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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_{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_{eff})
- demo11_5: Diagnostics with posterior and bayesplot packages

It's all about expectations (reminder)

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

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

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- Grid (equal spacing) evaluation with self-normalization

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

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

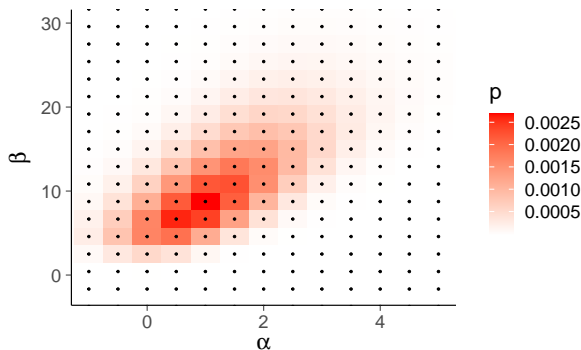
Monte Carlo

- 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)
 - Importance sampling is reliable only in special cases

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Posterior density evaluated in a grid

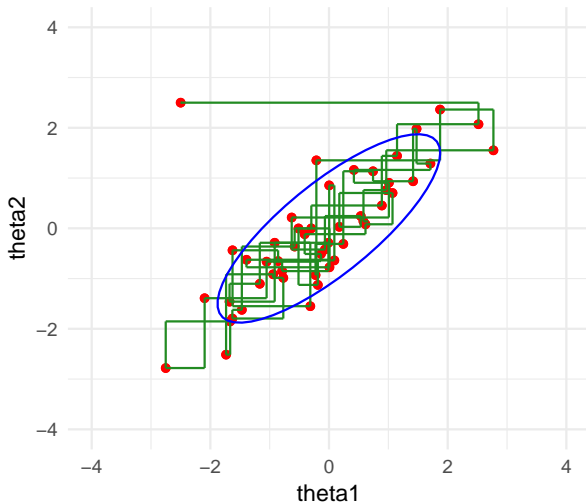


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- What to do in high dimensions?
 - Markov chain Monte Carlo (Ch 11-12)
 - Laplace, Variational*, EP* (Ch 4,13*)

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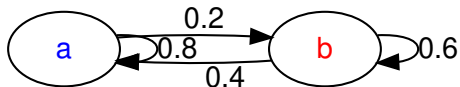
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- In Markov chain Monte Carlo we are not interested in the sequences directly, but how likely each state is in a long sequence

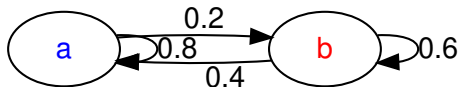
Markov chain

- Example of a simple Markov chain



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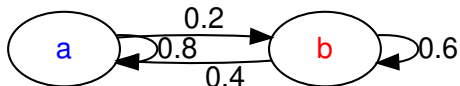
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- Given known transition probabilities, we can simulate the Markov process and count how often each state is visited

Markov chain

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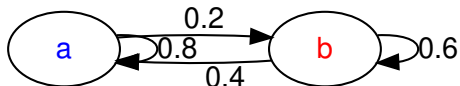


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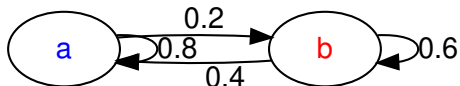
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$$p(a) \approx \frac{1}{S} \sum_{s=1}^S I(\text{state} = a)$$

Markov chain

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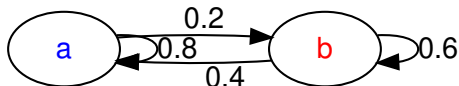
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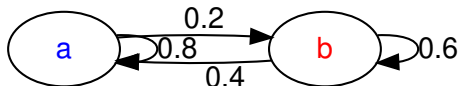
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- In discrete case we can also find the marginal probabilities by examining the transition probability matrix

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

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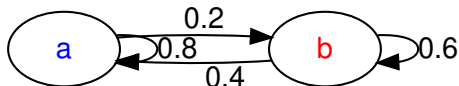
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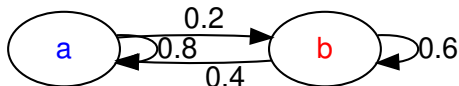
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- From A^S we get $p(\mathbf{a}) = 0.75$ and $p(\mathbf{b}) = 0.25$

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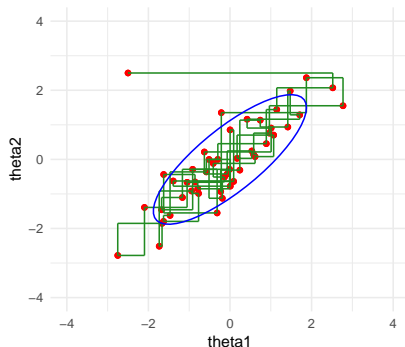
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 - + central limit theorem holds for expectations
 - draws are dependent
 - construction of efficient Markov chains is not always easy

Markov chain

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

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- 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 $p(\theta \mid y)$

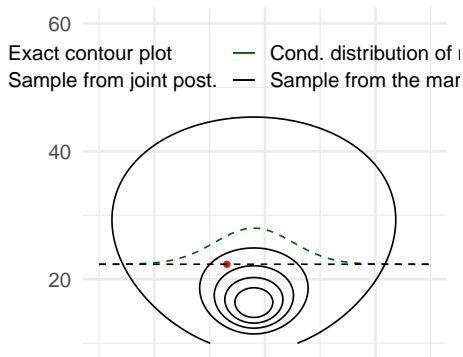
Gibbs sampling

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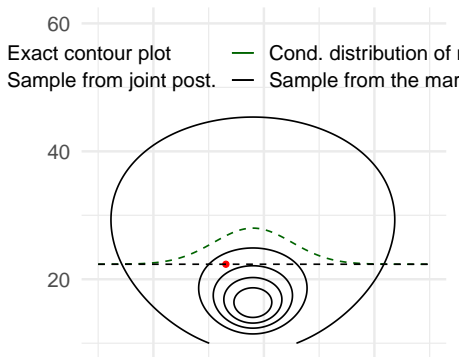
Joint posterior



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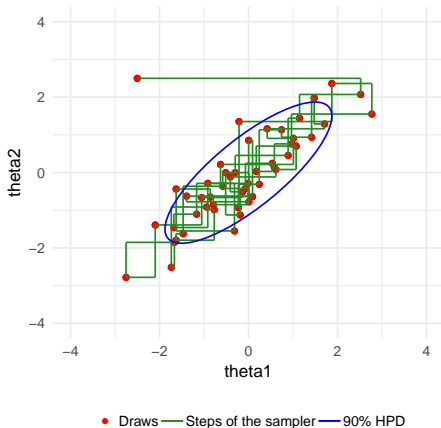
Joint posterior



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

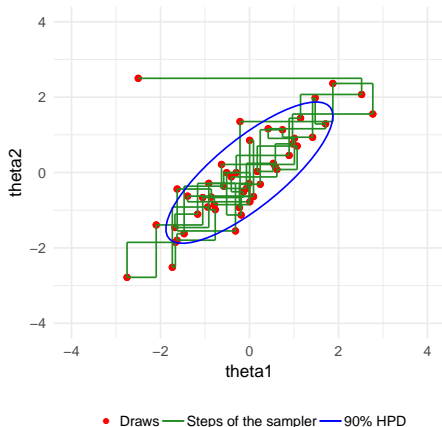
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- demo11_1



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- Basic algorithm

sample θ_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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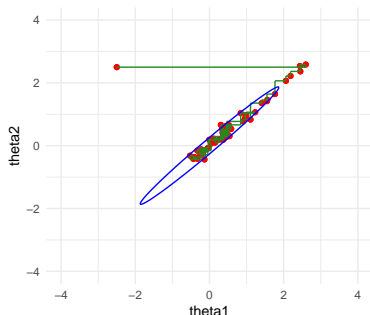
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- Slow if parameters are highly dependent in the posterior
 - demo11_1 continues



Conditional vs joint

- How about sampling θ jointly?
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Conditional vs joint

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 - 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 θ^0

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

- (a) pick a proposal θ^* 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

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- rejection of a proposal increments the time t also by one
ie, the new state is the same as previous

Metropolis algorithm

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

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

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$$\theta^t = \begin{cases} \theta^* & \text{with probability } \min(r, 1) \\ \theta^{t-1} & \text{otherwise} \end{cases}$$

- rejection of a proposal increments the time t also by one
ie, the new state is the same as previous
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Metropolis algorithm

- Algorithm

1. starting point θ^0

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

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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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 - = probability to return to a state i is 1
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- since their joint distribution is symmetric, θ^{t-1} and θ^t 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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 - many steps accepted, but the chain moves slowly due to small steps
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 - long steps proposed, but many of those rejected and again chain moves slowly

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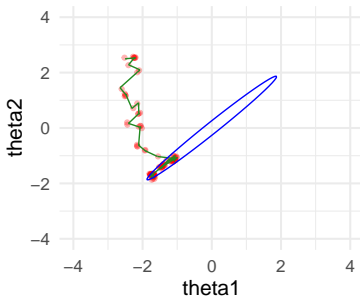
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- Generic rule for rejection rate is 60-90% (but depends on dimensionality and a specific algorithm variation)

Gibbs sampling

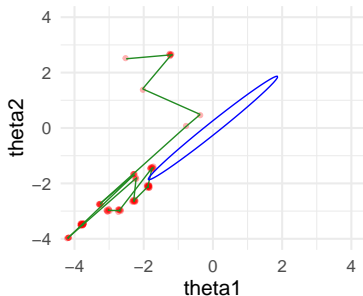
- Specific case of Metropolis-Hastings algorithm
 - single updated (or blocked)
 - proposal distribution is the conditional distribution
 - proposal and target distributions are same
 - acceptance probability is 1

Metropolis

- Usually doesn't scale well to high dimensions
 - if the shape doesn't match the whole distribution, the efficiency drops
 - demo11_2



• Draws — Steps of the sampler — 90% HPD



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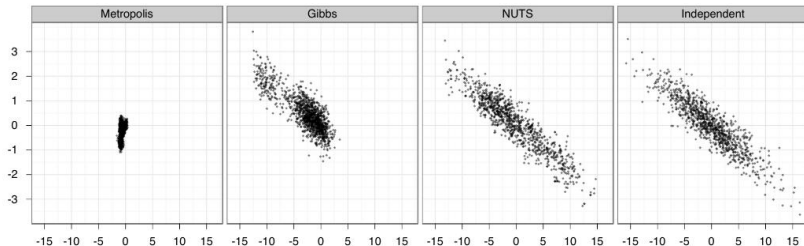
Dynamic Hamiltonian Monte Carlo and NUTS

- 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)

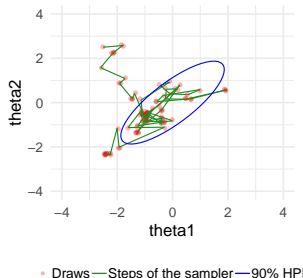


Warm-up and convergence diagnostics

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

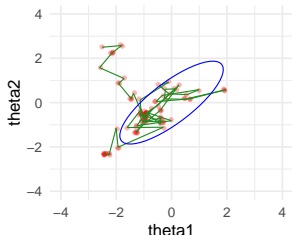
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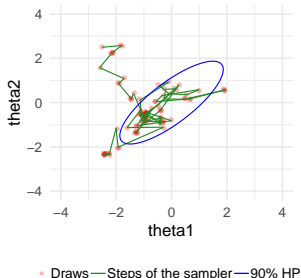


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- Warm-up = remove draws from the beginning of the chain
 - warm-up may include also phase for adapting algorithm parameters
- Convergence diagnostics
 - Is the sample representative of the target distribution?

MCMC draws are dependent

- Monte Carlo estimates still valid
(central limit theorem holds 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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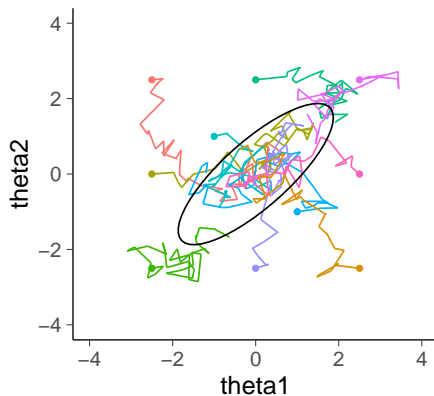
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 - evaluation of *effective* sample size (ESS)
 - given finite variance, the distribution of the expectation approaches normal distribution with variance $\sigma_\theta^2/\text{ESS}$

Several chains

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

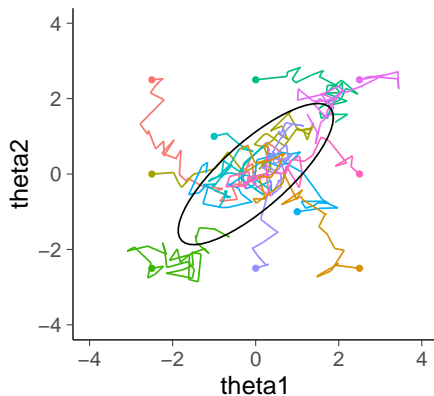
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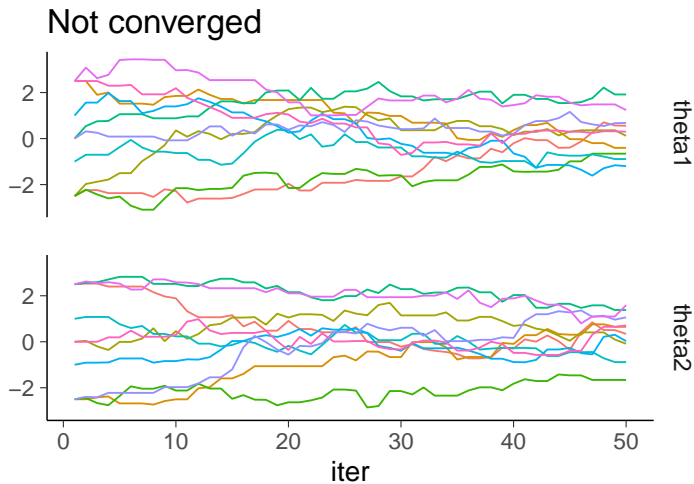
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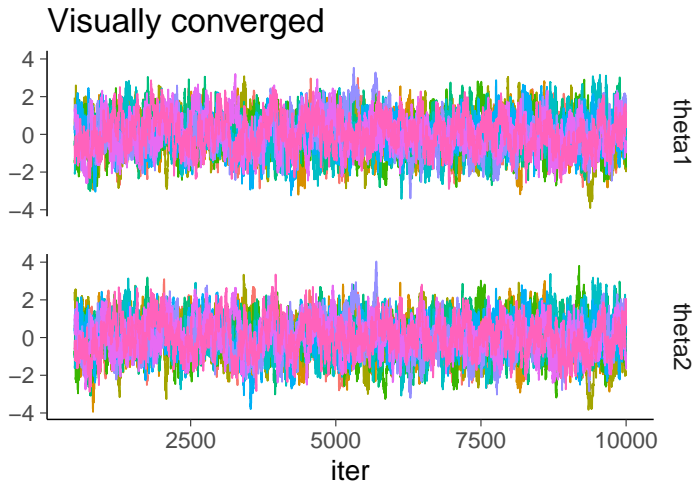


- Remove draws from the beginning of the chains and run chains long enough so that it is not possible to distinguish where each chain started and the chains are well mixed

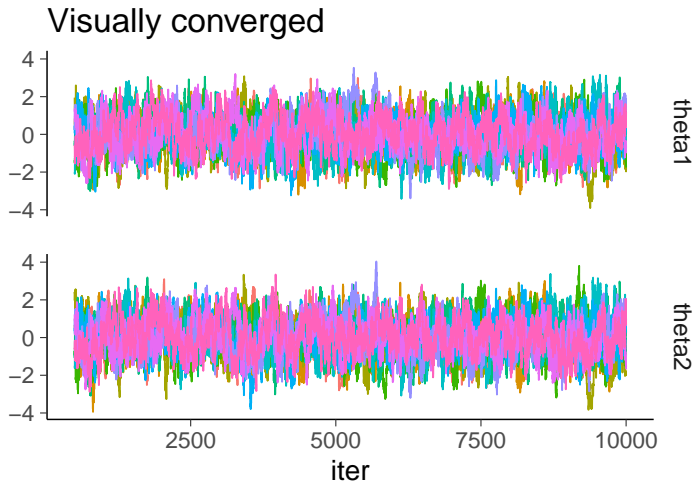
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Visual convergence check is not sufficient

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

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

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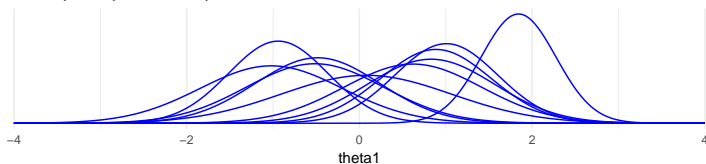
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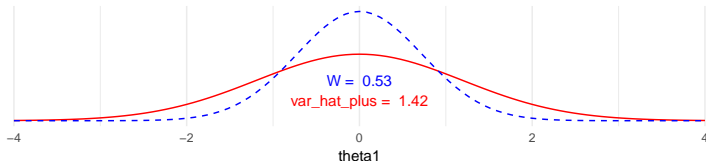
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var_hat_plus = total variance estimate

50 warmup, 50 post warmup iterations



Rhat = 1.64



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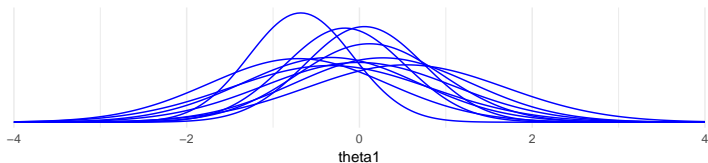
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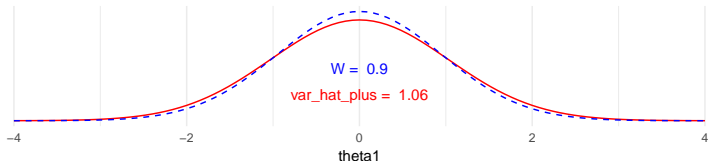
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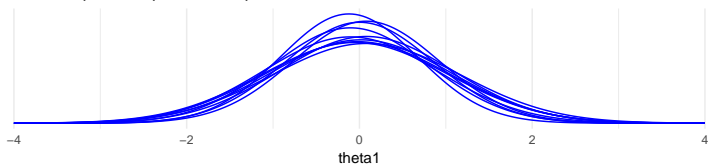
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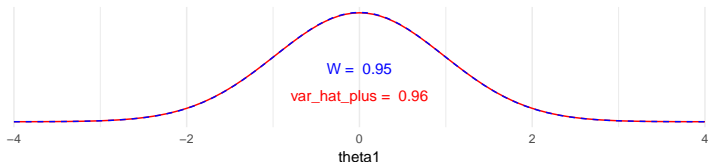
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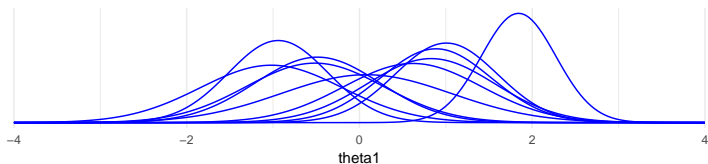
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- As $\widehat{\text{var}}^+(\theta \mid y)$ overestimates and W underestimates, compute

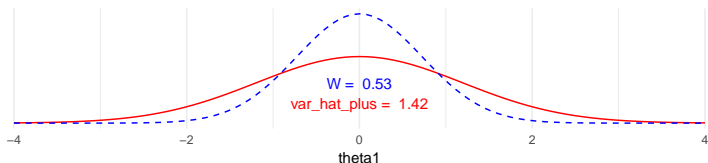
$$\hat{R} = \sqrt{\frac{\widehat{\text{var}}^+}{W}}$$

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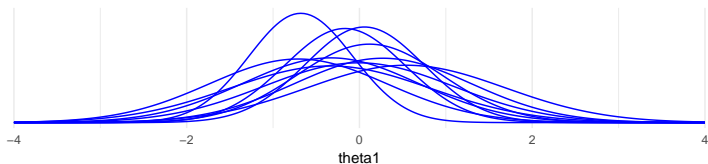


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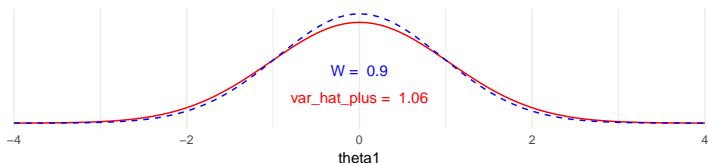


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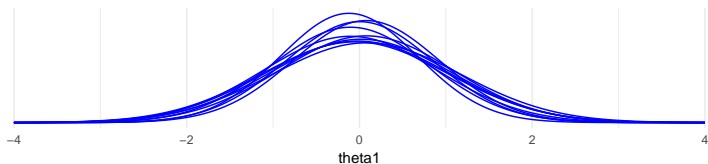


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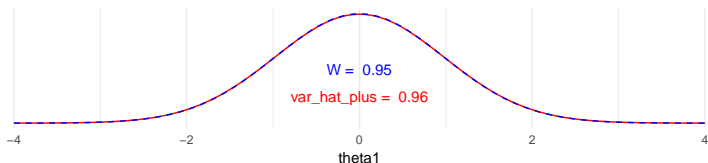


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5000 warmup, 5000 post warmup iterations



Rhat = 1



\widehat{R}

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

- Estimates how much the scale of ψ 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

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

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- $\hat{R} \rightarrow 1$, when $N \rightarrow \infty$
- if \hat{R} is big (e.g., $R > 1.01$), keep sampling
- If \hat{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 θ_{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.
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Rank normalized \hat{R}

- Original \hat{R} requires that the target distribution has finite mean and variance
- Rank normalization fixes this and is also more robust given finite but high variance
 - inverse normal-cdf of ranks

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- Notation updated compared to BDA3

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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"  
x |>  
  summarise_draws(mean, sd, mcse_mean, rhat_basic, rhat)
```


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

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x |>
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```

variable	mean	sd	mcse_mean	rhat_basic	rhat
N	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"
x |>
  summarise_draws(mean, sd, mcse_mean, pareto_khat,
                  rhat_basic, rhat)
```

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rhat_basic() without rank normalization

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x <- as_draws_matrix(x)
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```
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```
x |>
```

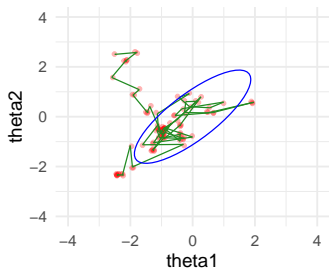
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                  rhat_basic, rhat)
```

variable	mean	sd	mcse_mean	pareto_khat	rhat_basic	rhat
t1	-1.11	42.1	1.23	1.07	1.01	1.47

Time series analysis

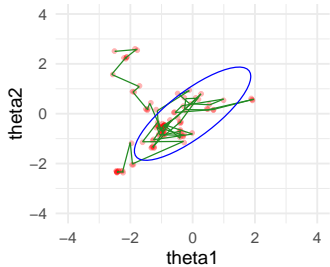
- Autocorrelation function
 - describes the correlation given a certain lag
 - can be used to compare efficiency of MCMC algorithms and parameterizations

Autocorrelation



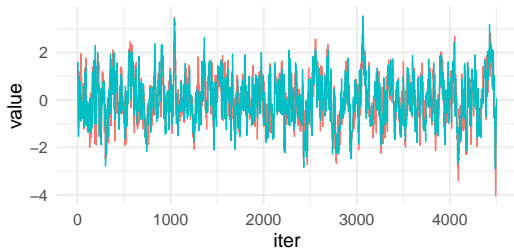
• Draws — Steps of the sampler — 90% HPI

Autocorrelation



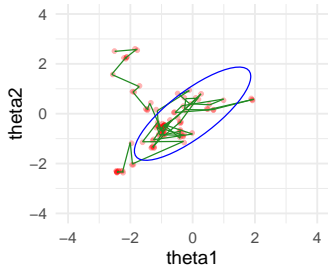
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Trends



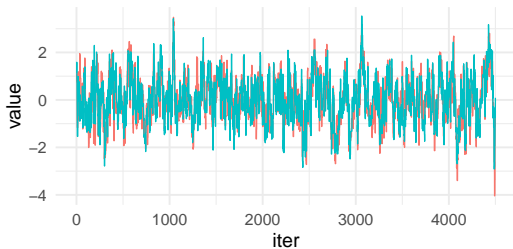
— θ_1 — θ_2

Autocorrelation



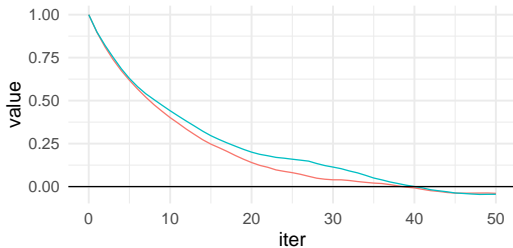
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Trends

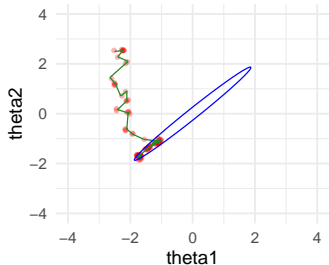


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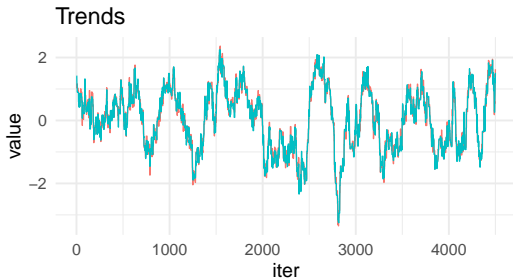
Autocorrelation function



Autocorrelation (slow mixing due to small step size)

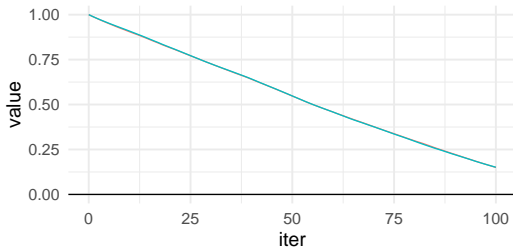


• Draws — Steps of the sampler — 90% HPI

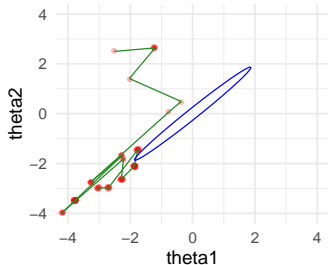


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Autocorrelation function

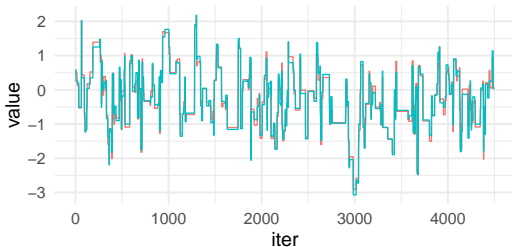


Autocorrelation (slow mixing due to many rejections)



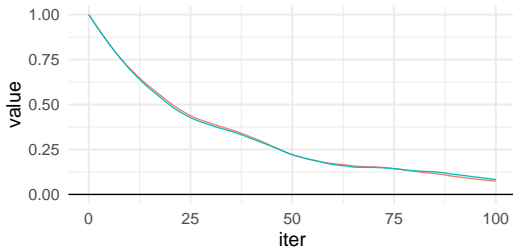
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Trends



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Autocorrelation function



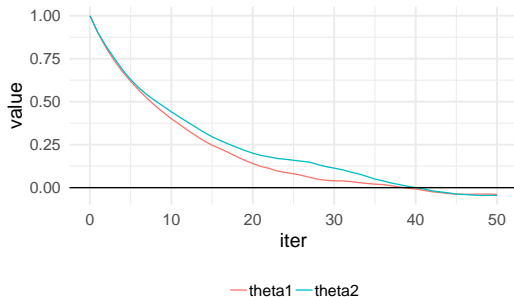
Time series analysis

- 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 τ is sum of autocorrelations

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

Time series analysis

- Estimation of the autocorrelation using several chains

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

where $\hat{\rho}_{n,m}$ is autocorrelation at lag n for chain m ,
and W and $\widehat{\text{var}}^+$ are the same as in \hat{R} (without rank
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- This combines \widehat{R} and autocorrelation estimates
 - 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 τ

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

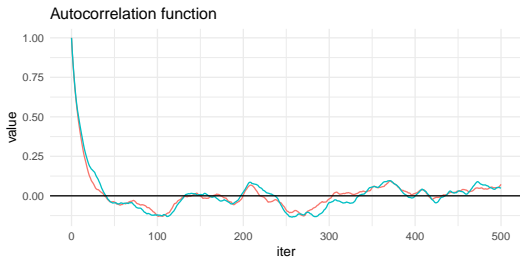
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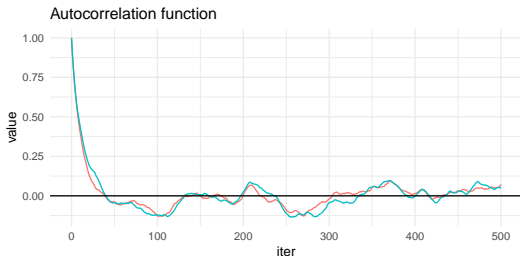


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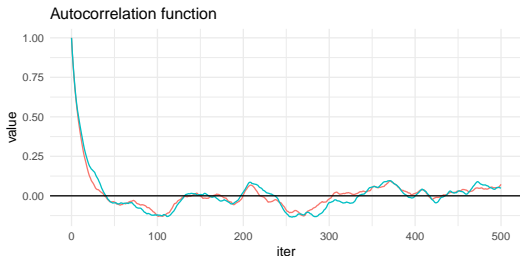
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- noise is larger for longer lags (less observations)

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

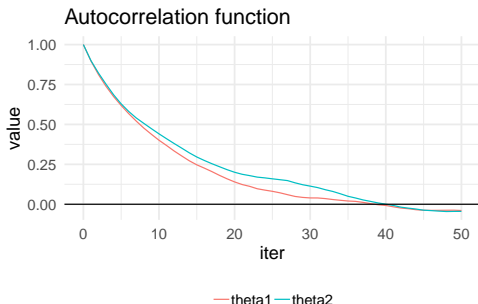
$$\hat{\tau} = 1 + 2 \sum_{t=1}^T \hat{\rho}_t$$

Geyer's adaptive window estimator

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



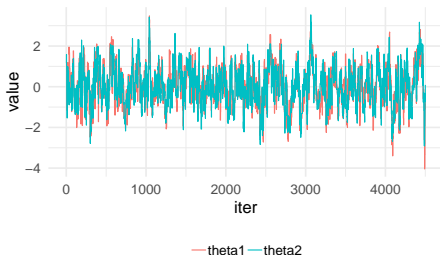
Effective sample size

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

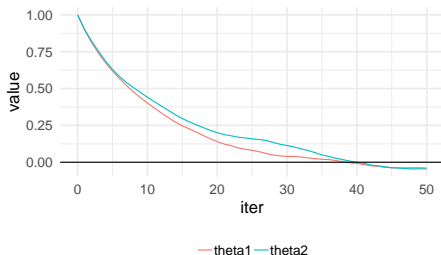
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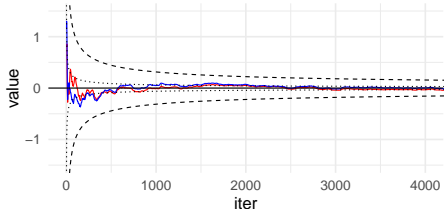
Trends



Autocorrelation function



Cumulative averages

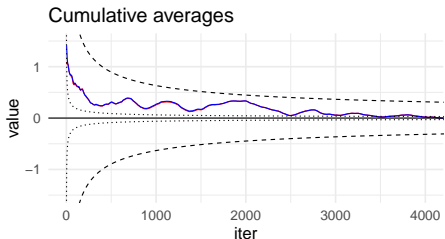
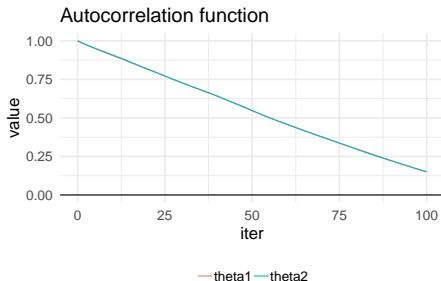
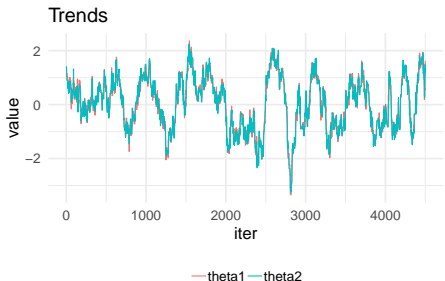


$$\hat{\tau} = 1 + 2 \sum_{t=1}^T \hat{\rho}_t$$
$$\approx 24$$

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

Effective sample size

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



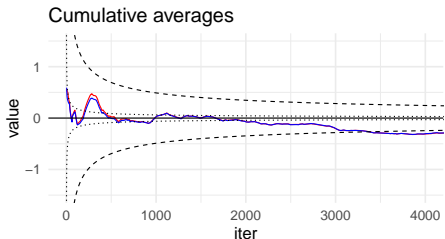
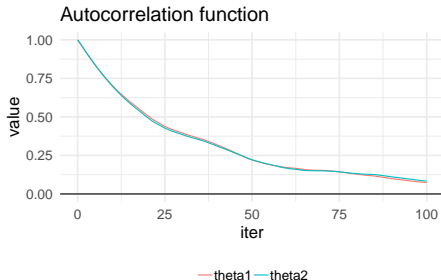
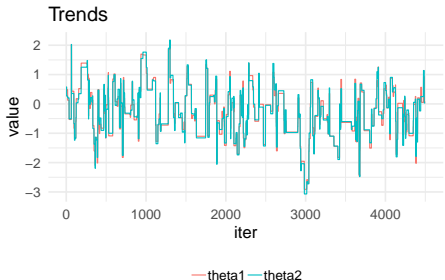
$$\hat{\tau} = 1 + 2 \sum_{t=1}^T \hat{\rho}_t$$

$$\approx 104$$

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

Effective sample size

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



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

$$\approx 63$$

— 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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```
drt |> summarise_draws(mean, pareto_khat,  
                        ess_mean, mcse_mean)  
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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.
xt1	0.33	0.00	93.	1.5	-5.8	6.1	1.00	2284.	3189.

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)`
 - `th |> summarize_draws(~quantile(.x, probs = c(0.05, 0.95)))`
 - see demo11_5 and Digits case study for the examples how to use these

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- trace, autocorrelation, density, scatter plots in R
 - `library(bayesplot)`
 - `mcmc_trace(th), mcmc_acf(th), mcmc_areas(th), ...`
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 - see demo11_5 for the examples for more bayesplot examples
- Python
 - see ArviZ package

Problematic distributions

- Nonlinear dependencies
 - optimal proposal depends on location

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- Nonlinear dependencies
 - optimal proposal depends on location
- Funnels
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Problematic distributions

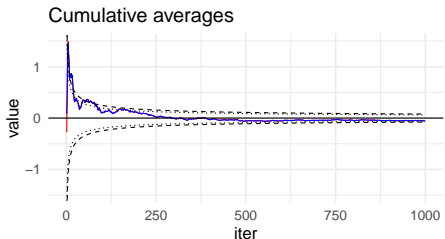
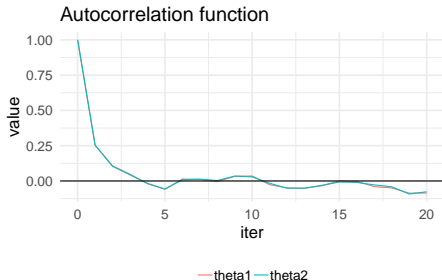
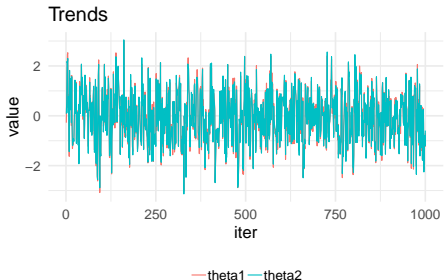
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- Multimodal
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Problematic distributions

- Nonlinear dependencies
 - optimal proposal depends on location
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- Multimodal
 - difficult to move from one mode to another
- 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 $ESS = S_{\text{eff}} \approx S/\hat{\tau}$



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

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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- Probabilistic programming frameworks
 - provide efficient MCMC algorithms that work well without manual tuning for many posterior distributions (more next week)