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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

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

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

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

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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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- Random variables $\theta_1, \theta_2, \ldots$ where 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 $N \to \infty$

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- Related to the (stochastic) EM algorithm

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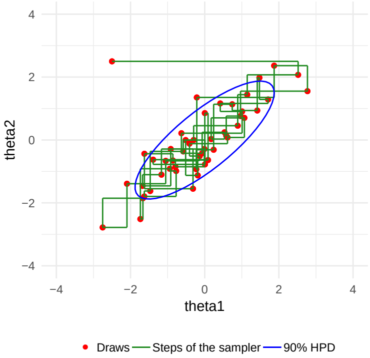

demo

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

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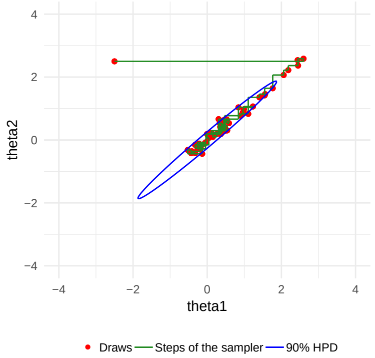

demo

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. $t = 1, 2, \ldots$
     (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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  - 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 $p(\theta|y)$

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

Metropolis-Hastings algorithm

- Ideal proposal distribution is the distribution itself
  - $J(\theta^*|\theta) \equiv p(\theta^*|y)$ for all θ
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demo

- Generic rule for rejection rate is 60-90%

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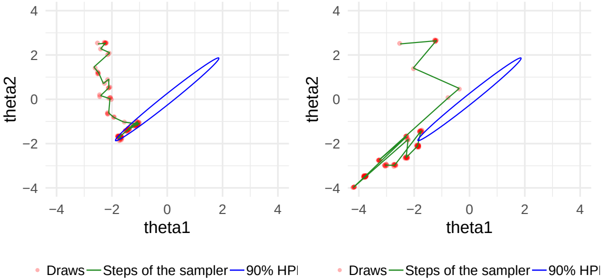
Gibbs sampling as a special case

- 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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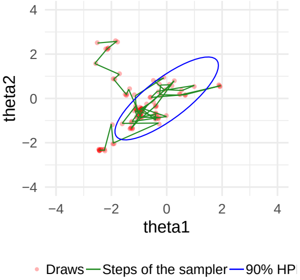

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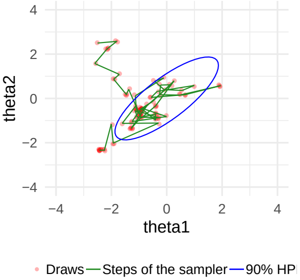

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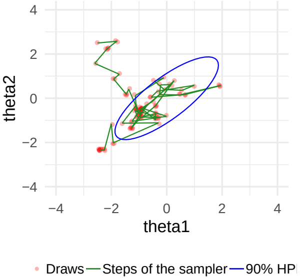

- Warm-up period = (non-representative) draws from the beginning of the Markov chain
  - remove warm-up before using samples for inference
  - warm-up may include also phase for adapting algorithm parameters
- Also called burn-in

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Assesing convergence

- Several Markov chains make convergence diagnostics easier

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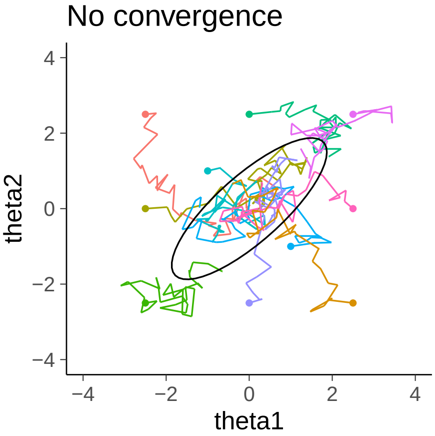
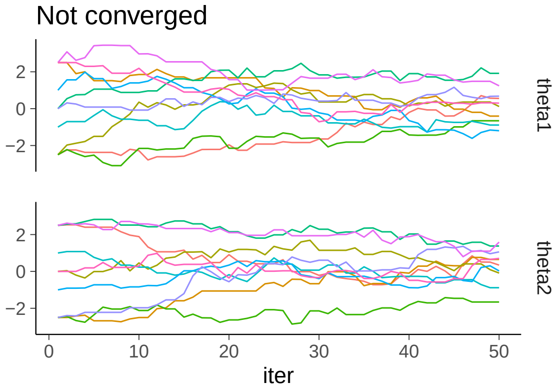
- Several Markov chains make convergence diagnostics easier
- Start chains from different starting points – preferably overdispersed



- Remove warm-up draws and run chains long enough

Several chains



Several chains

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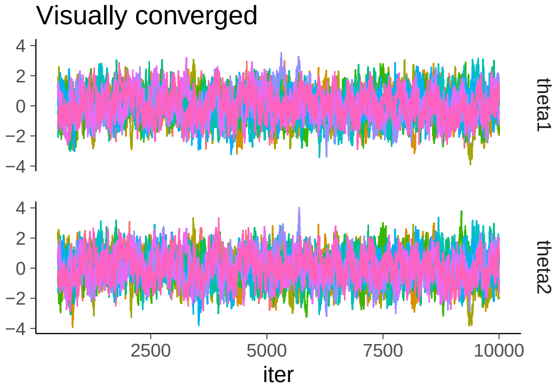

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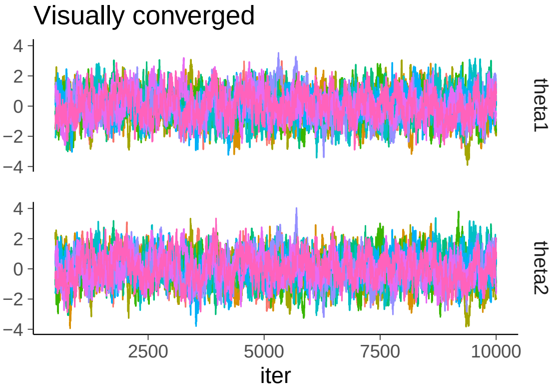

Visual convergence check is not sufficient

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- Compare means and variances of the chains

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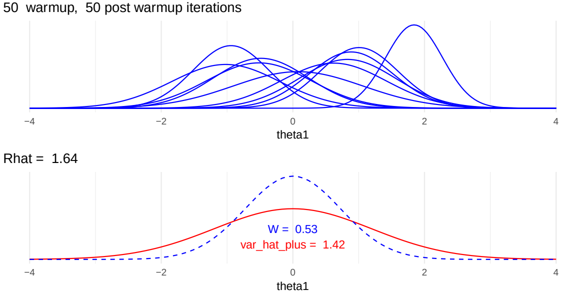

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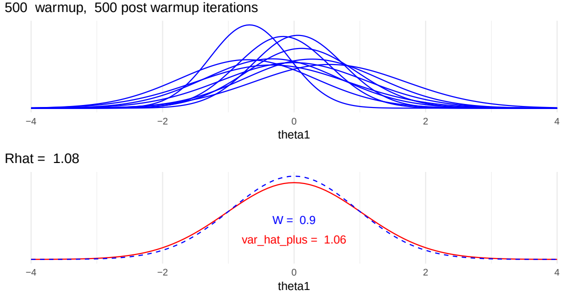

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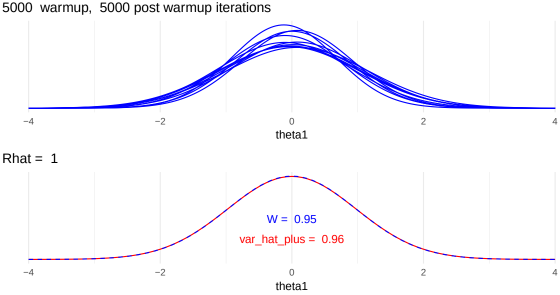

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- As $\widehat{\mathrm{var}}^{+}(\theta|y)$ overestimates and W underestimates, compute

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

$\widehat{R}$

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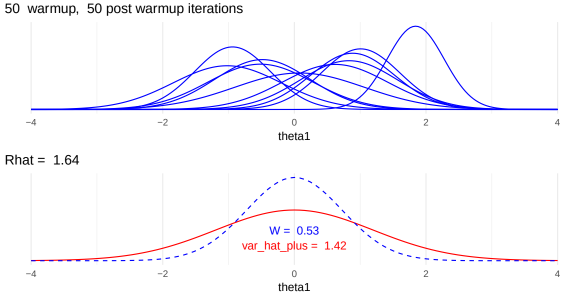

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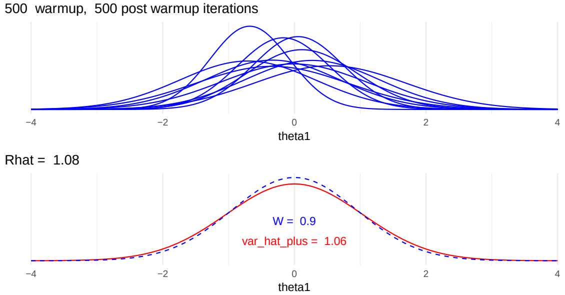

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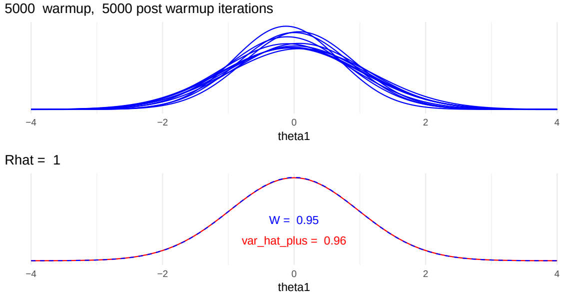

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- $\widehat{R} \to 1$, when $N \to \infty$
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- If $\widehat{R}$ close to 1, it is still possible that chains have not converged
  - if starting points were not overdispersed
  - distribution far from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

$\widehat{R}$

- 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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- 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
- 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

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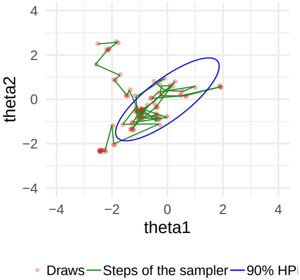

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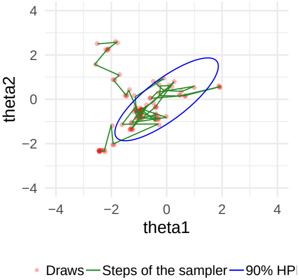

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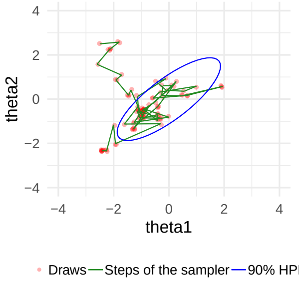

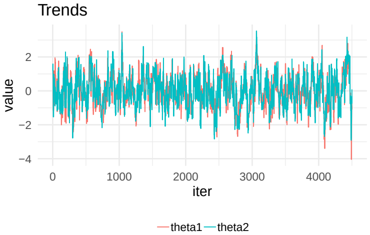

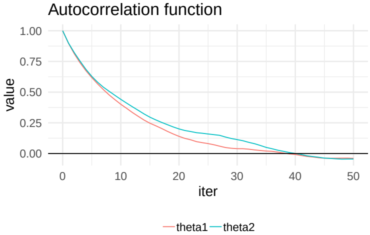

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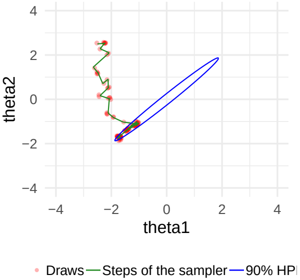

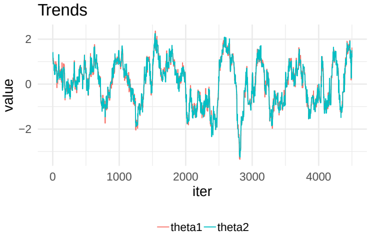

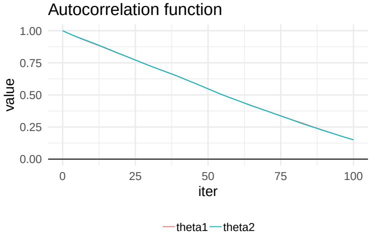

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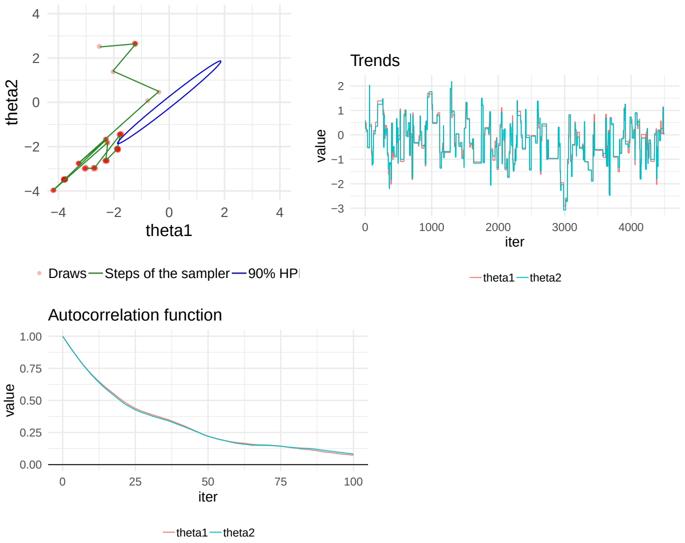

Autocorrelation

- The autocorrleation can be used to estimate Monte Carlo error in case of MCMC
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$$\mathrm{Var}[\bar{\theta}] = \frac{\sigma_\theta^2}{S_{\text{eff}}}$$

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

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Autocorrelation

- Estimation of the autocorrelation using several chains

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

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

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- BDA3 has slightly different and less accurate equation. The above equation is used in Stan 2.18+
- Compared to a method which computes the autocorrelation from a single chain, the multi-chain estimate has smaller variance

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Estimating τ

- Estimation of τ

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

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- less noisy estimate is obtained by truncating

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

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
  - Γ_m is positive, decreasing and convex function of m

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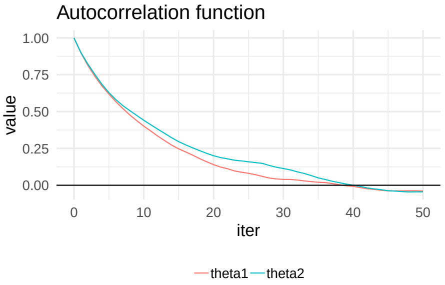
  - Γ_m is positive, decreasing and convex function of m
- Initial positive sequence estimator (Geyer's IPSE)
  - Choose the largest m so, that all values of the sequence $\hat{\Gamma}_1, \ldots, \hat{\Gamma}_m$ are positive



Effective sample size, S_{eff}

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

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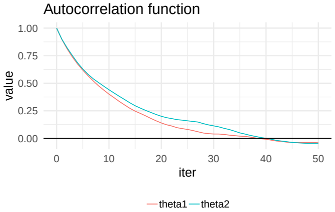

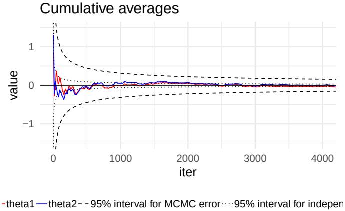

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$$\approx 24$$

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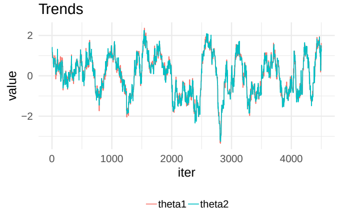
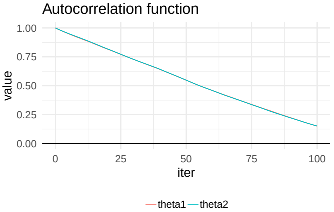
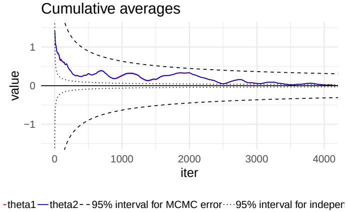
Effective sample size $\mathrm{ESS} = S_{\mathrm{eff}} \approx S/\hat{\tau}$





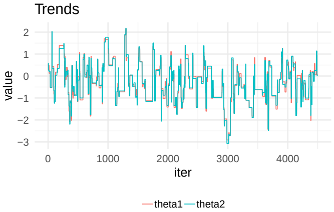


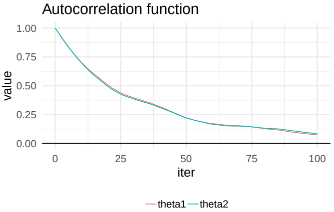
$$\hat{\tau} = 1 + 2\sum_{t=1}^{T} \hat{\rho}_t$$

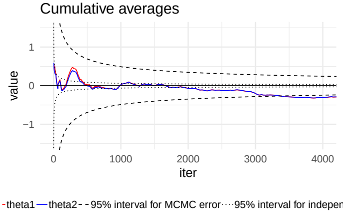
$$\approx 104$$

Effective sample size, S_{eff}

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







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

$$\approx 63$$

Problematic distributions

- Nonlinear dependencies
  - optimal proposal depends on location

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  - central limit theorem for expectations does not hold

demo