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- This lecture introduces also necessary diagnostics to check whether MCMC results are useful

# 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- $\hat{R}$  and effective sample size (ESS or  $S_{\text{eff}}$ )
- demo11\_5: Diagnostics with posterior and bayesplot packages

## It's all about expectations (reminder)

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

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

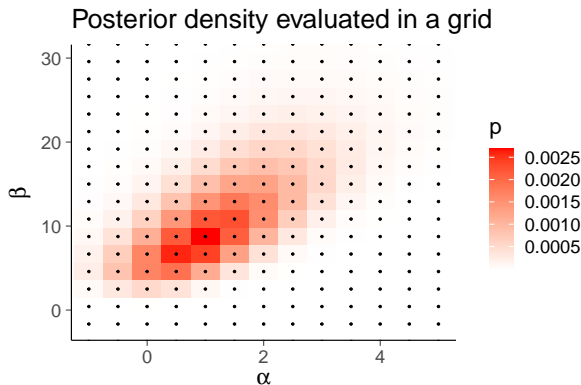
$$E_{p(\theta|y)}[f(\theta)] \approx \frac{1}{S} \sum_{s=1}^S f(\theta^{(s)})$$

# Monte Carlo

- Monte Carlo methods we have discussed so far
  - Inverse CDF works for 1D
  - 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)
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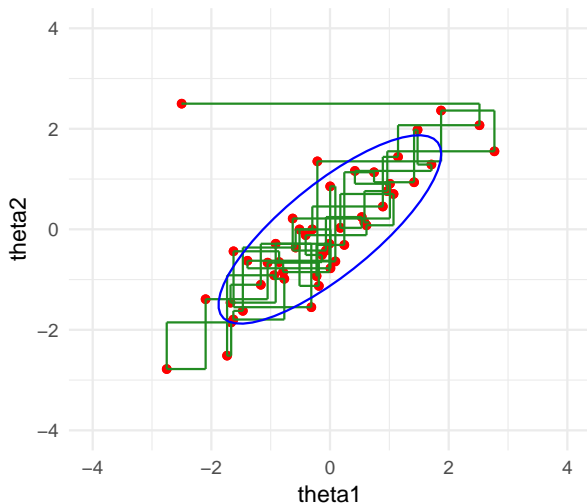


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- What to do in high dimensions?
  - Markov chain Monte Carlo (Ch 11-12)
  - Laplace, Variational\*, EP\* (Ch 4,13\*)

# Markov chain Monte Carlo (MCMC)

- Automatically focuses density evaluations where most of the posterior mass is



# 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



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  - Markov's model was a very small language model

## Markov chain and language models (off-topic)

- Deep learning language models are super big Markov models
- Brian Hayes (1983, *A progress report on the fine art of turning literature into drive!*), experimented with 0–8th order Markov chains for producing text. For example, using William Faulkner's story "Two Soldiers" to compute 8th order transition probabilities and then randomly generate text:

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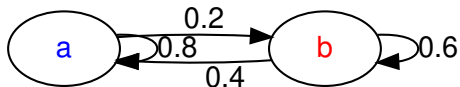
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- In Markov chain Monte Carlo we are not interested in the sequences directly, but how likely each state is in a long sequence

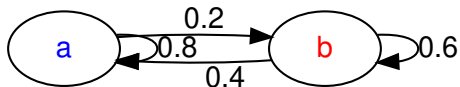
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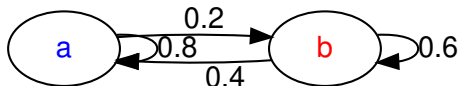


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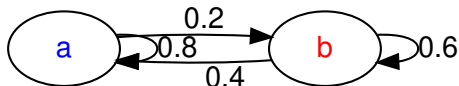


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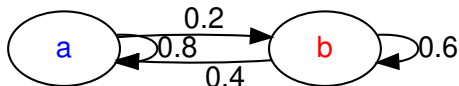
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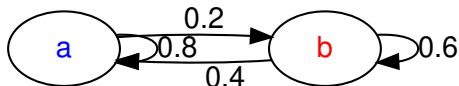
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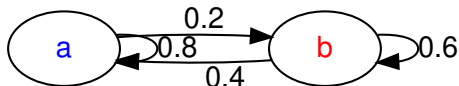
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$$A = \begin{pmatrix} 0.8 & 0.2 \\ 0.4 & 0.6 \end{pmatrix}$$

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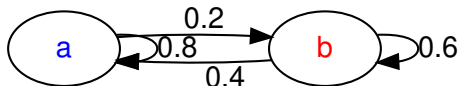
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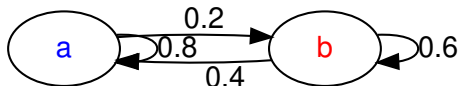
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- From  $A^S$  we get  $p(\text{a}) = 0.67$  and  $p(\text{b}) = 0.33$

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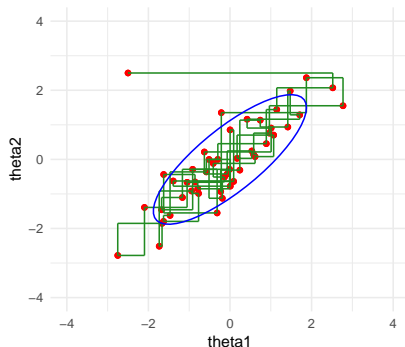
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    - draws are dependent
    - construction of efficient Markov chains is not always easy

# Markov chain

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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  $p(\theta \mid y)$



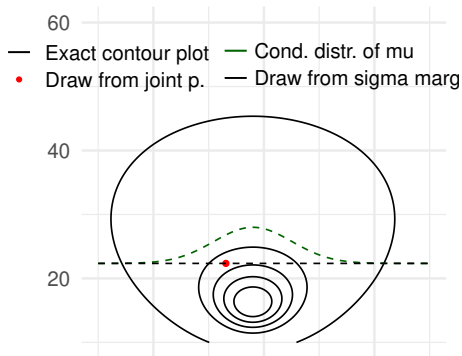
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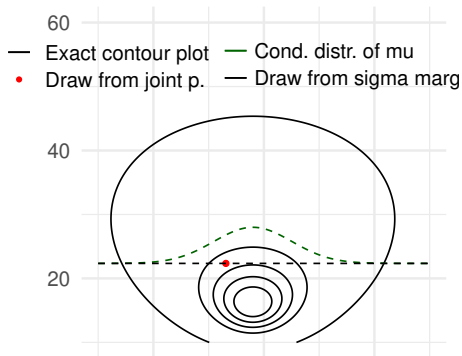
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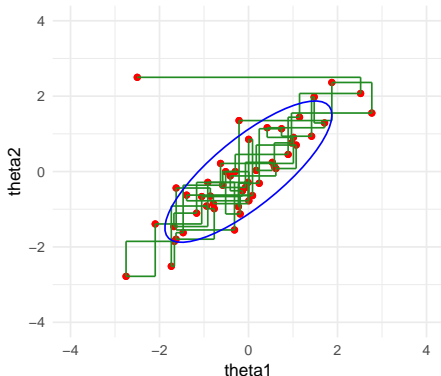
## Joint posterior



- 1D is easy even if no conjugate prior and analytic posterior

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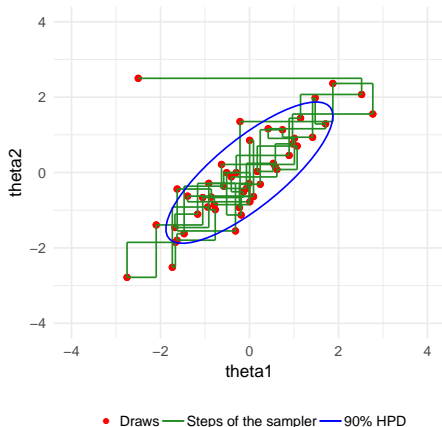
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- demo11\_1



• Draws — Steps of the sampler — 90% HPD

# Gibbs sampling

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- Basic algorithm

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

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

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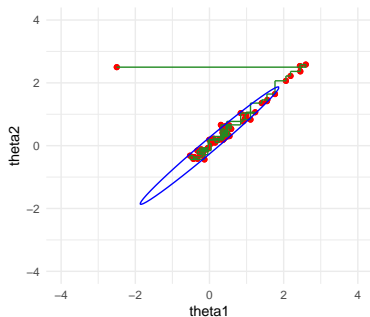


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- Several parameters can be updated in blocks (*blocking*)
- Slow if parameters are highly dependent in the posterior
  - demo11\_1 continues



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- 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.  $t = 1, 2, \dots$

- (a) pick a proposal  $\theta^*$  from the proposal distribution  $J_t(\theta^* \mid \theta^{t-1})$ .  
Proposal distribution has to be symmetric, i.e.

$$J_t(\theta_a \mid \theta_b) = J_t(\theta_b \mid \theta_a), \text{ for all } \theta_a, \theta_b$$

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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  $r$



# Metropolis algorithm

- Algorithm

1. starting point  $\theta^0$

2.  $t = 1, 2, \dots$

- (a) pick a proposal  $\theta^*$  from the proposal distribution  $J_t(\theta^* | \theta^{t-1})$ .  
Proposal distribution has to be symmetric, i.e.

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ie, the new state is the same as previous
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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

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

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- More examples <https://chi-feng.github.io/mcmc-demo/>

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- Theoretically
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  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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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,  $\theta^{t-1}$  and  $\theta^t$  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

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

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

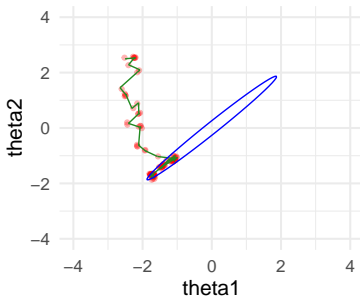
# Gibbs sampling

- Specific case of Metropolis-Hastings algorithm
  - single updated (or blocked)
  - proposal distribution is the conditional distribution
    - proposal and target distributions are same
    - acceptance probability is 1

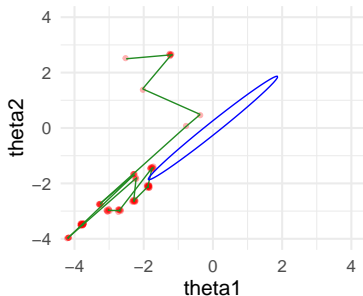


# Metropolis

- Usually doesn't scale well to high dimensions
  - if the shape doesn't match the whole distribution, the efficiency drops
  - demo11\_2



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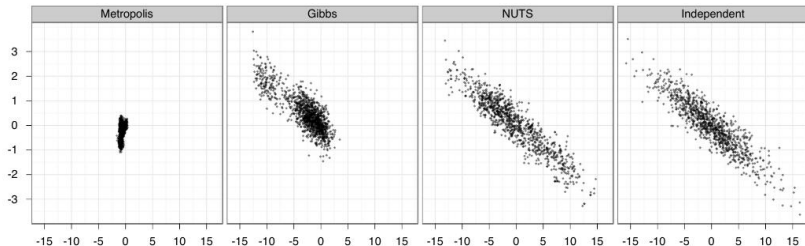
# Dynamic Hamiltonian Monte Carlo and NUTS

- 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)

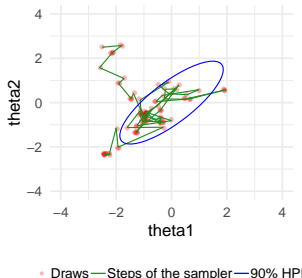


## Warm-up and convergence diagnostics

- Asymptotically chain spends the  $\alpha\%$  of time where  $\alpha\%$  posterior mass is

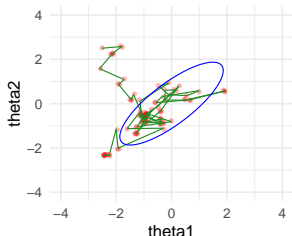
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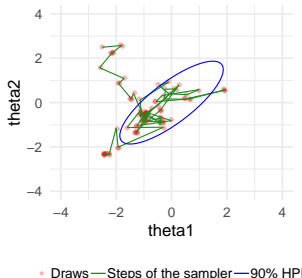


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  - warm-up may include also phase for adapting algorithm parameters
- Convergence diagnostics
  - Is the sample representative of the target distribution?

# MCMC draws are dependent

- Monte Carlo estimates still valid  
(central limit theorem holds as proved by Andrey Markov)

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

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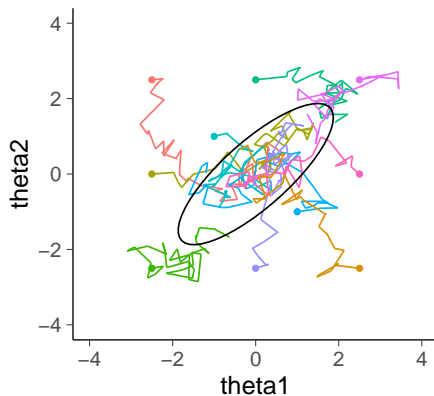
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  - evaluation of *effective* sample size (ESS)
  - given finite variance, the distribution of the expectation approaches normal distribution with variance  $\sigma_\theta^2/\text{ESS}$

## Several chains

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

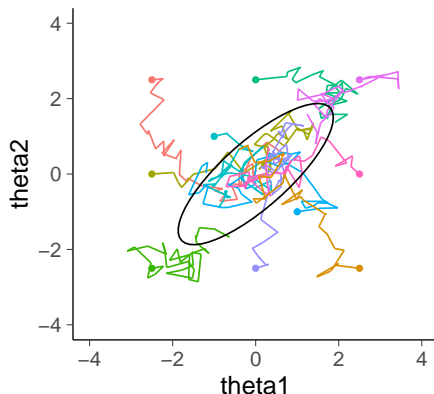
No convergence



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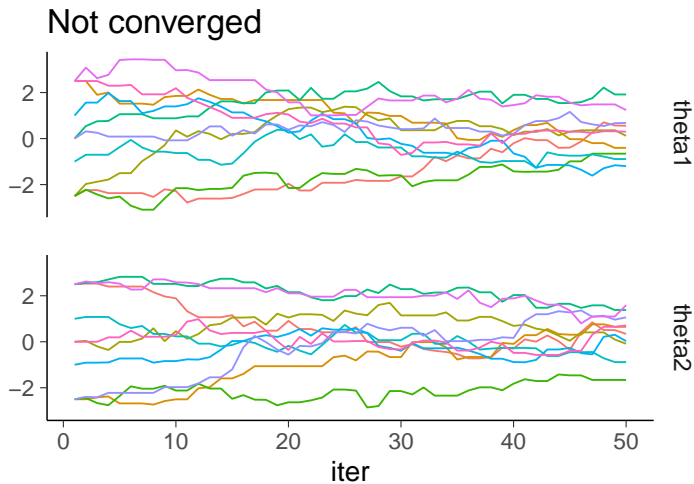
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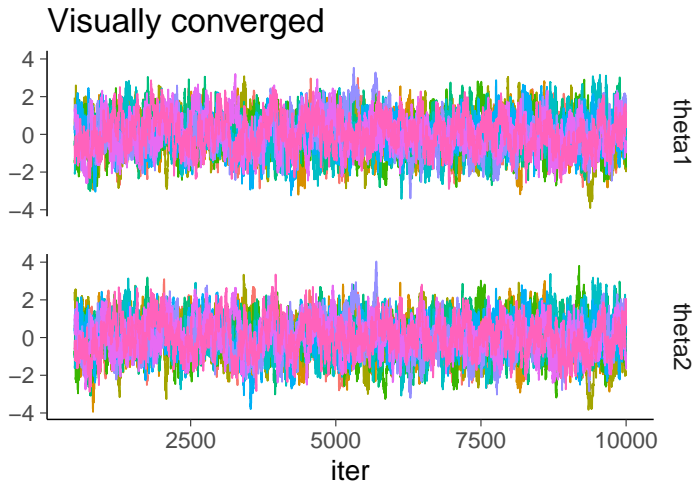


- Remove draws from the beginning of the chains and run chains long enough so that it is not possible to distinguish where each chain started and the chains are well mixed

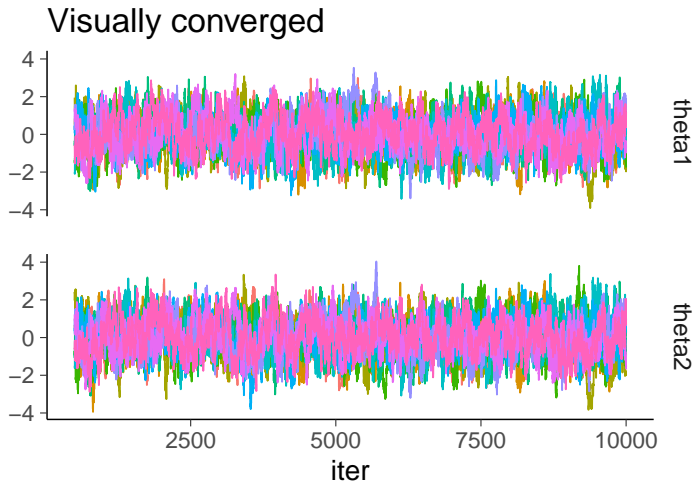
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Visual convergence check is not sufficient

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

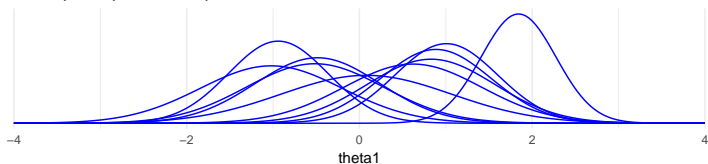
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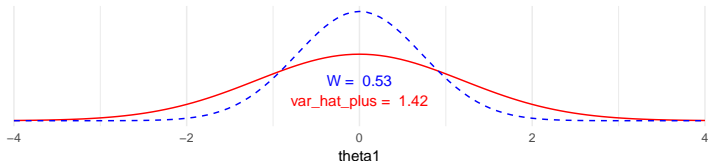
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 $\text{var\_hat\_plus}$  = total variance estimate

50 warmup, 50 post warmup iterations



Rhat = 1.64



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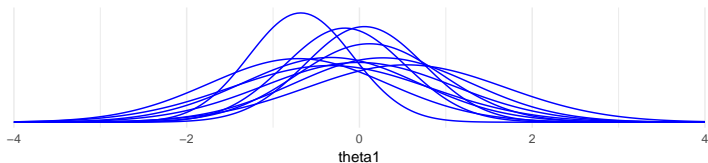
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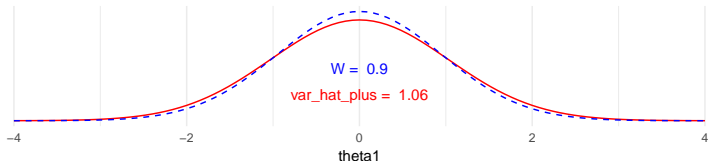
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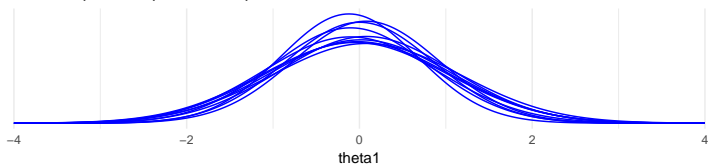
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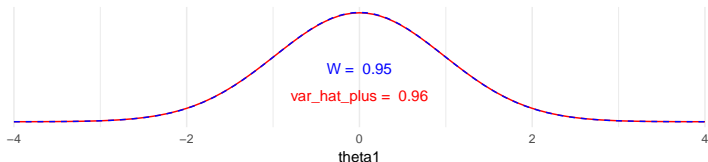
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$\hat{R}$

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- this **overestimates** marginal posterior variance if the starting points are overdispersed
- Given finite  $N$ ,  $W$  **underestimates** marginal posterior variance
  - single chains have not yet visited all points in the distribution
  - when  $N \rightarrow \infty$ ,  $E(W) \rightarrow \text{var}(\theta \mid y)$

- Estimate total variance  $\text{var}(\theta \mid y)$  as a weighted mean of  $W$  and  $B$

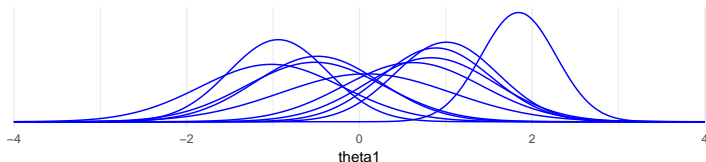
$$\widehat{\text{var}}^+(\theta \mid y) = \frac{N-1}{N} W + \frac{1}{N} B$$

- this **overestimates** marginal posterior variance if the starting points are overdispersed
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  - single chains have not yet visited all points in the distribution
  - when  $N \rightarrow \infty$ ,  $E(W) \rightarrow \text{var}(\theta \mid y)$
- As  $\widehat{\text{var}}^+(\theta \mid y)$  overestimates and  $W$  underestimates, compute

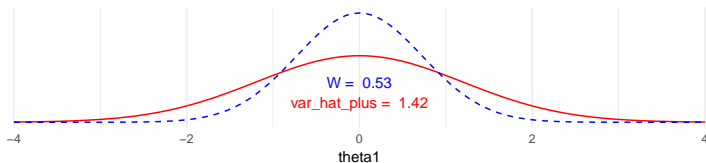
$$\hat{R} = \sqrt{\frac{\widehat{\text{var}}^+}{W}}$$

- BDA3:  $\hat{R}$  aka *potential scale reduction factor* (PSRF)
- Compare means and variances of the chains  
W = within chain variance estimate  
var\_hat\_plus = total variance estimate

50 warmup, 50 post warmup iterations

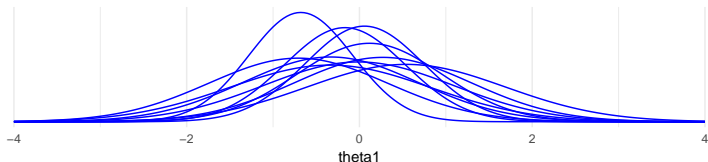


Rhat = 1.64

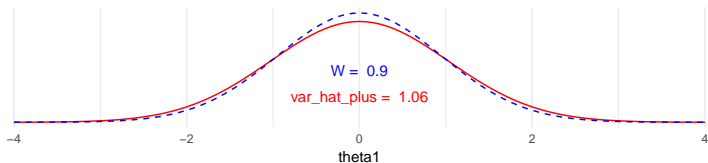


- BDA3:  $\hat{R}$  aka *potential scale reduction factor* (PSRF)
- Compare means and variances of the chains  
W = within chain variance estimate  
var\_hat\_plus = total variance estimate

500 warmup, 500 post warmup iterations

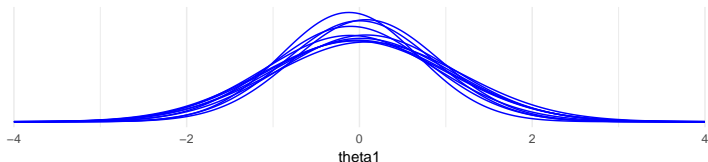


Rhat = 1.08

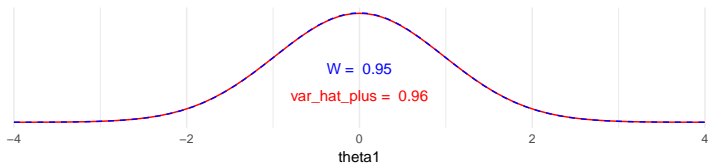


- BDA3:  $\hat{R}$  aka *potential scale reduction factor* (PSRF)
- Compare means and variances of the chains  
W = within chain variance estimate  
var\_hat\_plus = total variance estimate

5000 warmup, 5000 post warmup iterations



Rhat = 1



$\widehat{R}$ 

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

- Estimates how much the scale of  $\psi$  could reduce if  $N \rightarrow \infty$
- $\widehat{R} \rightarrow 1$ , when  $N \rightarrow \infty$
- if  $\widehat{R}$  is big (e.g.,  $R > 1.01$ ), keep sampling

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- $\widehat{R} \rightarrow 1$ , when  $N \rightarrow \infty$
- 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



## Split- $\hat{R}$

- BDA3: split- $\hat{R}$
- 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  $\theta_{nm}$  ( $n = 1, \dots, N; m = 1, \dots, M$ )
  - compare means and variances of the split chains

# Rank normalized $\hat{R}$

- Original  $\hat{R}$  requires that the target distribution has finite mean and variance

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

# Rank normalized $\hat{R}$

- Original  $\hat{R}$  requires that the target distribution has finite mean and variance
- Rank normalization fixes this, is also more robust given finite but high variance, and is more sensitive to differences in variance
  - inverse normal-cdf of ranks
  - inverse normal-cdf of ranks of absolute difference from median

Vehtari, Gelman, Simpson, Carpenter, Bürkner (2020). Rank-normalization, folding, and localization: An improved  $\hat{R}$  for assessing convergence of MCMC. Bayesian Analysis, doi:10.1214/20-BA1221.  
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- Notation updated compared to BDA3

Vehtari, Gelman, Simpson, Carpenter, Bürkner (2020). Rank-normalization, folding, and localization: An improved  $\hat{R}$  for assessing convergence of MCMC. Bayesian Analysis, doi:10.1214/20-BA1221.  
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## $\hat{R}$ and rank normalized $\hat{R}$ in posterior package

`rhat_basic()` without rank normalization

`rhat()` with rank normalization

## $\hat{R}$ and rank normalized $\hat{R}$ in posterior package

rhat\_basic() without rank normalization

rhat() with rank normalization

```
x <- array(data=c(rnorm(1000,mean=-3),  
                  rnorm(1000,mean=3)),  
           dim=c(1000, 2, 1))  
x <- as_draws_matrix(x)  
variables(x) <- "N_2"
```

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                  rnorm(1000,mean=3)),
           dim=c(1000, 2, 1))
x <- as_draws_matrix(x)
variables(x) <- "N_2"

x |>
  summarise_draws(mean, sd, mcse_mean, rhat_basic, rhat)
  variable    mean    sd mcse_mean rhat_basic  rhat
  N_2         0.0122  3.18      2.15      3.61  1.83
```



## $\hat{R}$ and rank normalized $\hat{R}$ in posterior package

rhat\_basic() without rank normalization

rhat() with rank normalization

```
x <- array(data=c(rt(1000,df=1)-6,  
                  rt(1000,df=1)+6),  
           dim=c(1000, 2, 1))  
x <- as_draws_matrix(x)  
variables(x) <- "t1_2"
```

## $\hat{R}$ and rank normalized $\hat{R}$ in posterior package

rhat\_basic() without rank normalization

rhat() with rank normalization

```
x <- array(data=c(rt(1000,df=1)-6,  
                  rt(1000,df=1)+6),  
           dim=c(1000, 2, 1))
```

```
x <- as_draws_matrix(x)
```

```
variables(x) <- "t1_2"
```

```
x |>
```

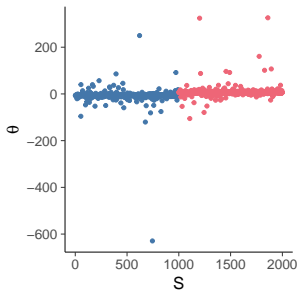
```
  summarise_draws(mean, sd, mcse_mean, pareto_khat,  
                  rhat_basic, rhat)
```

variable	mean	sd	mcse_mean	pareto_khat	rhat_basic	rhat
t1_2	-1.11	42.1	1.23	1.07	1.01	1.47

# Rank normalized $\hat{R}$

For example:

Cauchy mixture

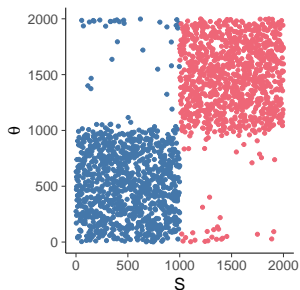
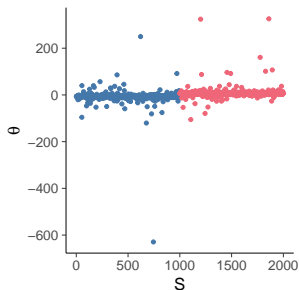


# Rank normalized $\hat{R}$

For example:

Cauchy mixture

→ ranks



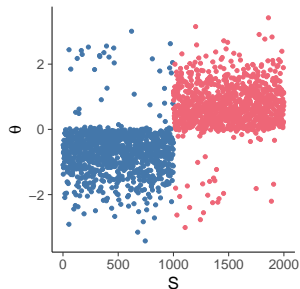
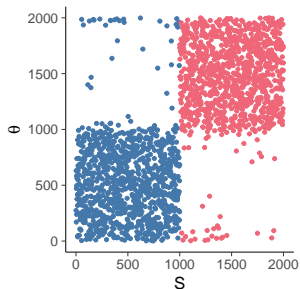
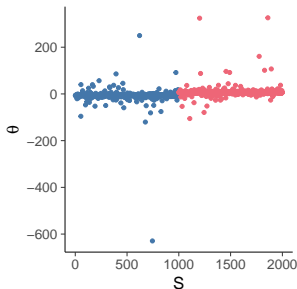
# Rank normalized $\hat{R}$

For example:

Cauchy mixture

→ ranks

→ inverse cdf



## $\hat{R}$ and rank normalized $\hat{R}$ in posterior package

rhat\_basic() without rank normalization

rhat() with **folding** and rank normalization

```
x <- array(data=c(normal(1000),  
                  normal(1000)*2),  
           dim=c(1000, 2, 1))  
x <- as_draws_matrix(x)  
variables(x) <- "N2v"
```

## $\hat{R}$ and rank normalized $\hat{R}$ in posterior package

rhat\_basic() without rank normalization

rhat() with **folding** and rank normalization

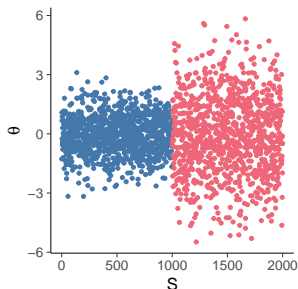
```
x <- array(data=c(normal(1000),
                    normal(1000)*2),
            dim=c(1000, 2, 1))
x <- as_draws_matrix(x)
variables(x) <- "N2v"

x |>
  summarise_draws(mean, sd, mcse_mean,
                  rhat_basic, rhat)
  variable  mean    sd mcse_mean rhat_basic  rhat
  N2v      -0.05   1.6    0.03      1.00   1.09
```

# Rank normalized $\hat{R}$ with folding

For example:

Normal variance mixture

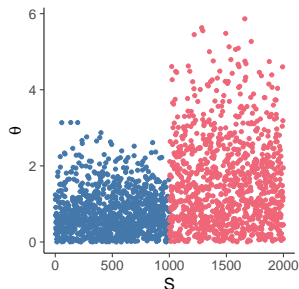
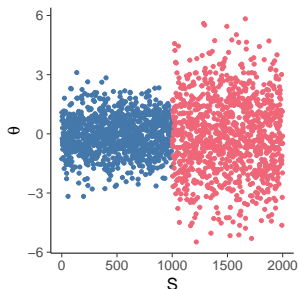




# Rank normalized $\hat{R}$ with folding

For example:

Normal variance mixture  $\rightarrow$  folded

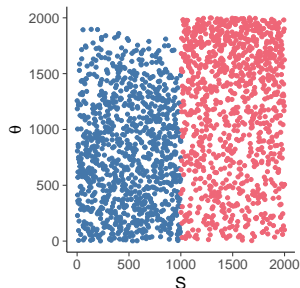
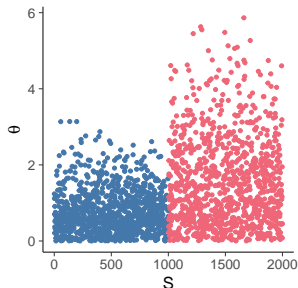
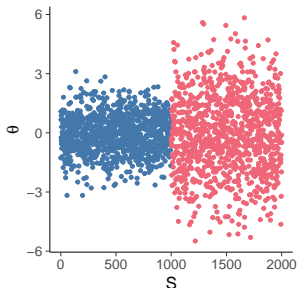


# Rank normalized $\hat{R}$ with folding

For example:

Normal variance mixture  $\rightarrow$  folded

$\rightarrow$  ranks

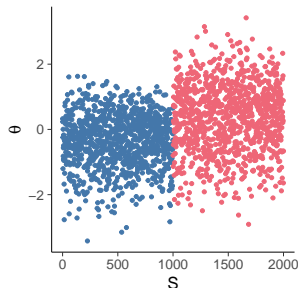
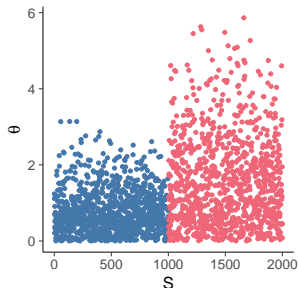
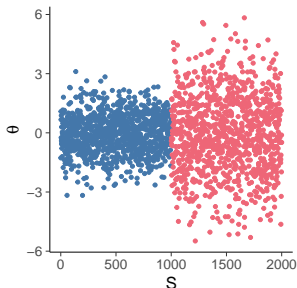


# Rank normalized $\hat{R}$ with folding

For example:

Normal variance mixture  $\rightarrow$  folded

$\rightarrow$  inverse cdf

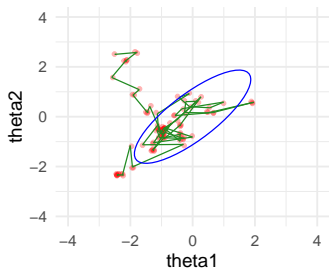


# Time series analysis

- Autocorrelation function
  - describes the correlation given a certain lag
  - can be used to compare efficiency of MCMC algorithms and parameterizations
  - For real valued, the correlation at lag  $n$

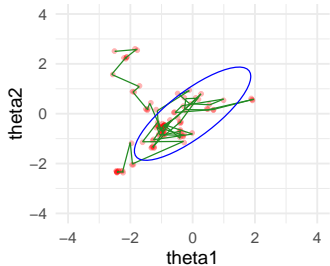
$$\frac{E [(X_{t+n} - E[X])(X_t - E[X])]}{\text{Var} [X]}$$

# Autocorrelation



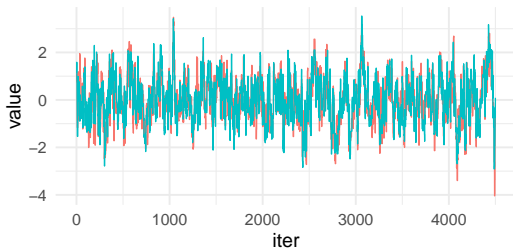
• Draws — Steps of the sampler — 90% HPI

# Autocorrelation



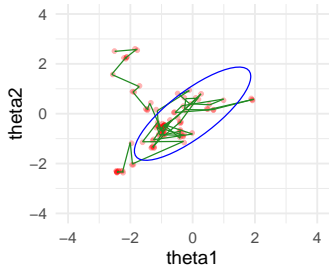
• Draws — Steps of the sampler — 90% HPD

## Trends



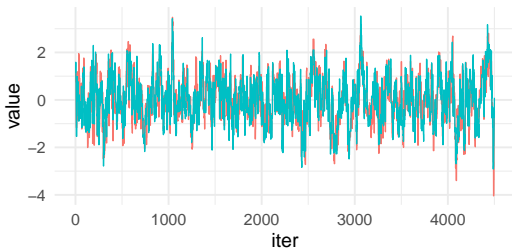
—  $\theta_1$  —  $\theta_2$

# Autocorrelation



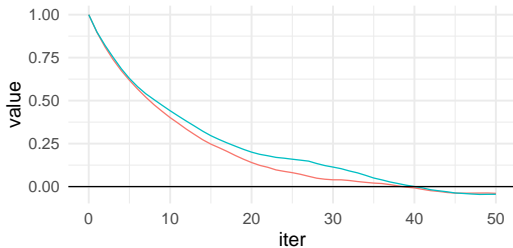
• Draws — Steps of the sampler — 90% HPD

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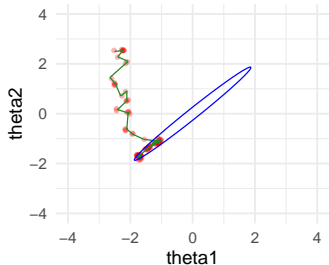


—  $\theta_1$  —  $\theta_2$

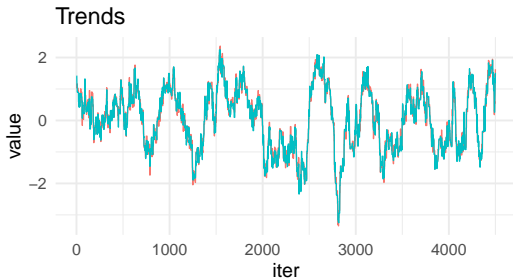
## Autocorrelation function



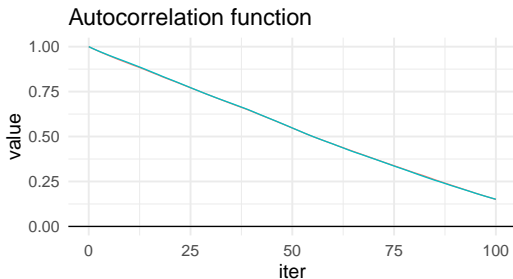
# Autocorrelation (slow mixing due to small step size)



• Draws — Steps of the sampler — 90% HPI

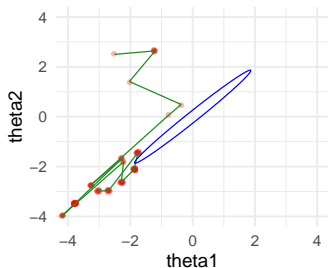


—  $\theta_1$  —  $\theta_2$

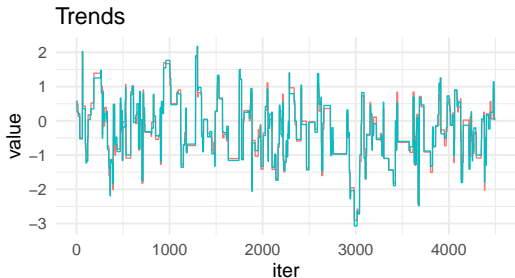




# Autocorrelation (slow mixing due to many rejections)

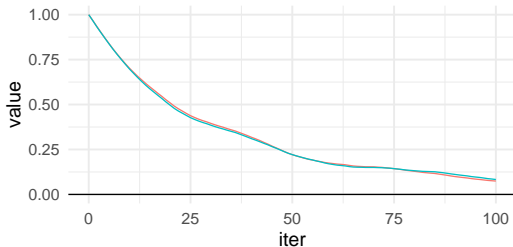


• Draws — Steps of the sampler — 90% HPI



—  $\theta_1$  —  $\theta_2$

## Autocorrelation function



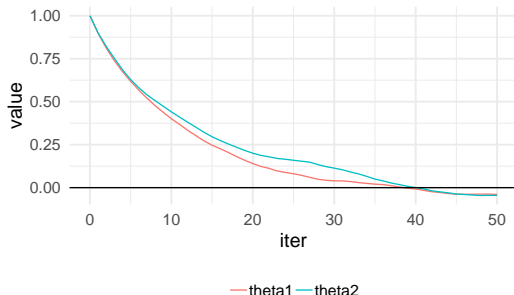
# Time series analysis

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

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

where  $S_{\text{eff}} = S/\tau$  (=ESS),  
and  $\tau$  is sum of autocorrelations

Autocorrelation function



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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

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

where  $\hat{\rho}_{n,m}$  is autocorrelation at lag  $n$  for chain  $m$ ,  
and  $\textcolor{blue}{W}$  and  $\widehat{\textcolor{red}{var}}^+$  are the same as in  $\widehat{R}$  (without rank normalization)

# Time series analysis

- Estimation of the autocorrelation using several chains

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

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  - takes into account if the chains are not mixing (the chains have not converged)

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  - takes into account if the chains are not mixing (the chains have not converged)
- 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

# Time series analysis

- Estimation of  $\tau$

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

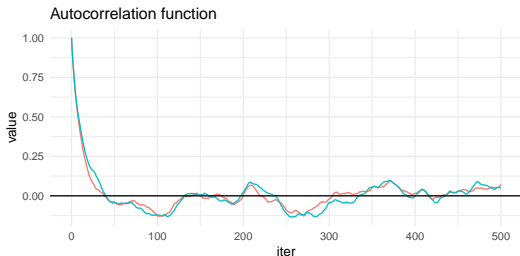
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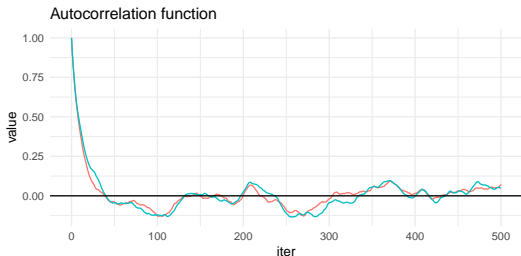
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- Estimation of  $\tau$

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



- empirical autocorrelation function is noisy and thus estimate of  $\tau$  is noisy
- noise is larger for longer lags (less observations)
- less noisy estimate is obtained by truncating

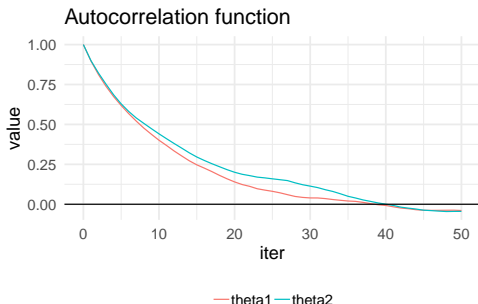
$$\hat{\tau} = 1 + 2 \sum_{t=1}^T \hat{\rho}_t$$

# Geyer's adaptive window estimator

- Truncation can be decided adaptively
  - for stationary, irreducible, recurrent Markov chain
  - let  $\Gamma_m = \rho_{2m} + \rho_{2m+1}$ , which is sum of two consequent autocorrelations
  - $\Gamma_m$  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
  - $\Gamma_m$  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  $\hat{\Gamma}_1, \dots, \hat{\Gamma}_m$  are positive



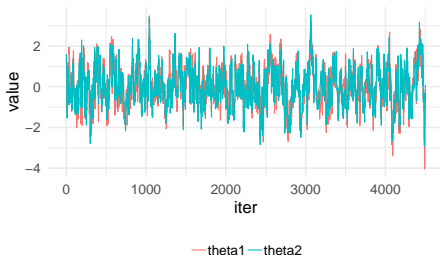
## Effective sample size

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

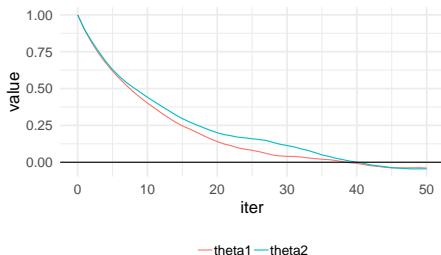
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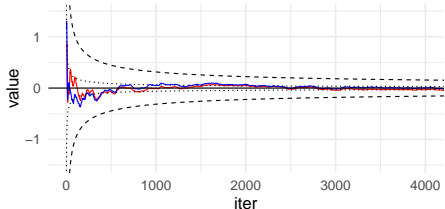
Trends



Autocorrelation function



Cumulative averages



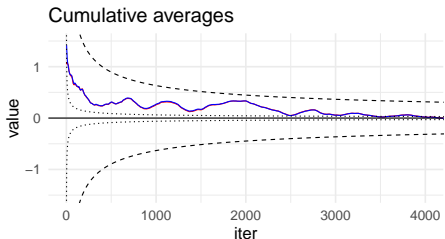
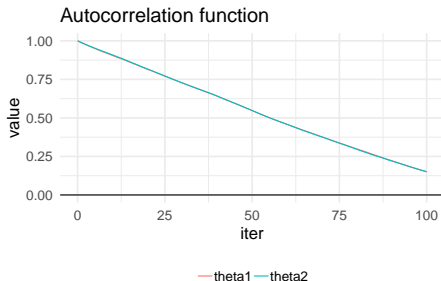
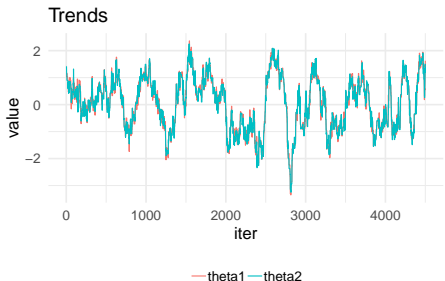
$$\hat{\tau} = 1 + 2 \sum_{t=1}^T \hat{\rho}_t$$

$$\approx 24$$



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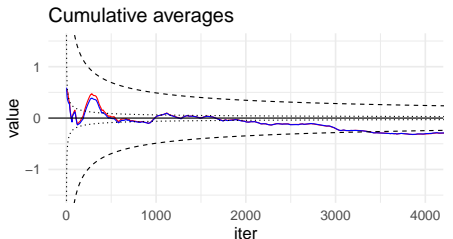
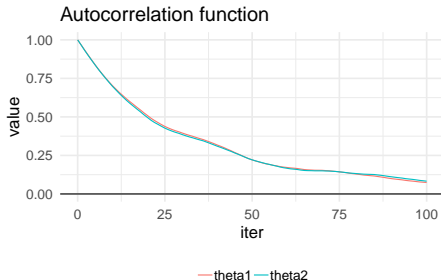
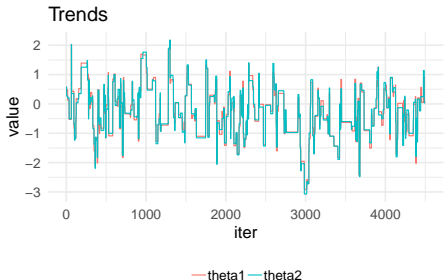


$$\hat{\tau} = 1 + 2 \sum_{t=1}^T \hat{\rho}_t$$

$$\approx 104$$

# Effective sample size

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



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

$$\approx 63$$

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

## Monte Carlo standard error (MCSE)

- MCSE is obtained as discussed in lecture 4, but replacing the sample size  $S$  with the effective sample size ESS.
- See Digits case study for how many iterations to run and how many digits to report  
<https://avehtari.github.io/casestudies/Digits/digits.html>

# ESS and MCSE in posterior package

Simulated 4 chains with AR(0.3) process

```
drt |> summarise_draws(mean, sd, pareto_khat,  
                        ess_mean, mcse_mean)
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variable	mean	sd	pareto_khat	ess_mean	mcse_mean
xn	0.01	0.99	-0.07	2280.	0.02
xt3	0.02	1.6	0.33	2452.	0.03
xt2	0.05	2.9	0.52	2903.	0.05
xt1	0.33	93.	1.0	3976.	1.5

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/variable	mean	pareto_khat	ess_mean	mcse_mean	ess_q95	mcse_q95
xn	0.01	-0.07	2280.	0.02	3251.	0.04
xt3	0.02	0.33	2452.	0.03	3251.	0.09
xt2	0.05	0.52	2903.	0.05	3251.	0.13
xt1	0.33	1.0	3976.	1.5	3251.	0.49

# Bulk-ESS and Tail-ESS in posterior package

- ESS depends on the quantity
- For quick diagnostic purposes the default summary shows
  - median and median absolute deviation (mad), which are valid in case of infinite mean and variance, too
  - if mad is much smaller than sd, suspect infinite variance
  - Rank-normalized  $\hat{R}$  rhat
  - Bulk-ESS (ess\_bulk) is generic ESS for sampling efficiency in bulk using rank normalized values (works for infinite variance)
  - Tail-ESS (ess\_tail) is the minimum ESS for 5%- and 95%-quantiles

```
drt |> summarise_draws()
```

variable	mean	median	sd	mad	q5	q95	rhat	ess_bulk	ess_tail
xn	0.01	0.00	0.99	0.99	-1.6	1.6	1.00	2284.	3189.
xt3	0.02	0.00	1.6	1.1	-2.3	2.3	1.00	2284.	3189.
xt2	0.05	0.00	2.9	1.2	-2.8	2.9	1.00	2284.	3189.
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# ESS and MCSE

- ESS and MCSE depend on the quantity
  - Bulk-ESS and Tail-ESS are useful diagnostic summaries, but eventually need to look at the ESS / MCSE for the quantity of interest



# Diagnostic tools

For this week's assignment:

- $\hat{R}$ , ESS, MCSE
  - `library(posterior)`
  - `th |> summarise_draws(Rhat=basic_rhat, ESS=mean_ess)`
  - `th |> summarise_draws(mean, mean_mcse)`
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  - see `demo11_5` and Digits case study for the examples how to use these

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- Python
  - see ArviZ package

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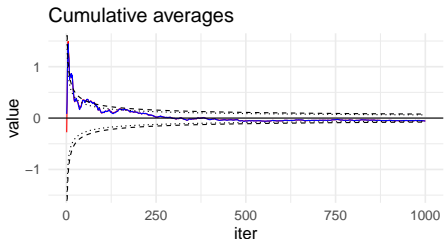
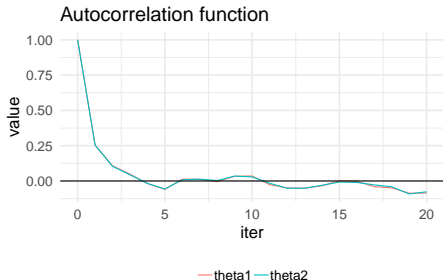
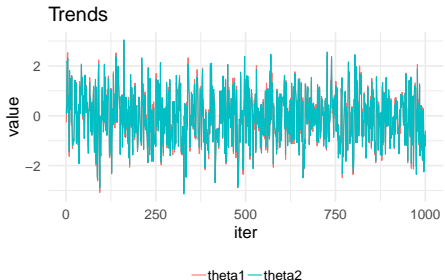
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- Multimodal
  - difficult to move from one mode to another
- Long-tailed with non-finite variance and mean
  - central limit theorem for expectations does not hold

# Next week: HMC, NUTS, and dynamic HMC

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



$$\hat{\tau} = 1 + 2 \sum_{t=1}^T \hat{\rho}_t$$
$$\approx 1.6$$

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



## Further diagnostics

- Pareto- $\hat{k}$  diagnostic for checking whether variance is finite
- Dynamic HMC/NUTS has additional diagnostics
  - divergences
  - tree depth exceedences

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- Construct a Markov chain which has desired stationary distribution
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- Probabilistic programming frameworks
  - provide efficient MCMC algorithms that work well without manual tuning for many posterior distributions (more next week)