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

Bayesian Statistics and Data Analysis
Lecture 5

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

Seminar today at 13.15

- Topic: posteriordb: Testing, Benchmarking and Developing Bayesian Inference Algorithms
- Where: H317 Ekonomikum
- Speaker Jakob Torgander, Department of Statistics, Uppsala University
- Opponent David Broman, EECS, KTH Royal Institute of Technology

Assignment 4

- "More explicit examples of proper weight normalization would help prevent implementation errors in importance sampling."

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- Minor suggestions and improvements

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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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- Monte Carlo methods we have discussed so far
  - Inverse CDF works mainly 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 an efficient Markov chains is not always easy

MCMC summary

- Random variables $\theta_1, \theta_2, \ldots$ where θ_t depends only on the previous $\theta_{(t-1)}$

$$p(\theta_t|\theta_1, \ldots, \theta_{(t-1)}) = p(\theta_t|\theta_{(t-1)})$$

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- Choose a transition distribution so the stationary distribution of the Markov chain is $p(\theta | y)$

Subsection 1

Gibbs sampling

Gibbs sampling

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

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

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- 1D sampling ($|j| = 1$) is generally easy

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- Popular for discrete parameters

Example: Bivariate Normal using Gibbs

$$p(\theta \mid y) \sim \mathcal{N}\left(\bar{y}, \tfrac{1}{n}\Sigma\right).$$

where Σ is known and $\theta \in \mathcal{R}^2$

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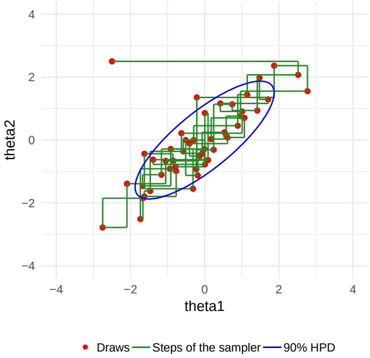
Using Gibbs sampling:

Given starting values $(\theta_1^{(0)}, \theta_2^{(0)})$, for $t = 1, 2, \ldots$:

$$\theta_1^{(t)} \sim \mathcal{N}\left(\bar{y}_1 + \frac{\rho}{\sigma_2}(\theta_2^{(t-1)} - \bar{y}_2),\ \frac{1}{n}\left(\sigma_1 - \frac{\rho^2}{\sigma_2}\right)\right),$$

$$\theta_2^{(t)} \sim \mathcal{N}\left(\bar{y}_2 + \frac{\rho}{\sigma_1}(\theta_1^{(t)} - \bar{y}_1),\ \frac{1}{n}\left(\sigma_2 - \frac{\rho^2}{\sigma_1}\right)\right).$$

Gibbs sampling



demo

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

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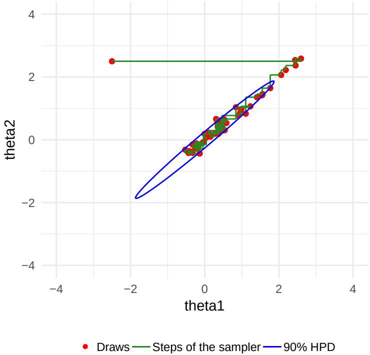

demo

Sampling conditional vs joint

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

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- How about sampling θ jointly?
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- Can we use that to form a Markov chain?

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Subsection 2

Metropolis-Hastings

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

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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

Why Metropolis algorithm works

- Intuitively more draws from the higher density areas as jumps to higher density are always accepted and only some of the jumps to the lower density are accepted

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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 $p(\theta|y)$

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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   b) aperiodic
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      - holds for a random walk on any proper distribution (except for trivial exceptions)
   c) recurrent / not transient
      = probability to return to a state i is 1 as $T \to \infty$
      - holds for a random walk on any proper distribution (except for trivial exceptions)

Why Metropolis algorithm works

2. Prove that this stationary distribution is the desired target distribution $p(\theta|y)$: see book
   - Show *detailed balance* with respect to $p(\theta|y)$:

     $$p(\theta|y)\, T(\theta|\theta') = p(\theta'|y)\, T(\theta'|\theta), \quad \forall \theta, \theta'.$$

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More indepth in a proper Markov Theory course!

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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demo

- Generic rule for rejection rate is 60-90%

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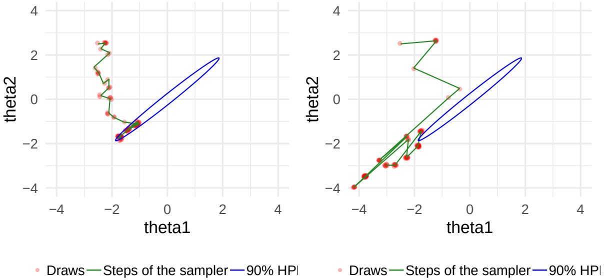
Gibbs sampling as a special case

- 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



Section 3

MCMC Diagnostics

What we want to know

1. Has the chains converged to the posterior distribution?

What we want to know

1. Has the chains converged to the posterior distribution?
2. How many efficient samples do I have?

Subsection 1

Warm-up

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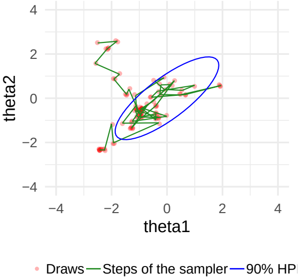
  - but in finite time the initial part of the Markov chain may be non-representative



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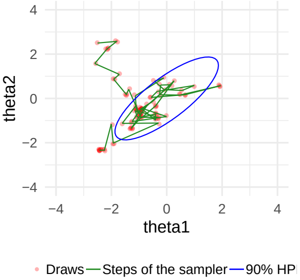

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  - warm-up may include phase for adapting algorithm parameters

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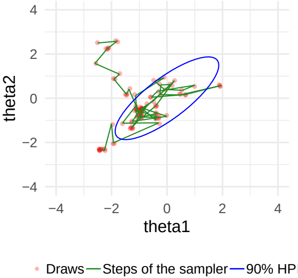


- Warm-up period = (non-representative) draws from the beginning of the Markov chain
  - remove warm-up before using samples for inference
  - warm-up may include phase for adapting algorithm parameters
- Also called burn-in

Subsection 2

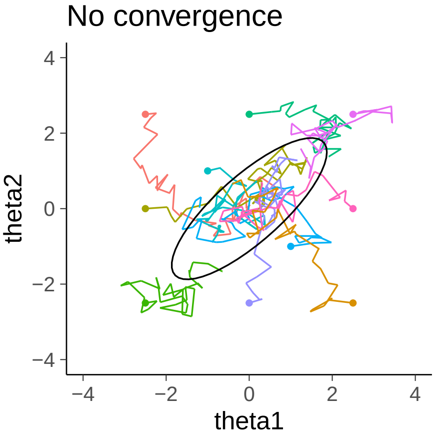
Convergence

Assesing convergence

- Several Markov chains make convergence diagnostics easier

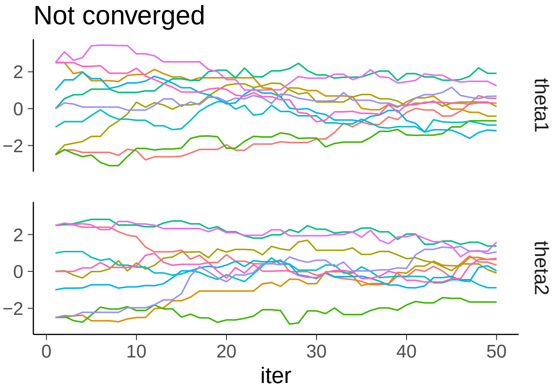
Assesing convergence

- 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



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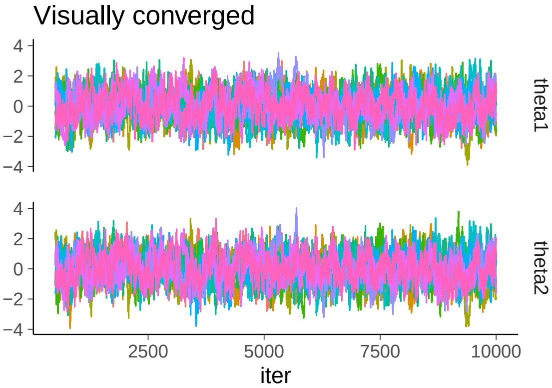

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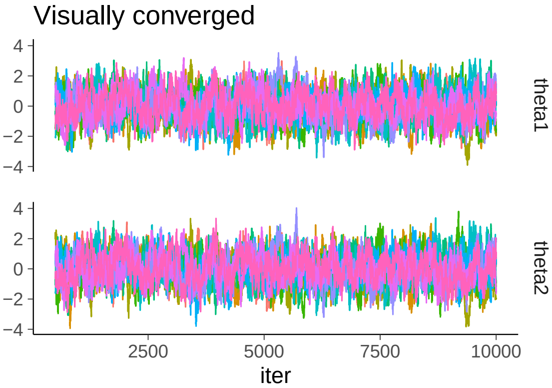

Visual convergence check is not sufficient

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

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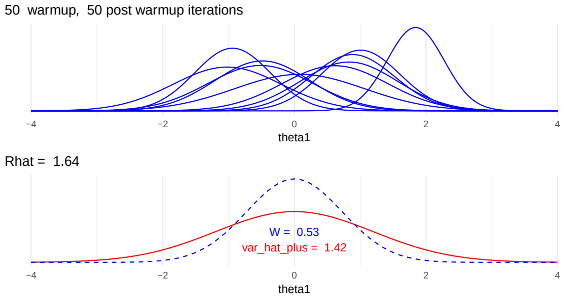

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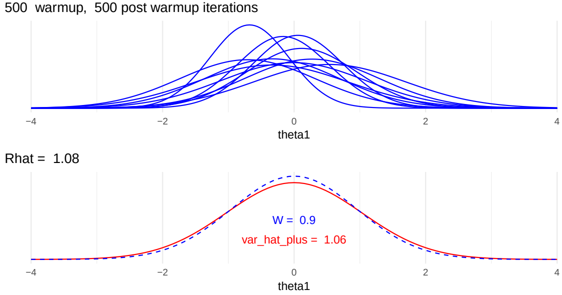

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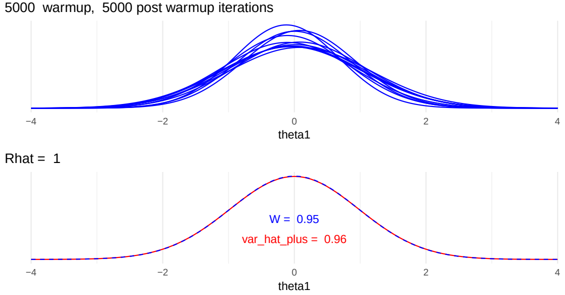

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- As $\widehat{\mathrm{var}}^{+}(\theta|y)$ overestimates and W underestimates, compute

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

Subsection 3

S_{eff}, MCSE, and autocorrelation

MCMC draws are dependent

- Monte Carlo estimates still valid (central limit theorem)

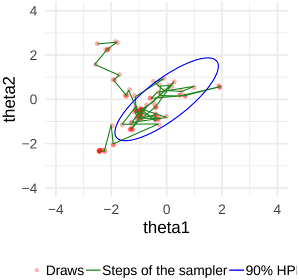
$$E_{p(\theta|y)}[f(\theta)] \approx \frac{1}{S}\sum_{s=1}^{S} f(\theta^{(s)})$$

- 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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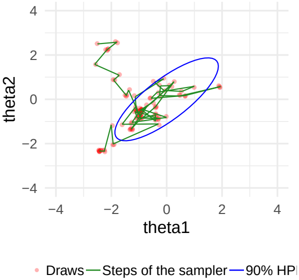

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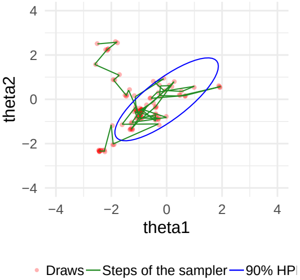

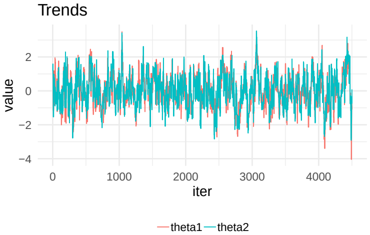

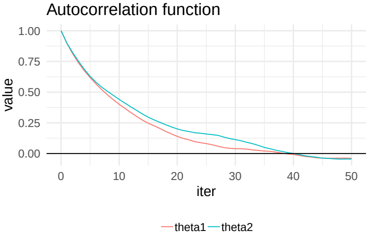

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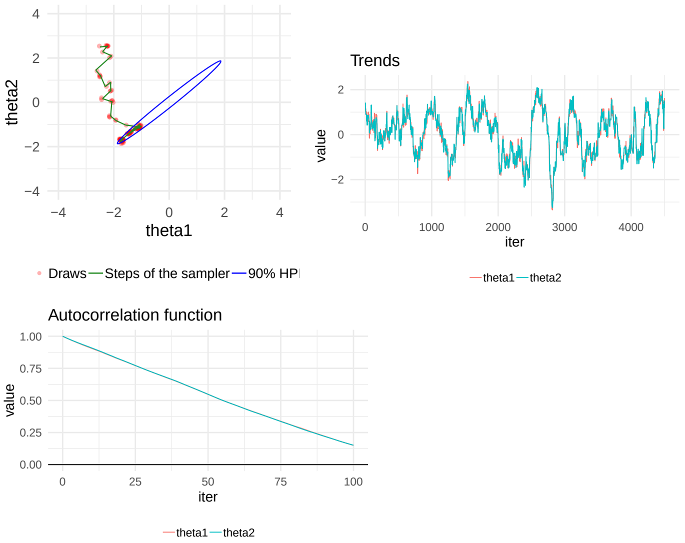

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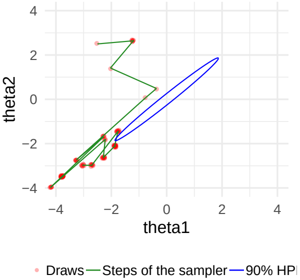

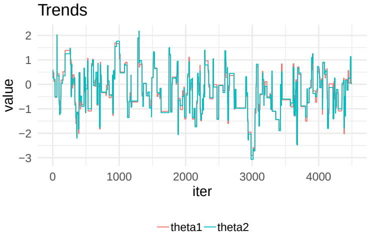

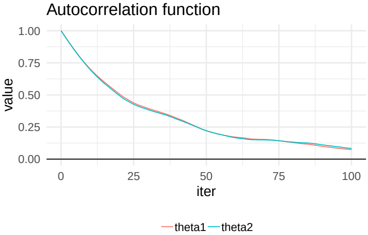

Autocorrelation

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

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

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

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

Estimating τ

- Estimation of τ

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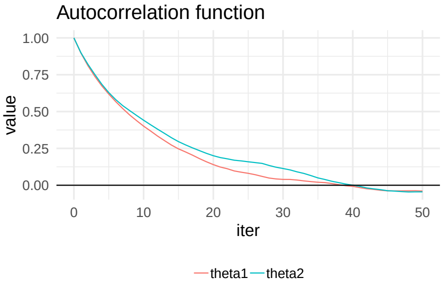
  - let $\Gamma_m = \rho_{2m} + \rho_{2m+1}$, which is sum of two consequent autocorrelations
  - Γ_m is positive, decreasing and convex function of m
- Initial positive sequence estimator (Geyer's IPSE)
  - Choose the largest m so, that all values of the sequence $\hat{\Gamma}_1, \ldots, \hat{\Gamma}_m$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



Effective sample size, S_{eff}

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

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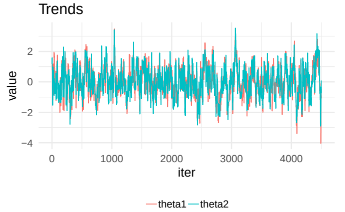
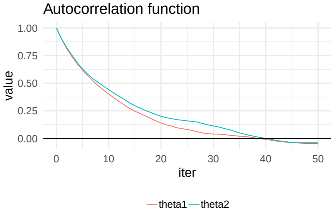
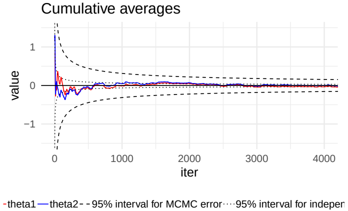






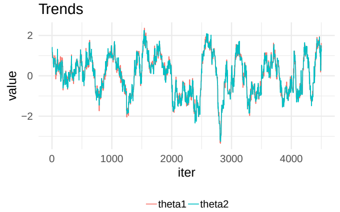
$$\hat{\tau} = 1 + 2\sum_{t=1}^{T} \hat{\rho}_t$$

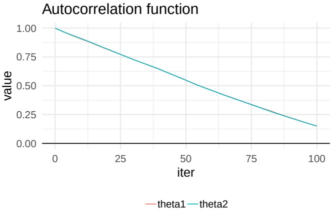
$$\approx 24$$

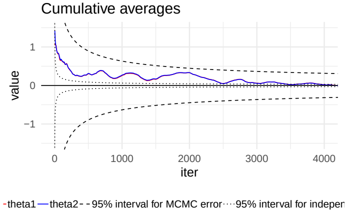
$$\hat{S}_{\text{eff}} = \frac{4500}{24} \approx 188$$

Effective sample size, S_{eff}

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







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

$$\approx 104$$

$$\hat{S}_{\text{eff}} = \frac{4500}{104} \approx 43$$

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- MCMC Diagnostics
  - Warm-up
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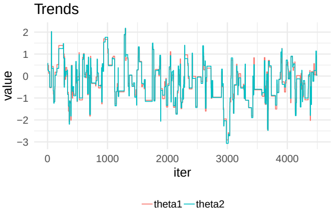
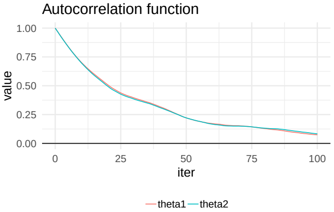
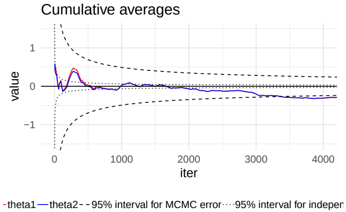
  - S_{eff}, MCSE, and autocorrelation
- Difficult geometries

Effective sample size, S_{eff}

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







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

$$\approx 63$$

$$\hat{S}_{\text{eff}} = \frac{4500}{63} \approx 71$$

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Section 4

Difficult geometries

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Problematic distributions

- Nonlinear dependencies
  - optimal proposal depends on location

demo

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demo

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demo

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demo

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demo

- Non-identifiable models
  - set of connected points is the mode

demo

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