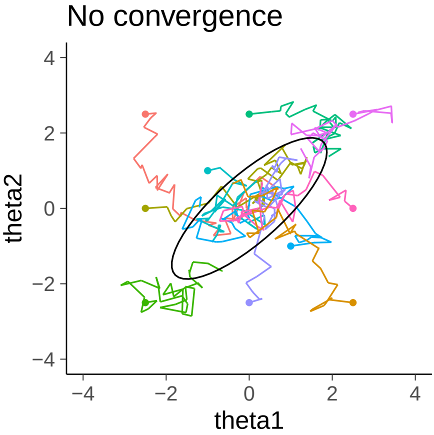
- Monte Carlo estimates still valid (central limit theorem holds)

$$E_{p(\theta|y)}[f(\theta)] \approx \frac{1}{S}\sum_{s=1}^{S} f(\theta^{(s)})$$

- Estimation of Monte Carlo error is more difficult
  - evaluation of *effective* sample size

Assesing convergence: Several chains

- Use of several chains make convergence diagnostics easier
- Start chains from different starting points – preferably overdispersed



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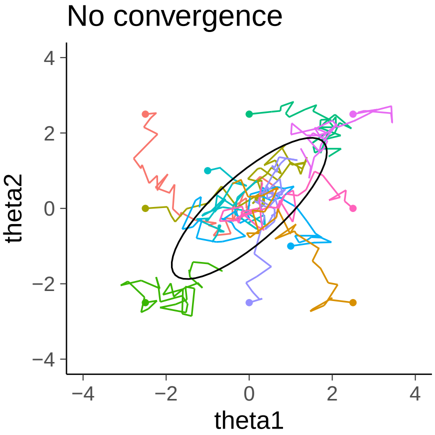

- Remove draws from the beginning of the chains and run chains long enough so that it is not possible to distinguish where each chain started and the chains are well mixed

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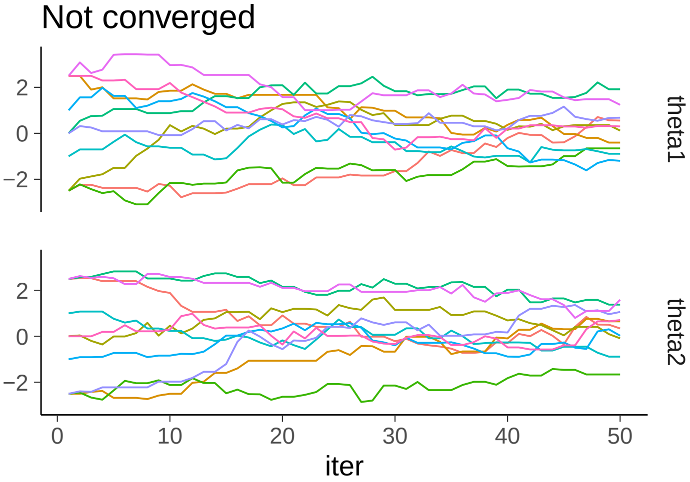

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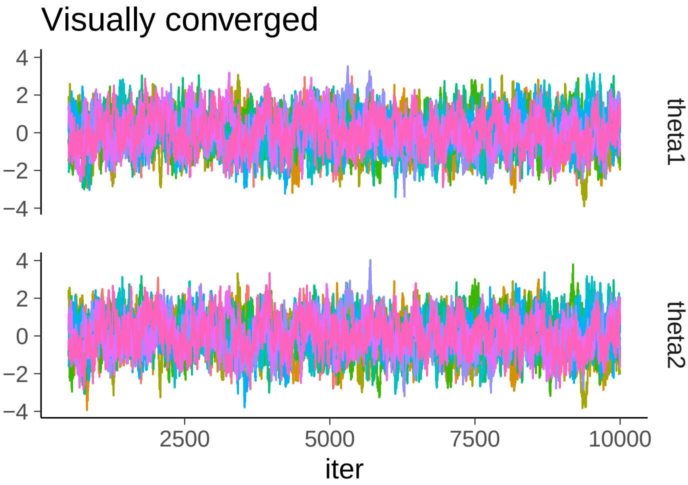

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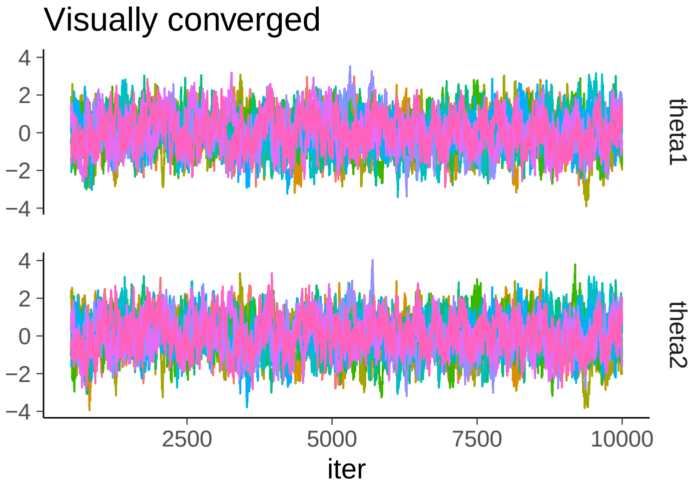

Visual convergence check is not sufficient

$\widehat{R}$: comparison of within and between variances of the chains

- BDA3: $\widehat{R}$ aka *potential scale reduction factor* (PSRF)
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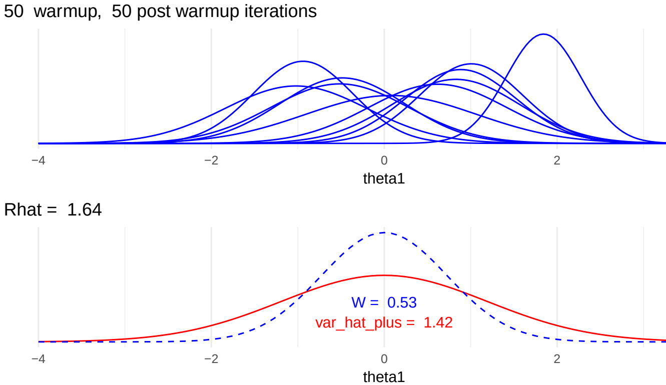

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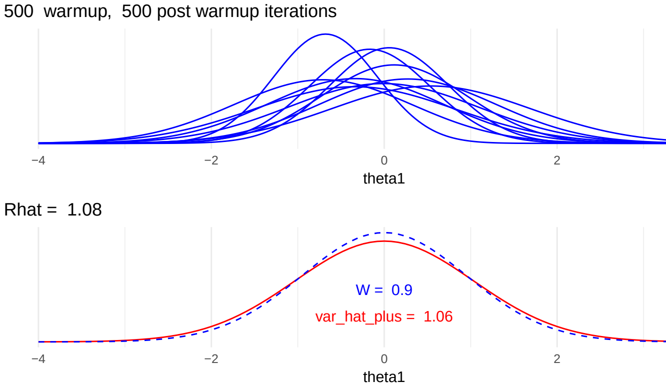

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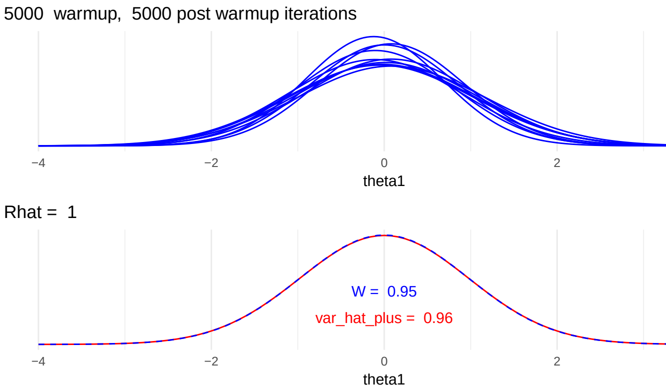

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  - when $N \to \infty, \quad \mathrm{E}(W) \to \mathrm{var}(\theta|y)$
- As $\widehat{\mathrm{var}}^{+}(\theta|y)$ overestimates and W underestimates, compute
$$\widehat{R} = \sqrt{\frac{\widehat{\mathrm{var}}^{+}}{W}}$$

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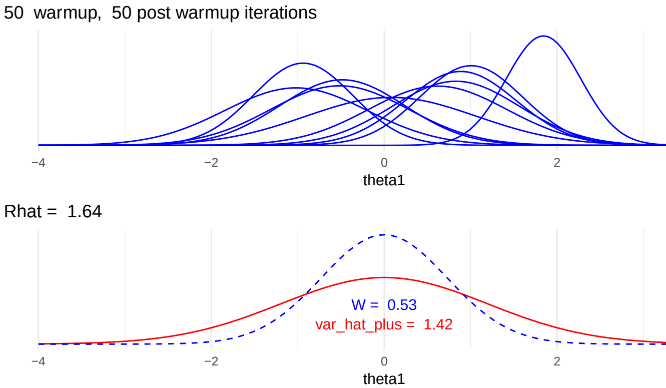

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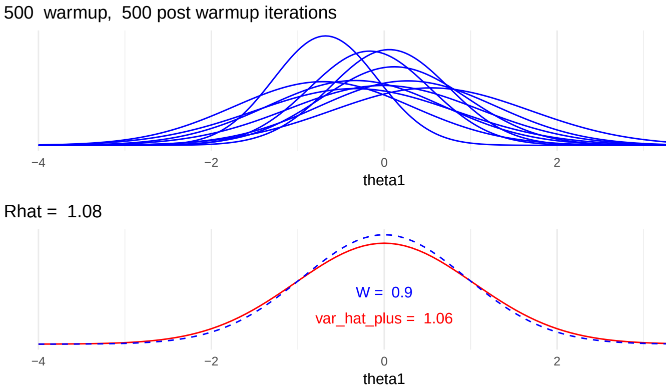

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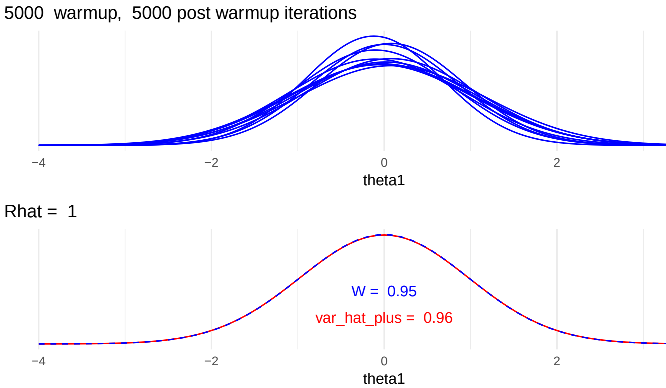

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- If $\widehat{R}$ close to 1, it is still possible that chains have not converged
  - if starting points were not overdispersed
  - distribution far from normal (especially if infinite variance)
  - just by chance when N is finite

Split-$\widehat{R}$

- BDA3: split-$\widehat{R}$
- Examines *mixing* and *stationarity* of chains
- To examine stationarity chains are split to two parts
  - after splitting, we have M chains, each having N draws
  - scalar draws $\theta_{nm} \quad (n = 1, \ldots, N; m = 1, \ldots, M)$
  - compare means and variances of the split chains

Rank normalized $\widehat{R}$

- Original $\widehat{R}$ requires that the target distribution has finite mean and variance

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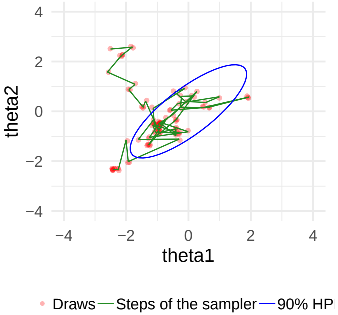
Time series analysis

- Auto correlation function
  - describes the correlation given a certain lag
  - can be used to compare efficiency of MCMC algorithms and parameterizations

Auto correlation



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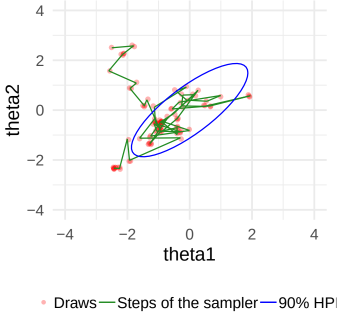

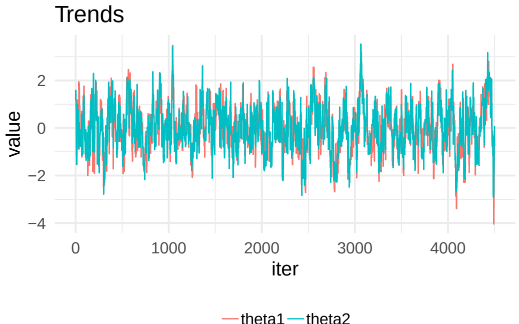

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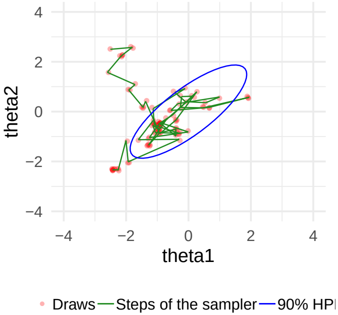

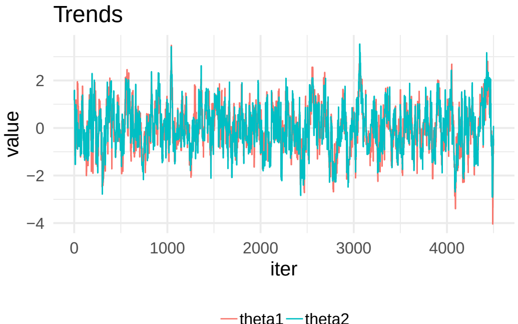

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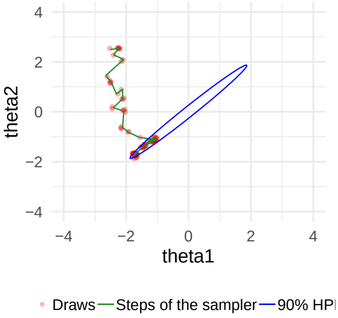

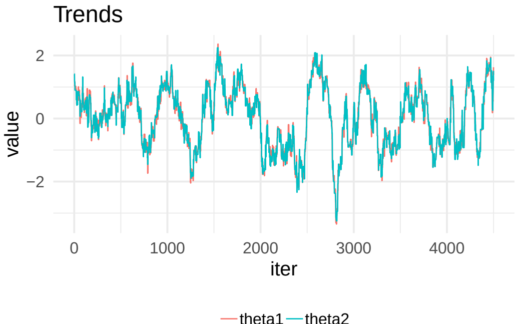

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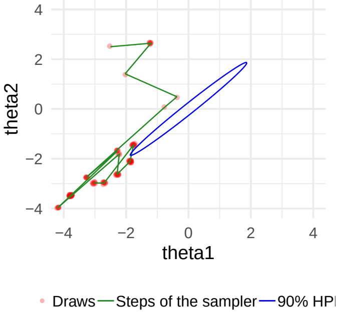

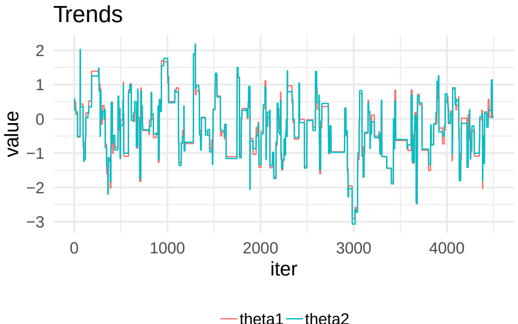

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- For expectation $\bar{\theta}$

$$\mathrm{Var}[\bar{\theta}] = \frac{\sigma_\theta^2}{S_{E_{\max}}}$$

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  - new R-hat paper $S = NM$ (in BDA3 $N = nm$ and $n_{E_{\max}} = N/\tau$)
  - BDA3 focuses on $S_{E_{\max}}$ and not the Monte Carlo error directly
    new R-hat paper discusses more about MCSEs for different quantities

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Time series analysis

- Estimation of the autocorrelation using several chains

$$\hat{\rho}_n = 1 - \frac{W - \frac{1}{M}\sum_{m=1}^{M} \hat{\rho}_{n,m}}{2\widehat{\text{var}}^{+}}$$

where $\hat{\rho}_{n,m}$ is autocorrelation at lag n for chain m

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  - takes into account if the chains are not mixing (the chains have not converged)
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- Compared to a method which computes the autocorrelation from a single chain, the multi-chain estimate has smaller variance

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Time series analysis

- Estimation of τ

$$\tau = 1 + 2\sum_{t=1}^{\infty} \hat{\rho}_t$$

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- empirical autocorrelation function is noisy and thus estimate of τ is noisy
- noise is larger for longer lags (less observations)

Time series analysis

- Estimation of τ

$$\tau = 1 + 2\sum_{t=1}^{\infty} \hat{\rho}_t$$

where $\hat{\rho}_t$ is empirical autocorrelation

- empirical autocorrelation function is noisy and thus estimate of τ is noisy
- noise is larger for longer lags (less observations)
- less noisy estimate is obtained by truncating

$$\hat{\tau} = 1 + 2\sum_{t=1}^{T} \hat{\rho}_t$$

Time series analysis

- Estimation of τ

$$\tau = 1 + 2\sum_{t=1}^{\infty} \hat{\rho}_t$$

where $\hat{\rho}_t$ is empirical autocorrelation

  - empirical autocorrelation function is noisy and thus estimate of τ is noisy
  - noise is larger for longer lags (less observations)
  - less noisy estimate is obtained by truncating

$$\hat{\tau} = 1 + 2\sum_{t=1}^{T} \hat{\rho}_t$$

- As τ is estimated from a finite number of draws, it's expectation is overoptimistic
  - if $\hat{\tau} > MN/20$ then the estimate is unreliable

Geyer's adaptive window estimator

- Truncation can be decided adaptively
  - for stationary, irreducible, recurrent Markov chain
  - let $\Gamma_m = \rho_{2m} + \rho_{2m+1}$, which is sum of two consequent autocorrelations
  - Γ_m is positive, decreasing and convex function of m

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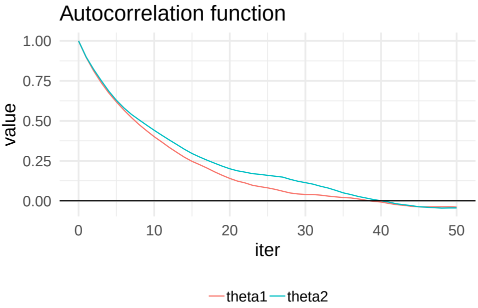
- Monte Carlo recap
- Markov Chain Monte Carlo (MCMC)
  - Gibbs sampling
  - Metropolis-Hastings
- Diagnostics
  - Warm-up
  - Convegernce
  - Convegernce
  - S_{eff}, MCSE, and autocorrelation

Geyer's adaptive window estimator

- Truncation can be decided adaptively
  - for stationary, irreducible, recurrent Markov chain
  - let $\Gamma_m = \rho_{2m} + \rho_{2m+1}$, which is sum of two consequent autocorrelations
  - Γ_m is positive, decreasing and convex function of m
- Initial positive sequence estimator (Geyer's IPSE)
  - Choose the largest m so, that all values of the sequence $\hat{\Gamma}_1, \ldots, \hat{\Gamma}_m$ are positive



Effective sample size

Effective sample size $\mathrm{ESS} = S_{E_{\max}} \approx S/\hat{\tau}$

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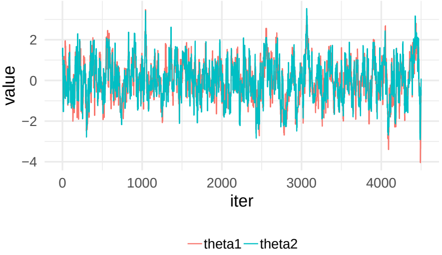
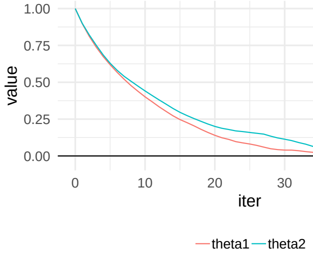
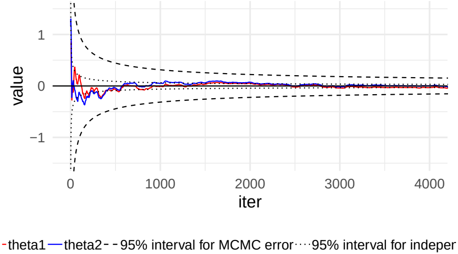
Trends



Autocorrelation function



Cumulative averages

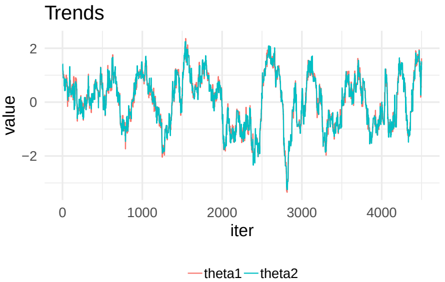


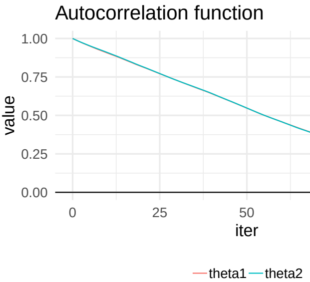
$$\hat{\tau} = 1 + 2\sum_{t=1}^{T} \hat{\rho}_t$$

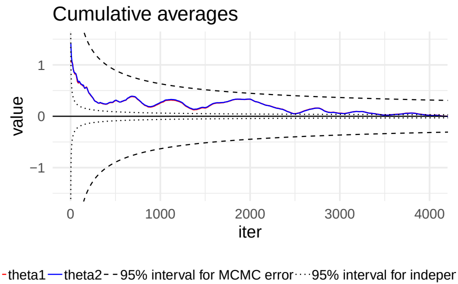
$$\approx 24$$

Effective sample size

Effective sample size $\mathrm{ESS} = S_{E_{\max}} \approx S/\hat{\tau}$







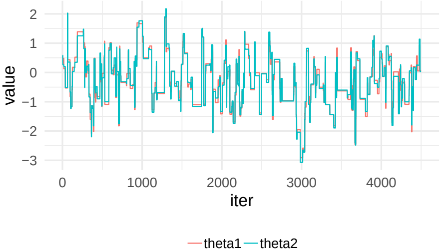
$$\hat{\tau} = 1 + 2\sum_{t=1}^{T} \hat{\rho}_t$$

$$\approx 104$$

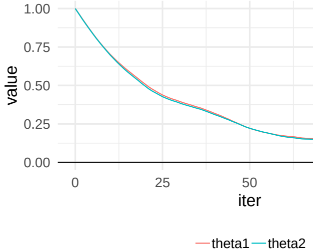
Effective sample size

Effective sample size $\mathrm{ESS} = S_{E_{\max}} \approx S/\hat{\tau}$

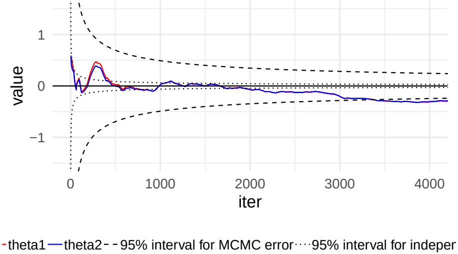
Trends



Autocorrelation function



Cumulative averages



$$\hat{\tau} = 1 + 2\sum_{t=1}^{T} \hat{\rho}_t$$

$$\approx 63$$

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Problematic distributions

- Nonlinear dependencies
  - optimal proposal depends on location

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  - difficult to move from one mode to another

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Problematic distributions

- Nonlinear dependencies
  - optimal proposal depends on location
- Funnels
  - optimal proposal depends on location
- Multimodal
  - difficult to move from one mode to another
- Long-tailed with non-finite variance and mean
  - central limit theorem for expectations does not hold