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

Bayesian Statistics and Data Analysis Lecture 5

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Thanks to Aki Vehtari, Aalto University

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It's all about expectations

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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

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

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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 $p(\theta|y)$

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Gibbs sampling

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

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

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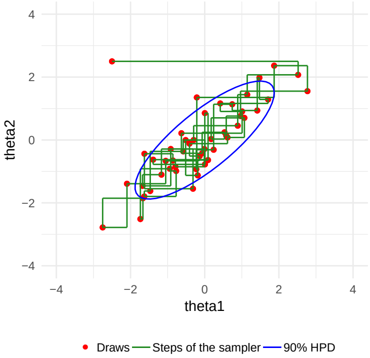
- Related to the (stochastic) EM algorithm

Gibbs sampling



demo

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

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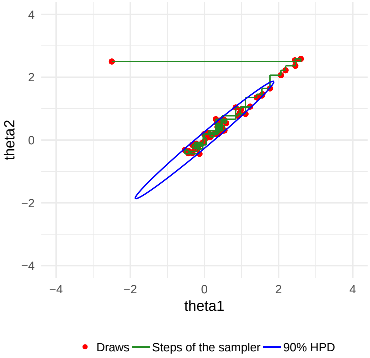

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Sampling conditional vs joint

- How about sampling θ jointly?
  - e.g. it is easy to sample from multivariate normal

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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?

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The Metropolis algorithm

- Algorithm
  1. starting point θ^0
  2. $t = 1, 2, \ldots$
     (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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  - $p(\theta^*|y)$ 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 $J_t(\theta^* | \theta_{t-1}) = \mathcal{N}(\theta^* | \theta_{t-1}, \sigma_p^2)$

demo

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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

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   c) recurrent / not transient
      = 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

$$r = \frac{p(\theta^*|y)/J_t(\theta^*|\theta_{t-1})}{p(\theta_{t-1}|y)/J_t(\theta_{t-1}|\theta^*)}$$

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Metropolis-Hastings algorithm

- Ideal proposal distribution is the distribution itself
  - $J(\theta^*|\theta) \equiv p(\theta^*|y)$ for all θ
  - acceptance probability is 1
  - independent draws
  - not usually feasible

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  - $J(\theta^*|\theta) \equiv p(\theta^*|y)$ for all θ
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demo

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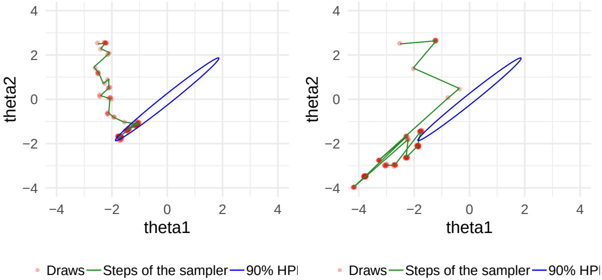
  demo
- Generic rule for rejection rate is 60-90%

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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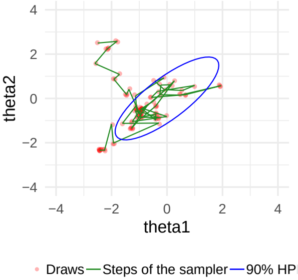

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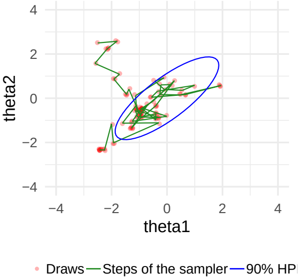

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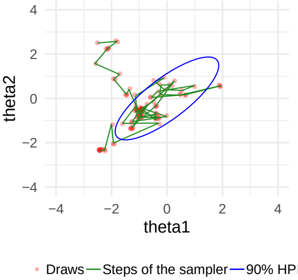

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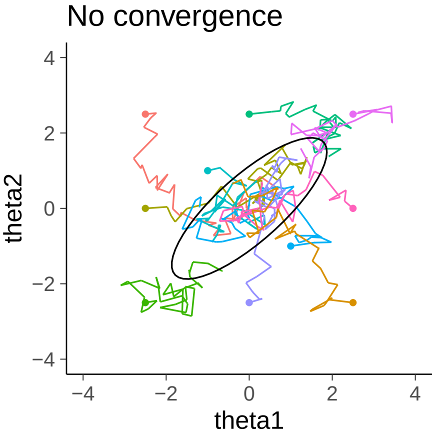
  - warm-up may include also phase for adapting algorithm parameters
- Also called burn-in

Assesing convergence: Several chains

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



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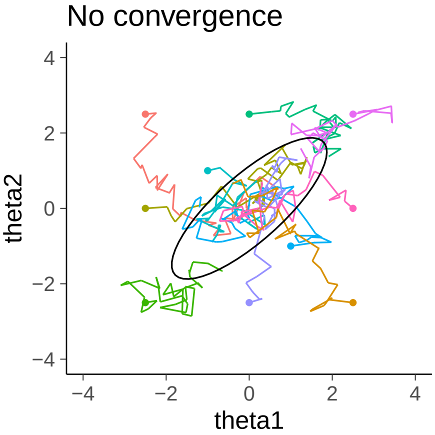
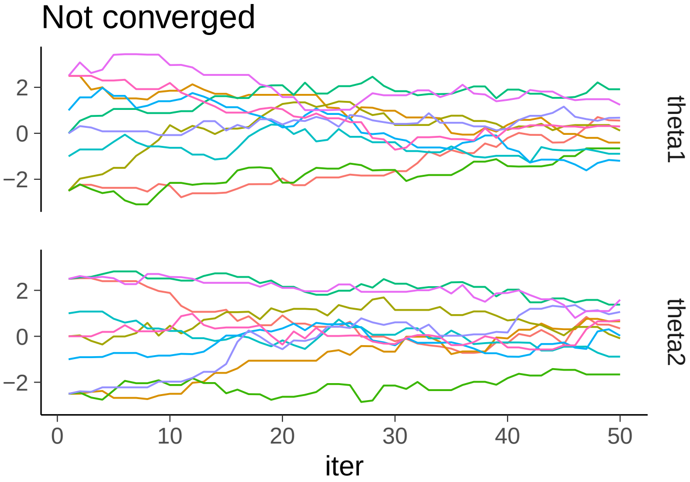


- Remove draws from the beginning of the chains and run chains long enough so that it is not possible to distinguish where each chain started and the chains are well mixed

Several chains



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- Monte Carlo recap
- Markov Chain Monte Carlo (MCMC)
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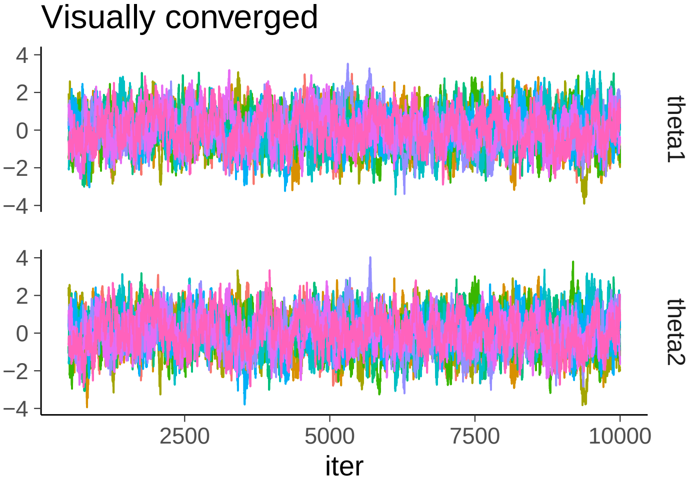

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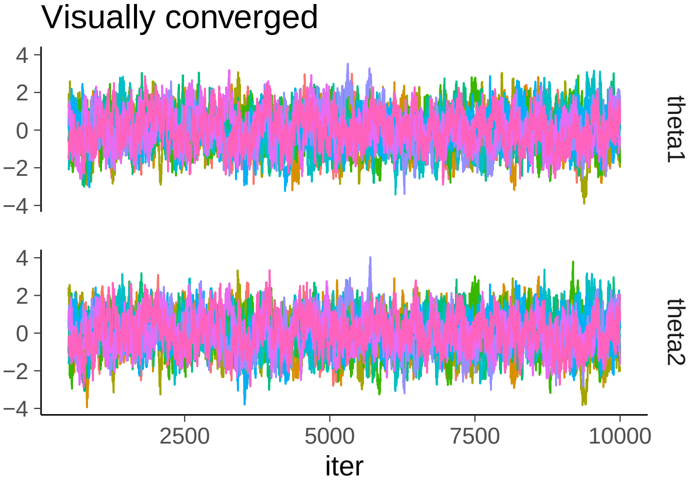

Visual convergence check is not sufficient

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

- BDA3: $\widehat{R}$ aka *potential scale reduction factor* (PSRF)
- Compare means and variances of the chains

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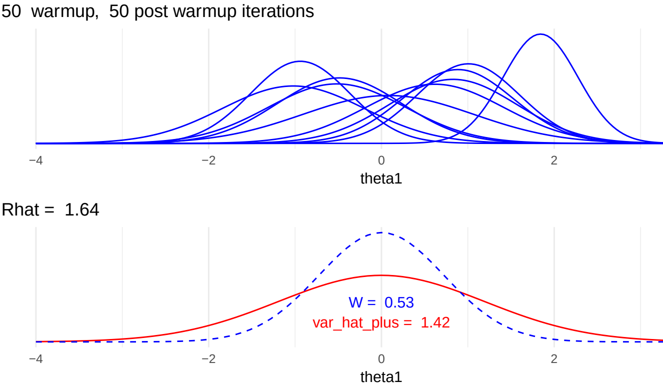

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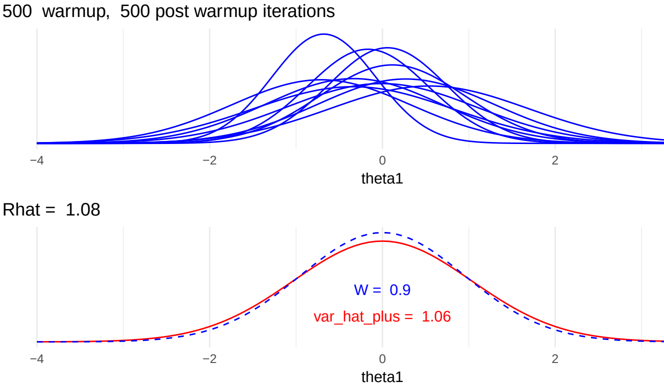

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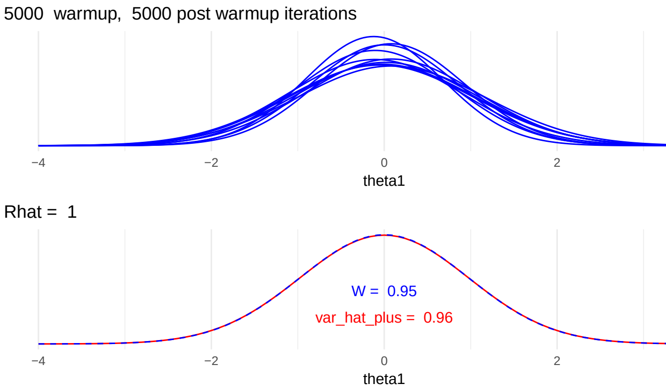

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- As $\widehat{\mathrm{var}}^{+}(\theta|y)$ overestimates and W underestimates, compute

$$\widehat{R} = \sqrt{\frac{\widehat{\mathrm{var}}^{+}}{W}}$$

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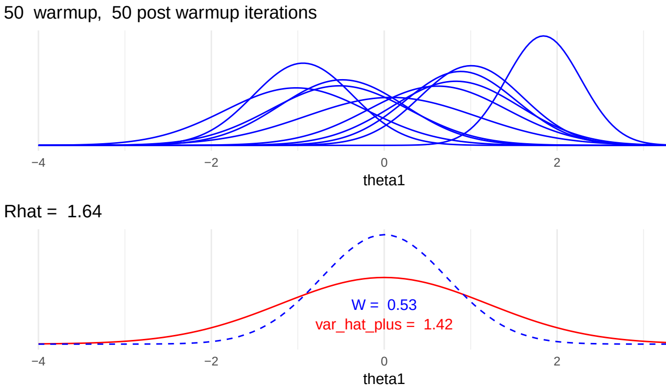

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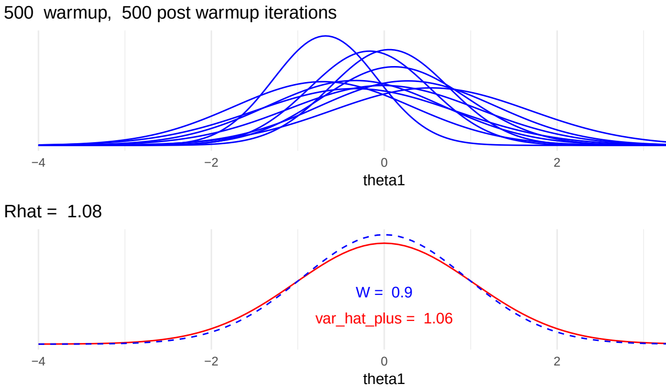

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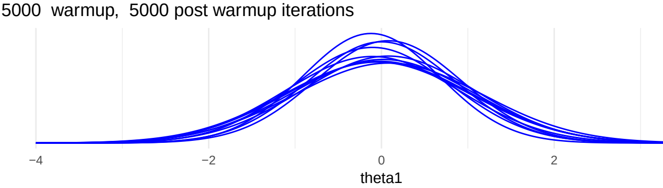

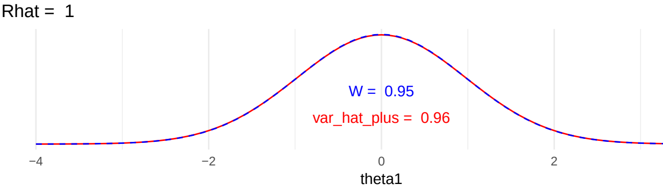

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- If $\widehat{R}$ close to 1, it is still possible that chains have not converged
  - if starting points were not overdispersed
  - distribution far from normal (especially if infinite variance)
  - just by chance when N is finite

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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MCMC draws are dependent

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

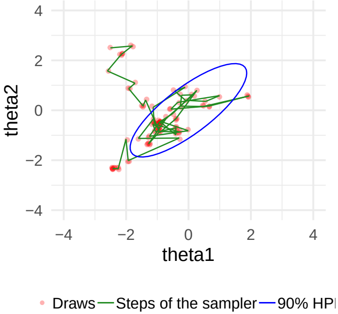
$$E_{p(\theta|y)}[f(\theta)] \approx \frac{1}{S}\sum_{s=1}^{S} f(\theta^{(s)})$$

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

MCMC Autocorrelation

- 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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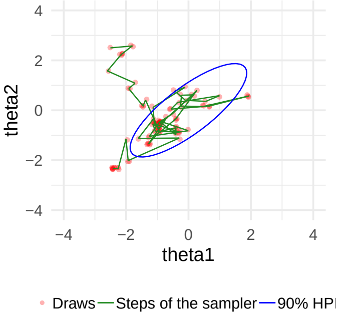

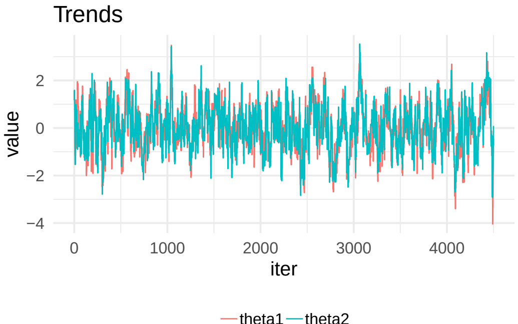

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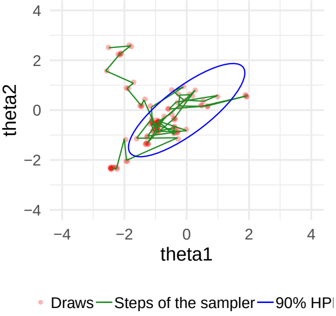

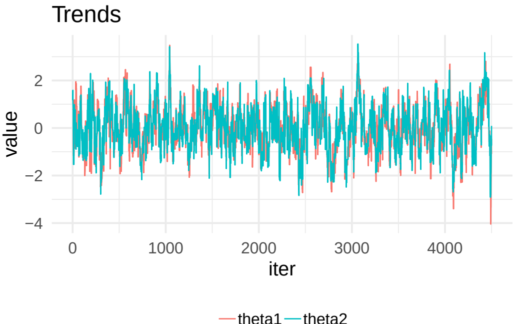

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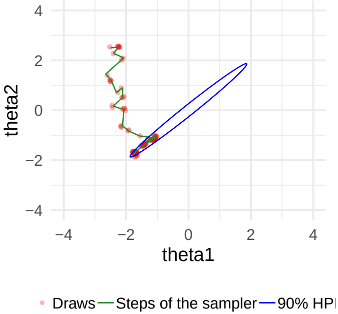

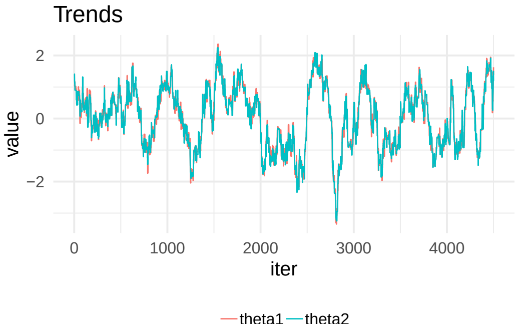

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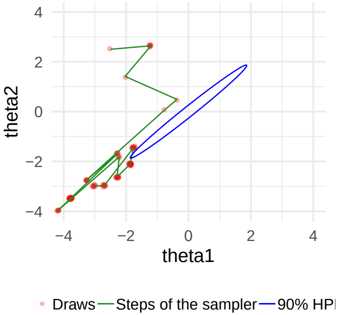

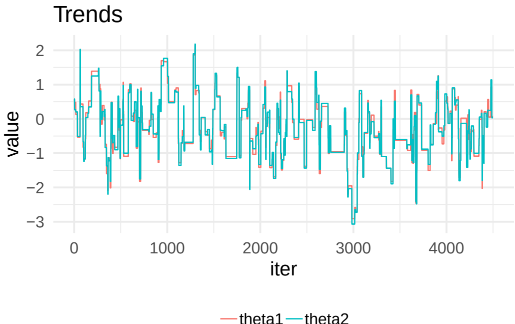

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- Time series analysis can be used to estimate Monte Carlo error in case of MCMC
- For expectation $\bar{\theta}$

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

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- BDA3 focuses on $S_{E_{\max}}$ and not the Monte Carlo error directly
  new R-hat paper discusses more about MCSEs for different quantities

Time series analysis

- Estimation of the autocorrelation using several chains

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

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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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- Estimation of τ

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

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

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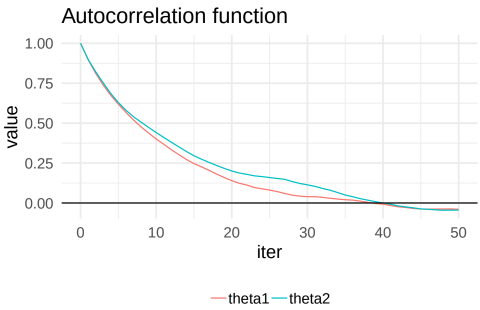
  - let $\Gamma_m = \rho_{2m} + \rho_{2m+1}$, which is sum of two consequent autocorrelations
  - Γ_m is positive, decreasing and convex function of m
- Initial positive sequence estimator (Geyer's IPSE)
  - Choose the largest m so, that all values of the sequence $\hat{\Gamma}_1, \ldots, \hat{\Gamma}_m$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



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Effective sample size

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

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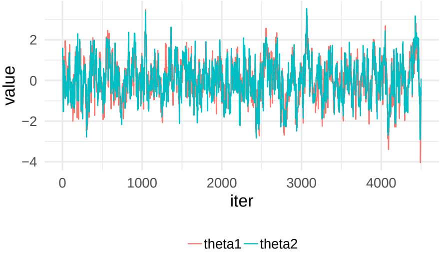
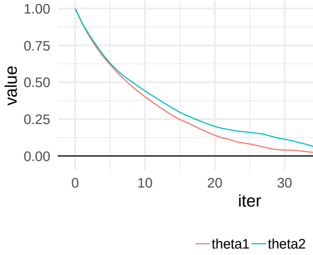
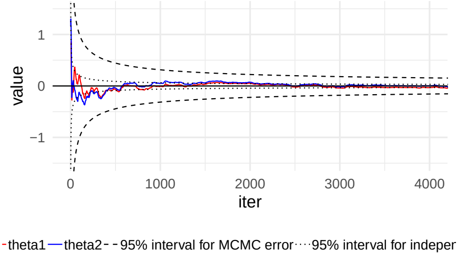
Trends



Autocorrelation function



Cumulative averages



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

$$\approx 24$$

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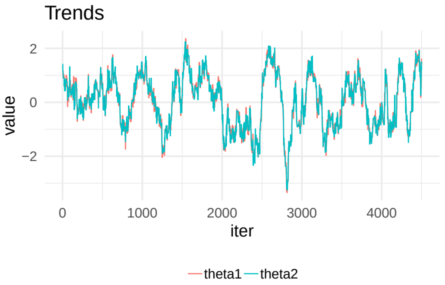
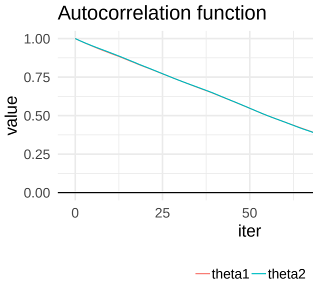
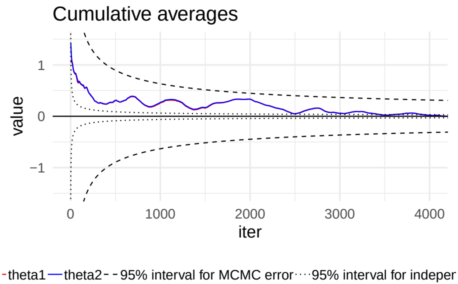
- Monte Carlo recap
- Markov Chain Monte Carlo (MCMC)
  - Gibbs sampling
  - Metropolis-Hastings
- Diagnostics
  - Warm-up
  - Convergence
  - Convergence
  - S_{eff}, MCSE, and autocorrelation

Effective sample size

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





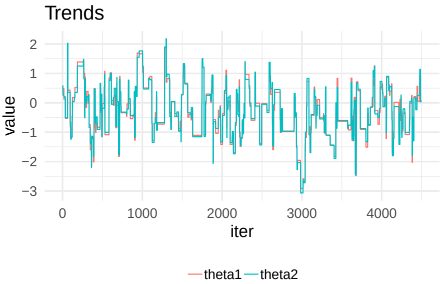


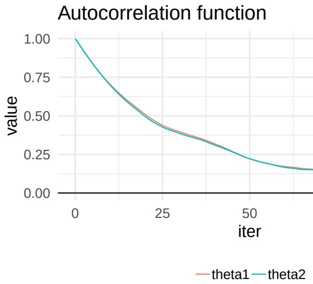
$$\hat{\tau} = 1 + 2\sum_{t=1}^{T} \hat{\rho}_t$$

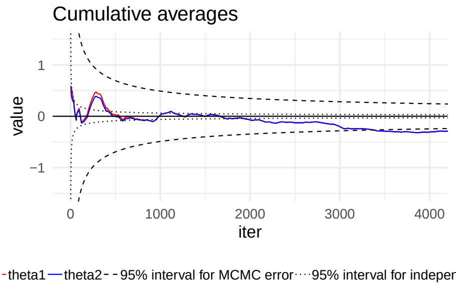
$$\approx 104$$

Effective sample size

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







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

$$\approx 63$$

Problematic distributions

- Nonlinear dependencies
  - optimal proposal depends on location

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- Long-tailed with non-finite variance and mean
  - central limit theorem for expectations does not hold