# Chapter 11

- 11.1 Gibbs sampler
- 11.2 Metropolis and Metropolis-Hastings
- 11.3 Using Gibbs and Metropolis as building blocks
- 11.4 Inference and assessing convergence (important)
  - potential scale reduction $\widehat{R}$ (R-hat)
- 11.5 Effective number of simulation draws (important)
  - effective sample size (ESS / $S_{\text{eff}}$)
- 11.6 Example: hierarchical normal model (quick glance)

# Chapter 11 demos

- demo11_1: Gibbs sampling
- demo11_2: Metropolis sampling
- demo11_3: Convergence of Markov chain
- demo11_4: split-$\widehat{R}$ and effective sample size (ESS or $S_{\text{eff}}$)

# It's all about expectations (reminder)

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

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

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- Grid (equal spacing) evaluation with self-normalization

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

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

# Monte Carlo

- Monte Carlo methods we have discussed so far
  - Inverse CDF works for 1D
  - Analytic transformations work for only certain distributions
  - Factorization works only for certain joint distributions
  - Grid evaluation and sampling works in a few dimensions
  - Rejection sampling works mostly in 1D (truncation is a special case)
  - Importance sampling is reliable only in special cases

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  - Importance sampling is reliable only in special cases
- What to do in high dimensions?
  - Markov chain Monte Carlo (Ch 11-12)
  - Laplace, Variational*, EP* (Ch 4,13*)

# Markov chain

- Andrey Markov proved weak law of large numbers and central limit theorem for certain dependent-random sequences, which were later named Markov chains
  - CLT saying the sum / mean converges towards normal if the variance is finite (we come back to this in the end of the course)

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  - Deep learning language models are super big Markov models

# Markov chain

- Example of a simple Markov chain

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

# Markov chain

- Set of random variables $\theta^1, \theta^2, \ldots$, so that with all values of $t$, $\theta^t$ depends only on the previous $\theta^{(t-1)}$

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- Chain has to be initialized with some starting point $\theta^0$
- Transition distribution $T_t(\theta^t \mid \theta^{t-1})$ (may depend on $t$)
  - by choosing a suitable transition distribution, the stationary distribution of Markov chain is $p(\theta \mid y)$

# Gibbs sampling

- Alternate sampling from 1D conditional distributions
  - e.g. normal distribution, sample alternating from
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    - 1D is easy even if no conjugate prior and analytic posterior

# Gibbs sampling

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- demo11_1
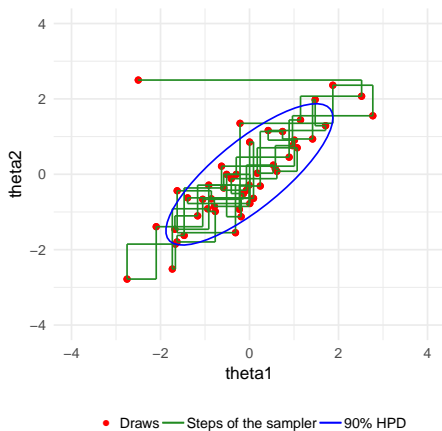


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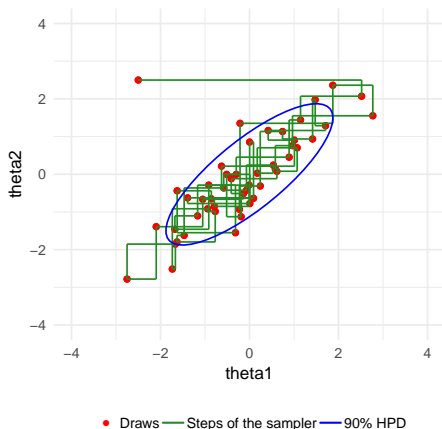
- Basic algorithm

  sample $\theta_j^t$ from $\quad p(\theta_j \mid \theta_{-j}^{t-1}, y)$,

  $\quad\quad$ where $\quad \theta_{-j}^{t-1} = (\theta_1^t, \ldots, \theta_{j-1}^t, \ \theta_{j+1}^{t-1}, \ldots, \theta_d^{t-1})$

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  (cf. proposal distribution in Metropolis algorithm)
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- Several parameters can be updated in blocks (*blocking*)
- Slow if parameters are highly dependent in the posterior
  - demo11_1 continues
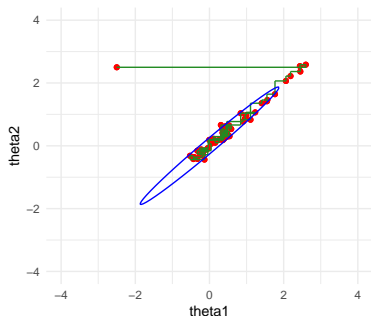


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# Conditional vs joint

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

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

# Metropolis algorithm

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

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

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      $U(0, 1)$
    - $p(\theta^* \mid y)$ and $p(\theta^{t-1} \mid y)$ have the same normalization terms,
      and thus instead of $p(\cdot \mid y)$, unnormalized $q(\cdot \mid y)$ 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

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

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- More examples https://chi-feng.github.io/mcmc-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
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   &= p(\theta_a \mid y)J_t(\theta_a \mid \theta_b),
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     which is the same as the probability of transition from $\theta_a$ to $\theta_b$, since we have required that $J_t(\cdot \mid \cdot)$ is symmetric
   - since their joint distribution is symmetric, $\theta^t$ and $\theta^{t-1}$ have the same marginal distributions, and so $p(\theta \mid y)$ is the stationary distribution of the Markov chain of $\theta$

# Metropolis-Hastings algorithm

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

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

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# Metropolis-Hastings algorithm

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

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- Generic rule for rejection rate is 60-90% (but depends on dimensionality and a specific algorithm variation)

# Gibbs sampling

- 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
  - demo11_2
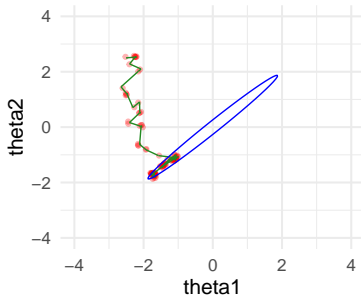


Draws ● Steps of the sampler — 90% HP[     Draws ● Steps of the sampler — 90% HP[
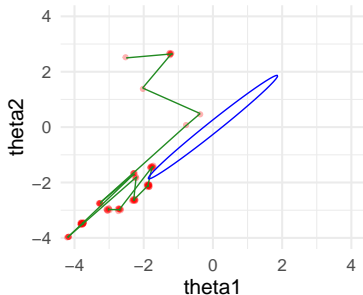
# Dynamic Hamiltonian Monte Carlo and NUTS

- Chapter 12 presents some more advanced methods
  - Chapter 12 includes Hamiltonian Monte Carlo and NUTS, which is one of the most efficient methods
    - uses gradient information
    - Hamiltonian dynamic simulation reduces random walk
    - state-of-the-art MCMC used by most modern probabilistic programming frameworks
- More next week

# HMC / NUTS

Comparison of algorithms on **highly correlated** 250-dimensional Gaussian distribution

- Do **1,000,000** draws with both Random Walk Metropolis and Gibbs, thinning by 1000

- Do **1,000** draws using Stan's NUTS algorithm (no thinning)

- Do 1,000 independent draws (we can do this for multivariate normal)
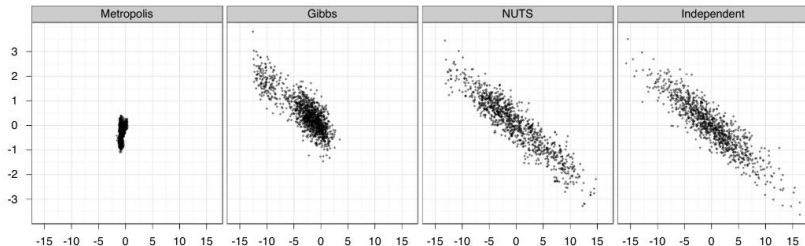


from Hoffman & Gelman (2014)

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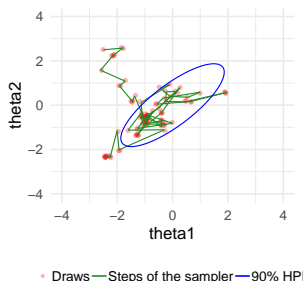
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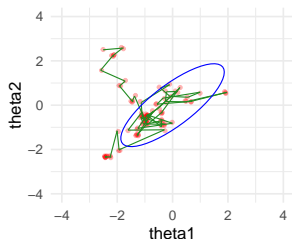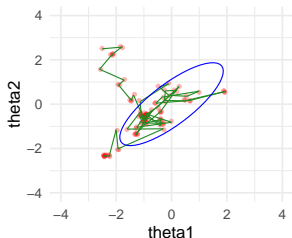


Draws — Steps of the sampler — 90% HPD

- Warm-up = remove draws from the beginning of the chain
  - warm-up may include also phase for adapting algorithm parameters
- Convergence diagnostics
  - Is the sample representative of 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

# Several chains

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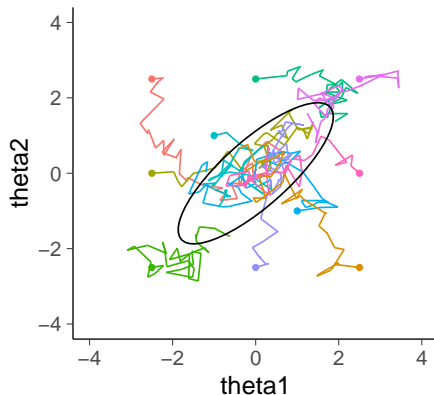


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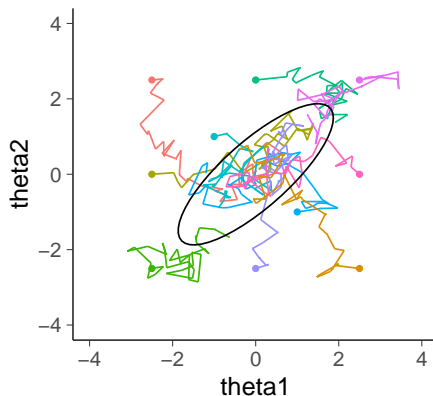


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- Remove draws from the beginning of the chains and run chains long enough so that it is not possible to distinguish where each chain started and the chains are well mixed

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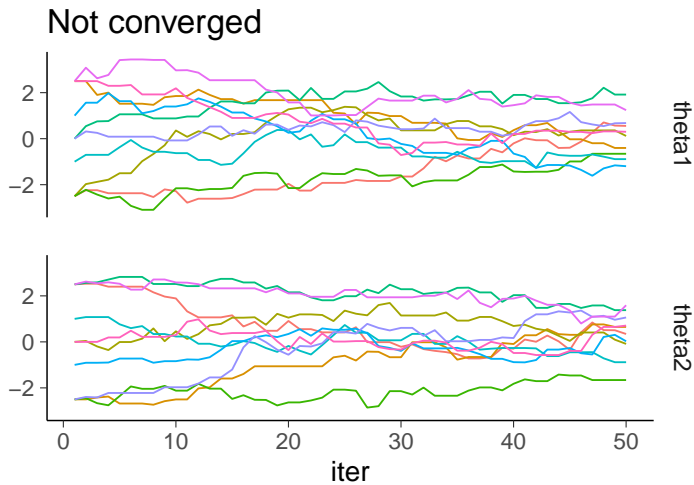
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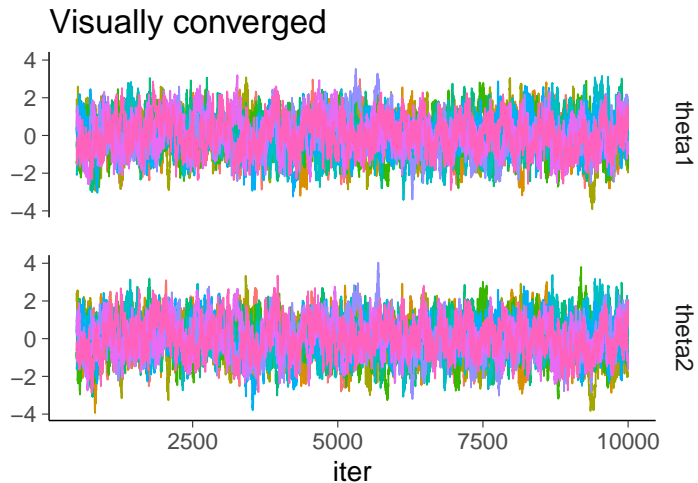
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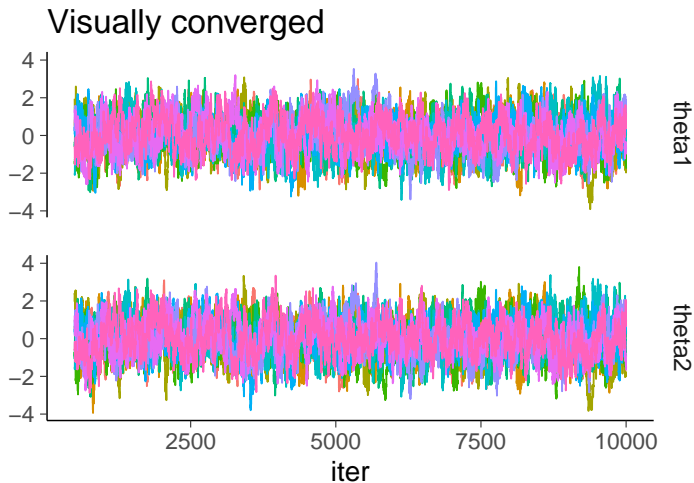


Visual convergence check is not sufficient

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50 warmup, 50 post warmup iterations

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Rhat = 1.64

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- As $\widehat{\mathrm{var}}^+(\theta \mid y)$ overestimates and $W$ underestimates, compute
  $$\widehat{R} = \sqrt{\frac{\widehat{\mathrm{var}}^+}{W}}$$

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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 $\theta_{nm}$ $(n = 1, \ldots, N; m = 1, \ldots, M)$
  - 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

Vehtari, Gelman, Simpson, Carpenter, Bürkner (2020). Rank-normalization, folding, and localization: An improved $\widehat{R}$ for assessing convergence of MCMC. Bayesian Analysis, doi:10.1214/20-BA1221. https://projecteuclid.org/euclid.ba/1593828229.

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# Time series analysis

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

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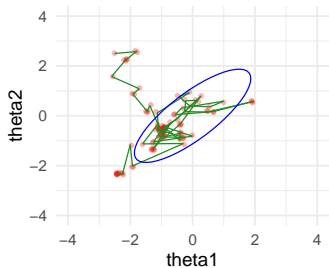


Draws ——Steps of the sampler——90% HPI
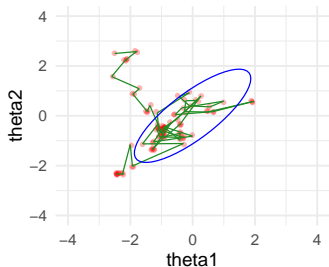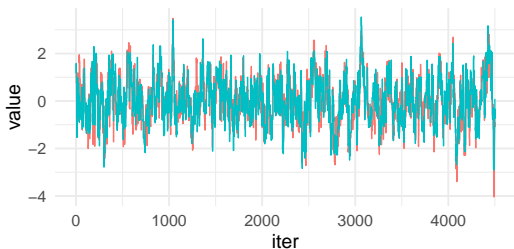
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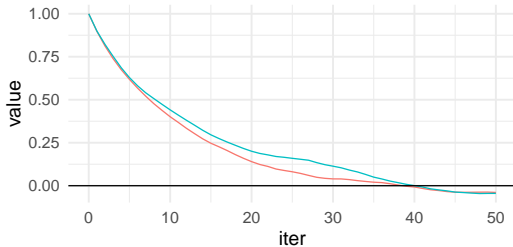
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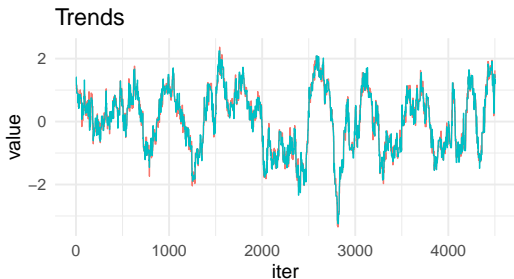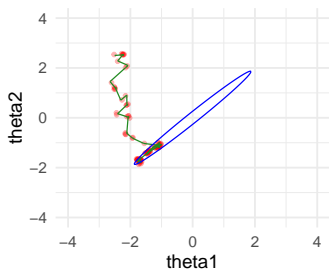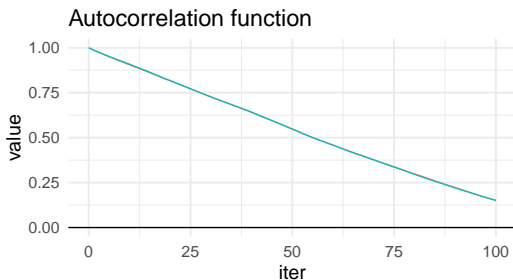
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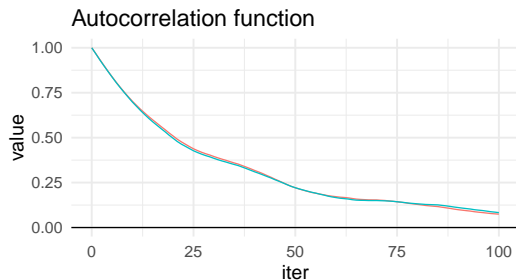
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Autocorrelation function



theta1 — theta2
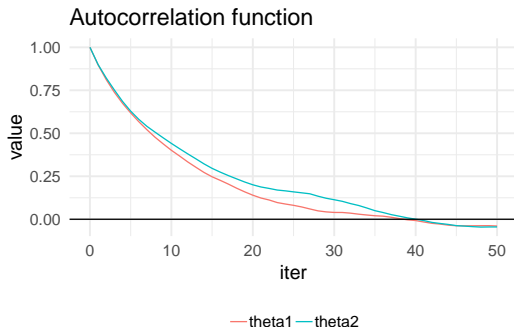
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  - new $\widehat{R}$ paper $S = NM$ (in BDA3 $N = nm$ and $n_{\text{eff}} = N/\tau$)
  - BDA3 focuses on $S_{\text{eff}}$ and not the Monte Carlo error directly new $\widehat{R}$ paper discusses more about MCSEs for different quantities

# 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

# Time series analysis

- Estimation of $\tau$

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

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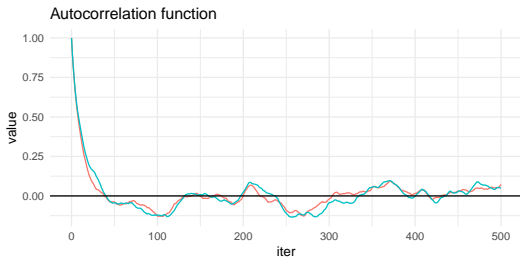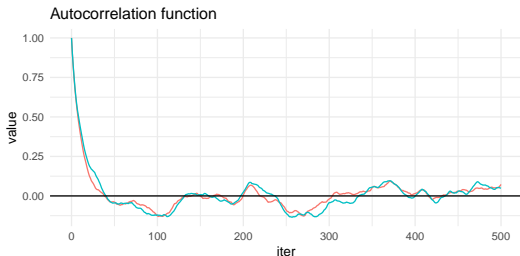
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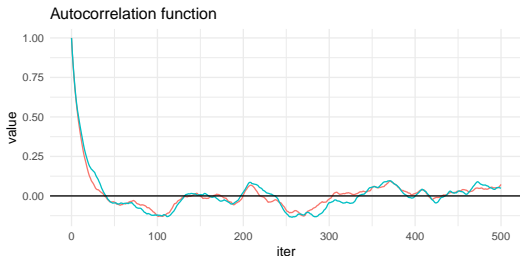
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- noise is larger for longer lags (less observations)
- less noisy estimate is obtained by truncating

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

# Geyer's adaptive window estimator

- Truncation can be decided adaptively
  - for stationary, irreducible, recurrent Markov chain
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- 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



Autocorrelation function
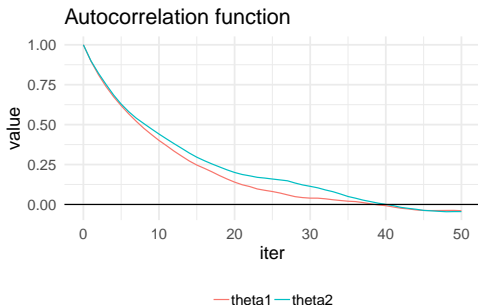
theta1 — theta2

# Effective sample size

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

# Effective sample size

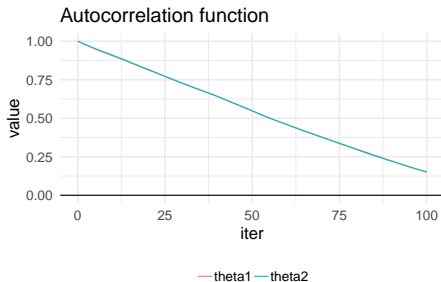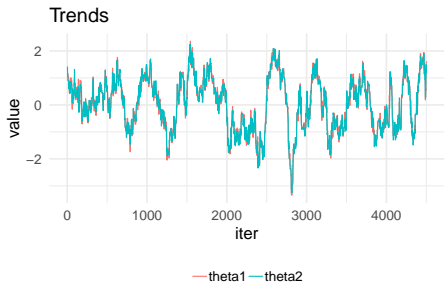Effective sample size ESS $= S_{\text{eff}} \approx S/\hat{\tau}$



Trends

Autocorrelation function

—theta1 —theta2

—theta1 —theta2

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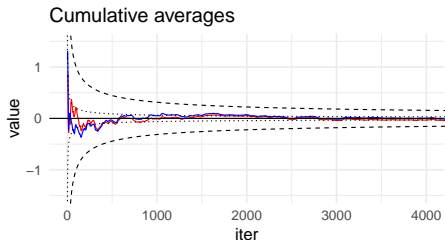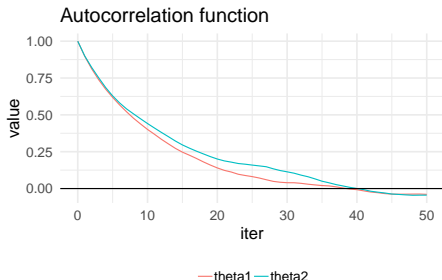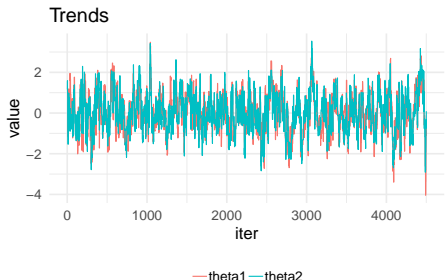
$$\hat{\tau} = 1 + 2 \sum_{t=1}^{T} \hat{\rho}_t$$

$$\approx 24$$

-theta1 —theta2 - -95% interval for MCMC error ⋯⋯95% interval for indeper

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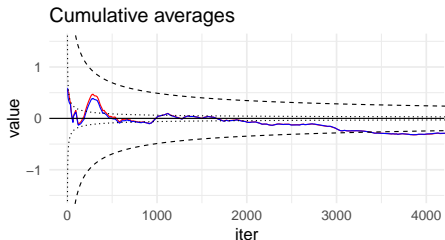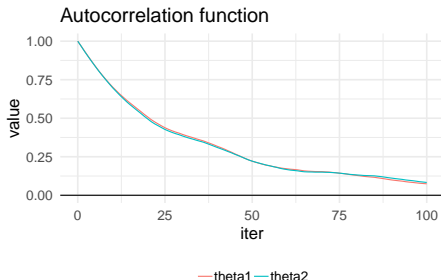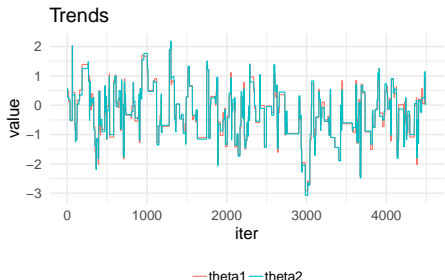
Effective sample size ESS $= S_{\text{eff}} \approx S/\hat{\tau}$
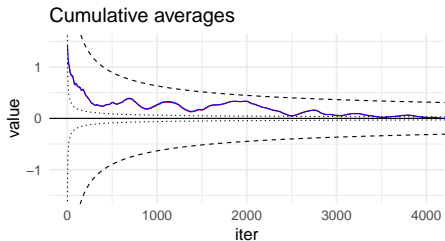


$$\hat{\tau} = 1 + 2\sum_{t=1}^{T} \hat{\rho}_t$$

$$\approx 104$$

# Effective sample size

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


Trends


Autocorrelation function

— theta1 — theta2

— theta1 — theta2


Cumulative averages

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

$$\approx 63$$

--theta1 —theta2 - - 95% interval for MCMC error····95% interval for indeper

# Problematic distributions

- Nonlinear dependencies
  - optimal proposal depends on location

# Problematic distributions

- Nonlinear dependencies
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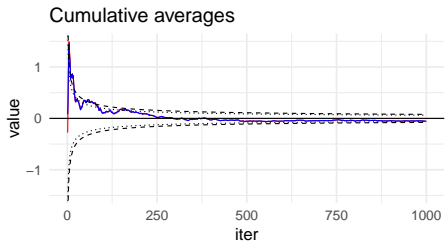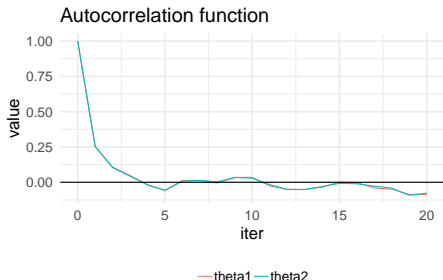
# Problematic distributions

- Nonlinear dependencies
  - optimal proposal depends on location
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- Multimodal
  - difficult to move from one mode to another
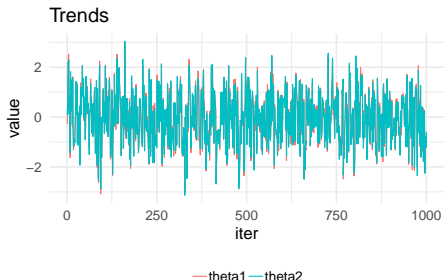
# Problematic distributions

- 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

# Next week: HMC, NUTS, and dynamic HMC

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



Trends

Autocorrelation function

— theta1 — theta2

— theta1 — theta2

Cumulative averages

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

$$\approx 1.6$$

- theta1 —theta2 - - 95% interval for MCMC error ···· 95% interval for indeper

# Further diagnostics

- Dynamic HMC/NUTS has additional diagnostics
  - divergences
  - tree depth exceedences
  - fraction of missing information