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Bayesian Statistics and Data Analysis
Lecture 5

Måns Magnusson
Department of Statistics, Uppsala University
Thanks to Aki Vehtari, Aalto University

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It's all about expectations

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

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

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

Monte Carlo

- Monte Carlo methods we have discussed so far
  - 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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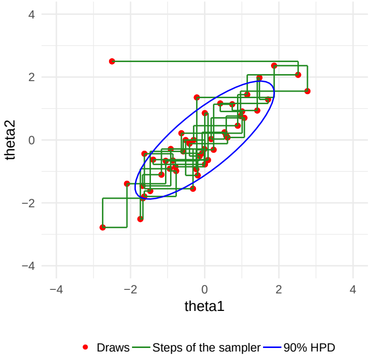
- Related to the (stochastic) EM algorithm

Gibbs sampling



demo

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

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

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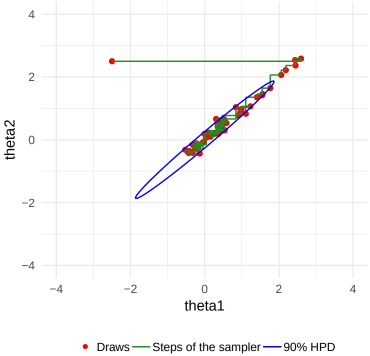

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Sampling conditional vs joint

- How about sampling θ jointly?
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  - 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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     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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  - rejection of a proposal increments the time t also by one ie, the new state is the same as previous
  - 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

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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

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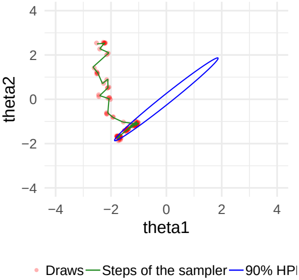
  demo
- Generic rule for rejection rate is 60-90%

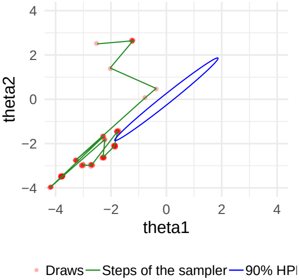
Gibbs sampling as a special case

- 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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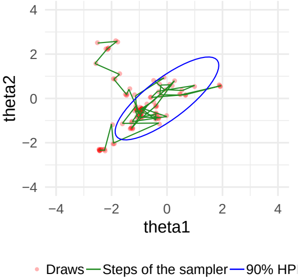

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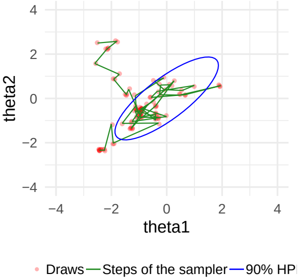

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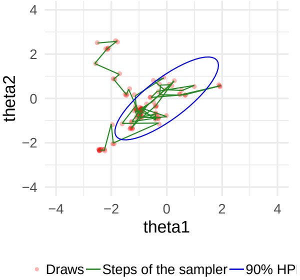

- Warm-up period = (non-representative) draws from the beginning of the Markov chain
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- Also called burn-in

Assesing convergence

- Several Markov chains make convergence diagnostics easier

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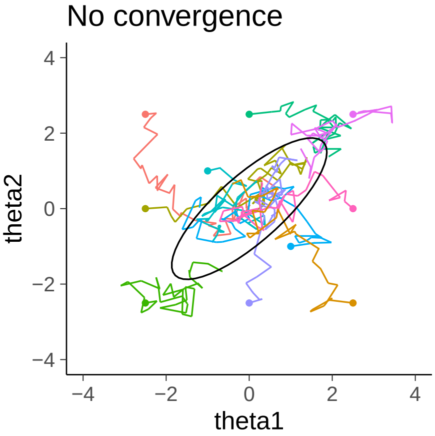
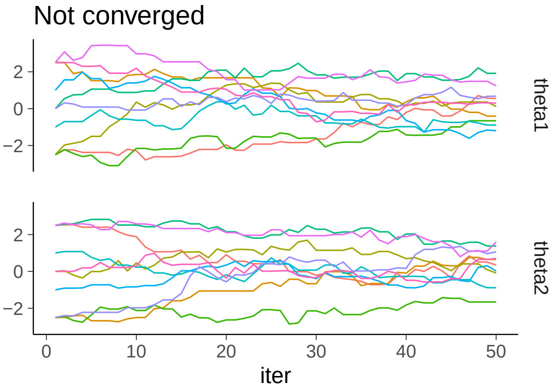
- Start chains from different starting points – preferably overdispersed



- Remove warm-up draws and run chains long enough

Several chains



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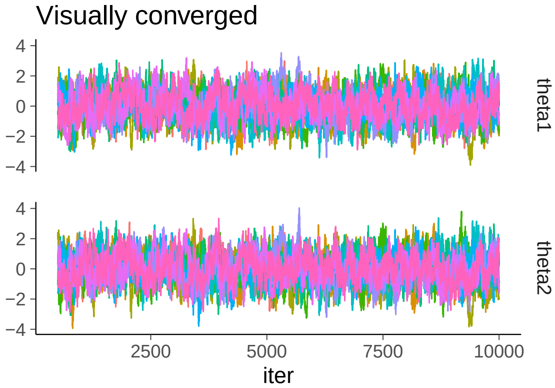

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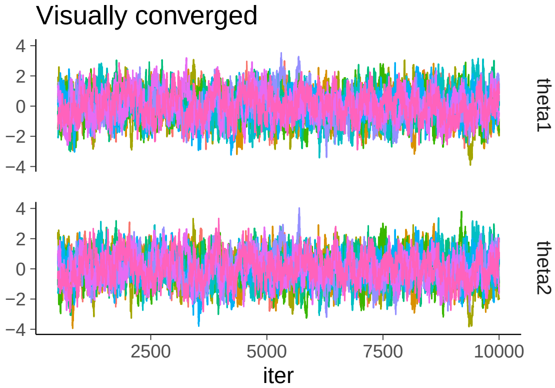

Visual convergence check is not sufficient

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

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

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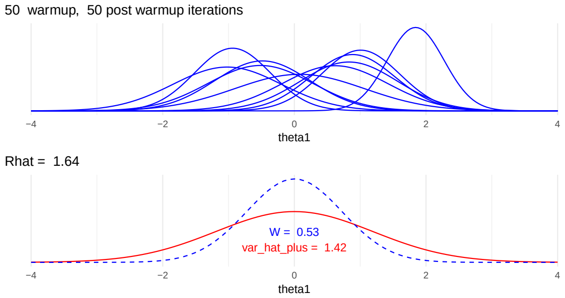

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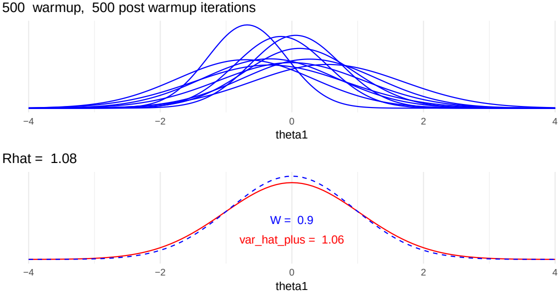

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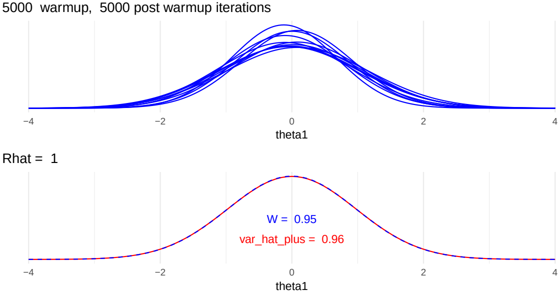

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- Given finite N, W *underestimates* marginal posterior variance
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  - when $N \to \infty, \quad \mathrm{E}(W) \to \mathrm{var}(\theta|y)$
- As $\widehat{\mathrm{var}}^{+}(\theta|y)$ overestimates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

$\widehat{R}$

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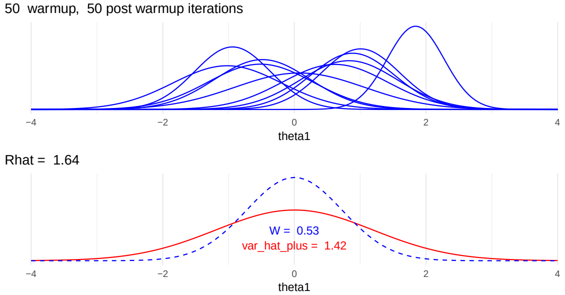

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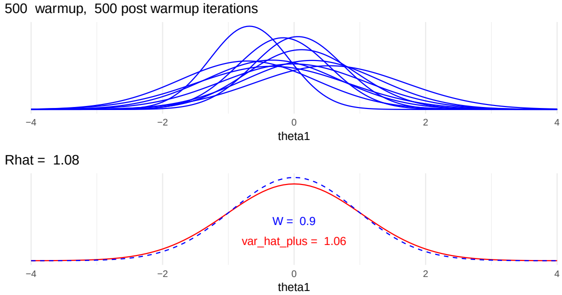

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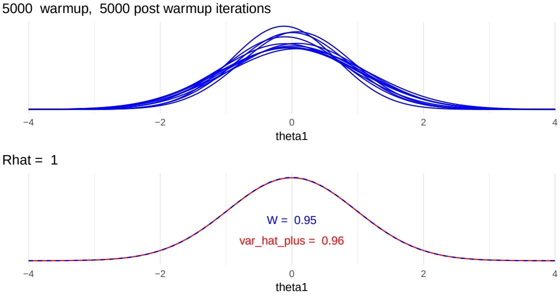

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- If $\widehat{R}$ is big (e.g., $R > 1.01$), keep sampling
- If $\widehat{R}$ close to 1, it is still possible that chains have not converged
  - if starting points were not overdispersed
  - distribution far from normal (especially if infinite variance)
  - just by chance when N is finite

$\widehat{R}$

- Additional $\widehat{R}$ methods to assess convergence
- Split-$\widehat{R}$
  - Examines *mixing* and *stationarity* of chains
  - To examine stationarity chains are split to two parts: compare means and variances of the split chains

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  - Examines *mixing* and *stationarity* of chains
  - To examine stationarity chains are split to two parts: compare means and variances of the split chains
- Rank normalized $\widehat{R}$
  - Does not requires that the target distribution has finite mean and variance

MCMC draws are dependent

- Monte Carlo estimates still valid (central limit theorem)

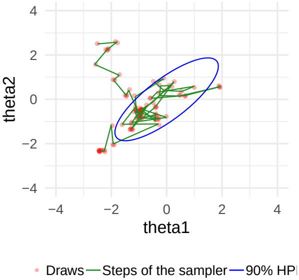
$$E_{p(\theta|y)}[f(\theta)] \approx \frac{1}{S}\sum_{s=1}^{S} f(\theta^{(s)})$$

- Estimation of Monte Carlo error is more difficult
  - evaluation of *effective* sample size, S_{eff}.

MCMC Autocorrelation

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

Autocorrelation



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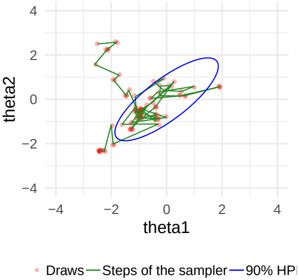

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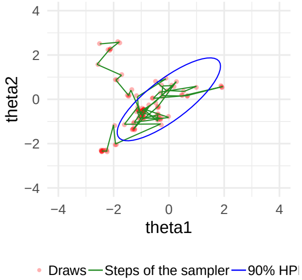

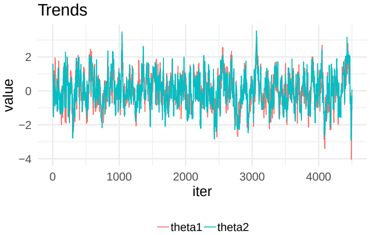

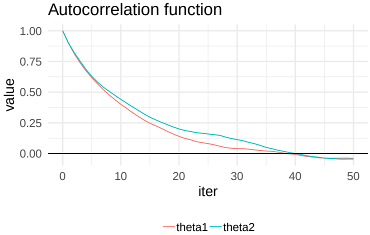

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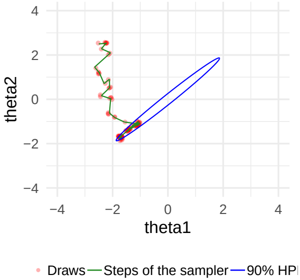

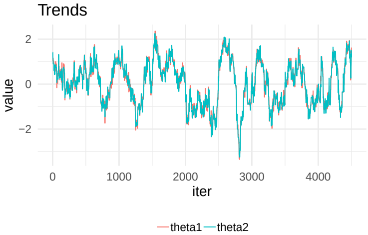

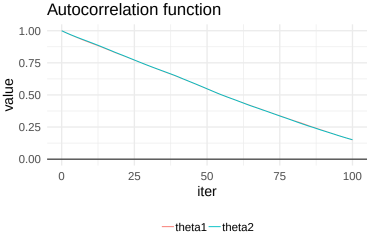

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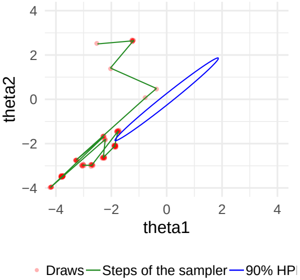

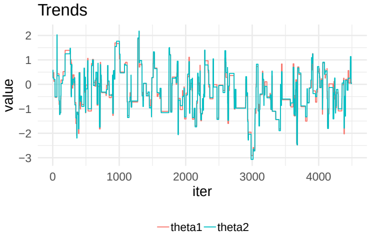

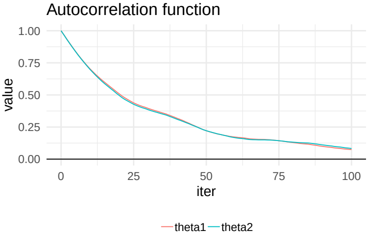

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Autocorrelation

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

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  - BDA3 focuses on S_{eff} and not the Monte Carlo error directly

Autocorrelation

- Estimation of the autocorrelation using several chains

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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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- less noisy estimate is obtained by truncating

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

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Geyer's adaptive window estimator of τ

- Truncation T 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
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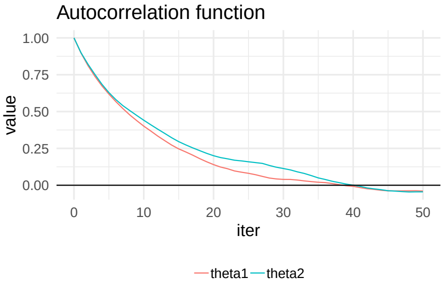
  - Γ_m is positive, decreasing and convex function of m
- Initial positive sequence estimator (Geyer's IPSE)
  - Choose the largest m so, that all values of the sequence $\hat{\Gamma}_1, \ldots, \hat{\Gamma}_m$ are positive



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Effective sample size, S_{eff}

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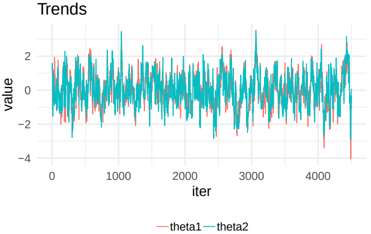
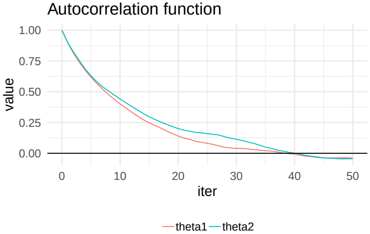
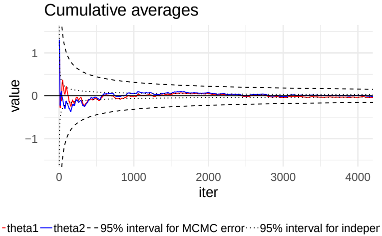




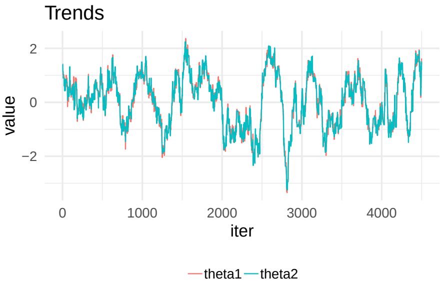


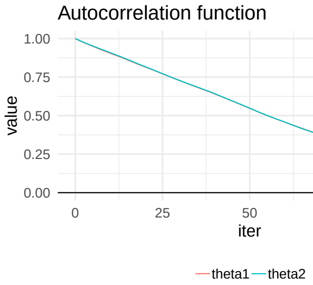
$$\hat{\tau} = 1 + 2\sum_{t=1}^{T} \hat{\rho}_t$$

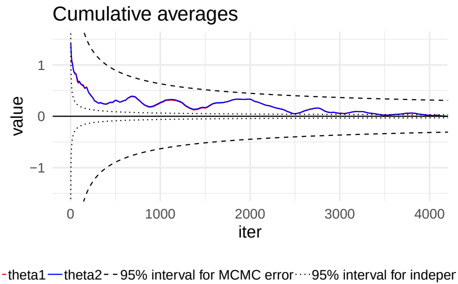
$$\approx 24$$

Effective sample size

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





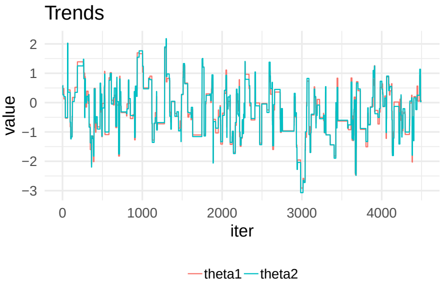


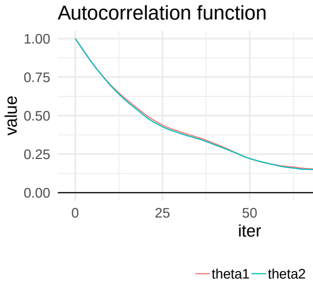
$$\hat{\tau} = 1 + 2\sum_{t=1}^{T} \hat{\rho}_t$$

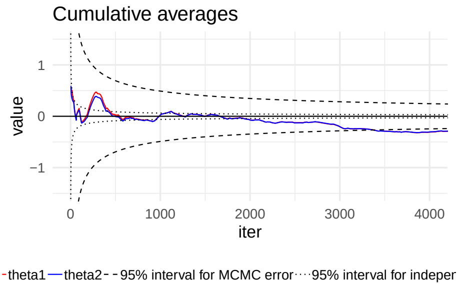
$$\approx 104$$

Effective sample size

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







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

$$\approx 63$$

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Problematic distributions

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  - 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