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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-$\widehat{R}$ and effective sample size (ESS or S_{eff})
- demo11_5: Diagnostics with `posterior` and `bayesplot` packages

It's all about expectations (reminder)

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

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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)
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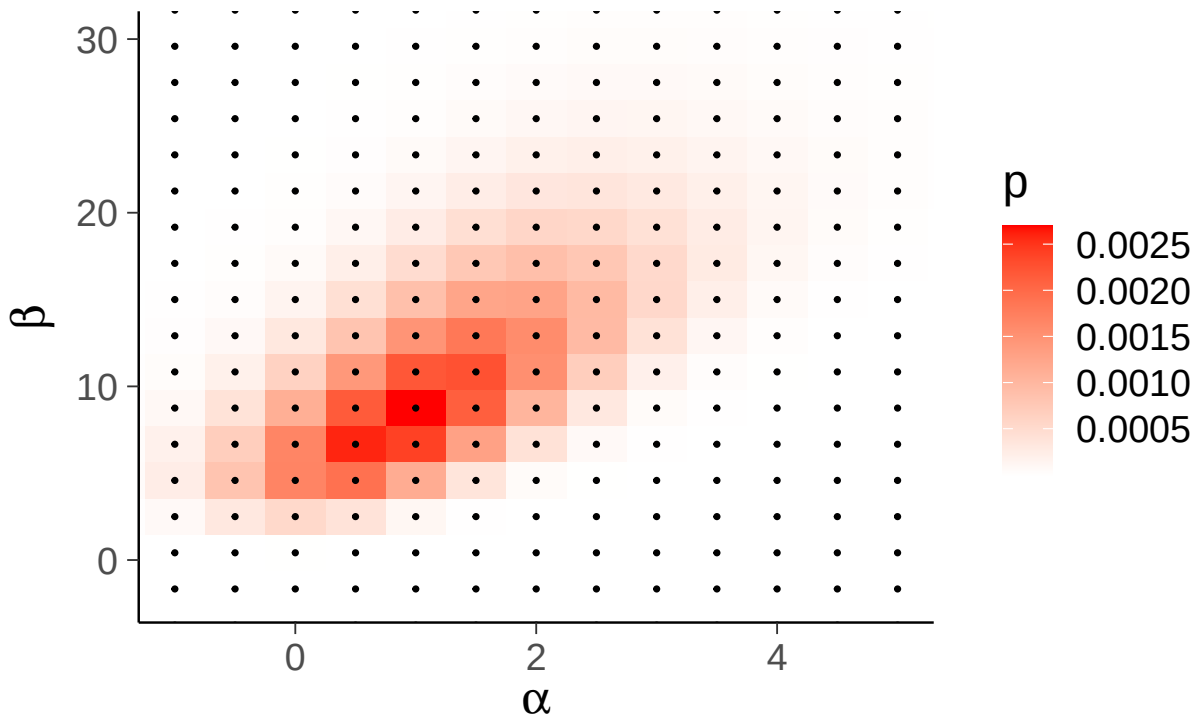
Posterior density evaluated in a grid



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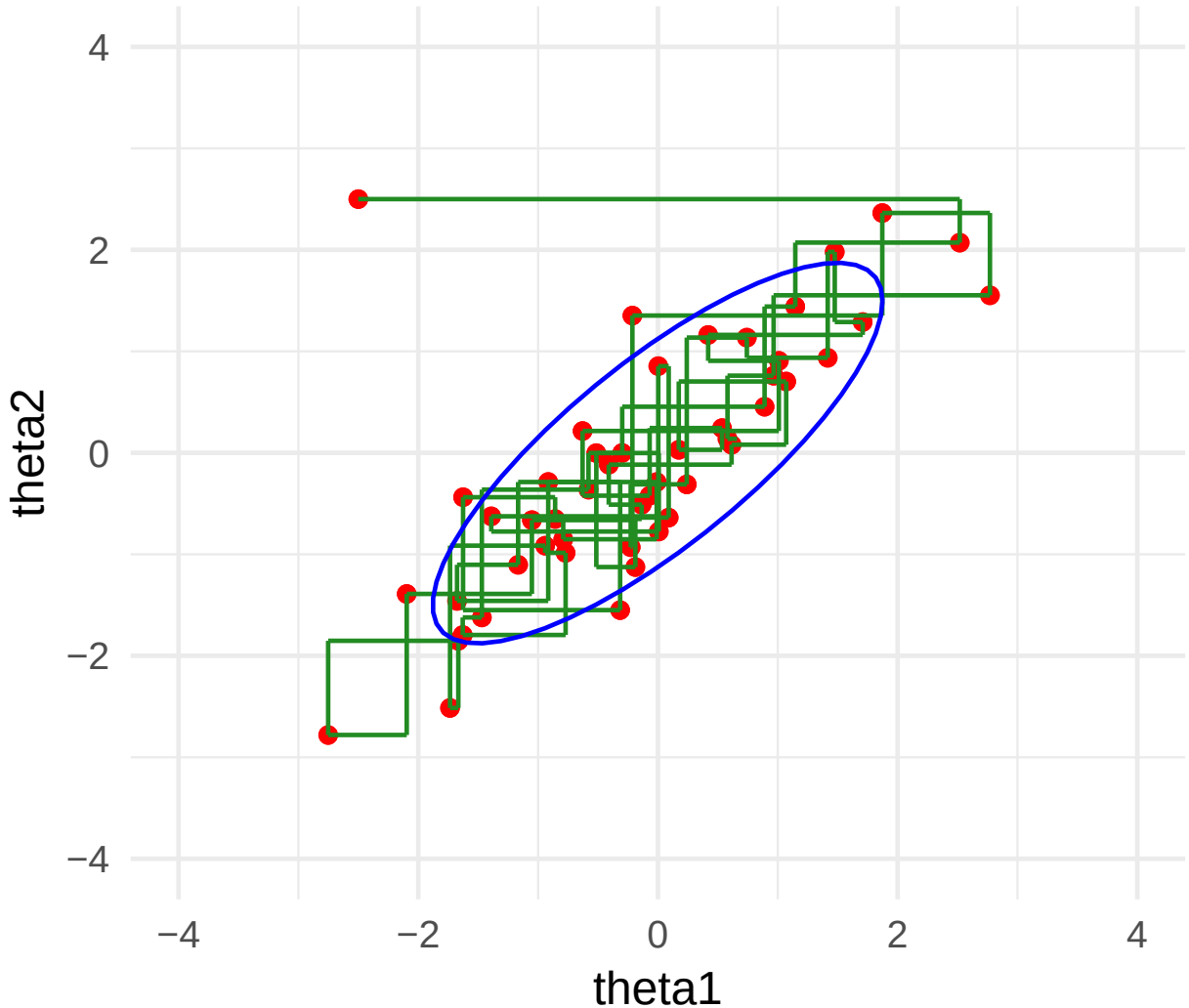
- What to do in high dimensions?
  - Markov chain Monte Carlo (Ch 11-12)
  - Laplace, Variational*, EP* (Ch 4,13*)

Markov chain Monte Carlo (MCMC)

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



Markov chain

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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 drivel*), 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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- 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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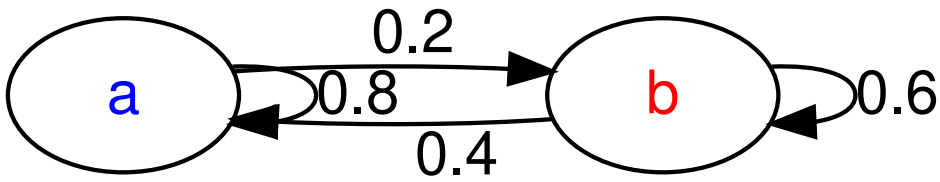
- Example of a simple Markov chain



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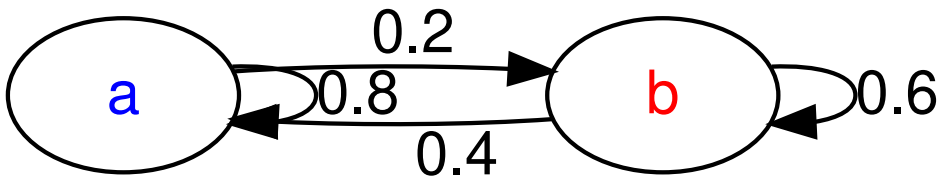

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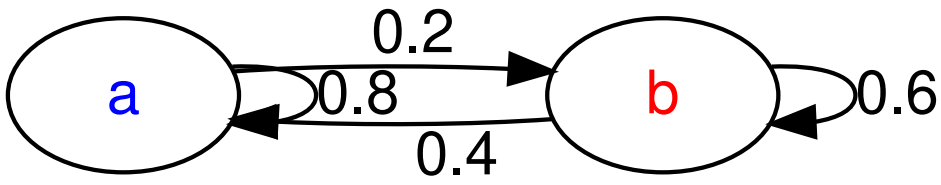

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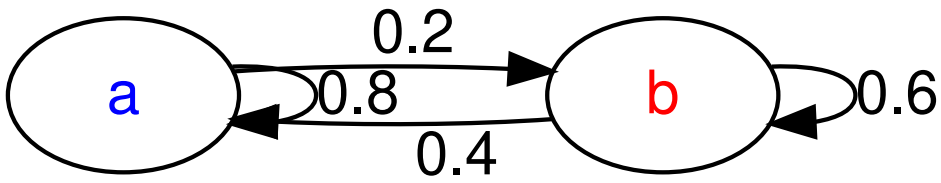

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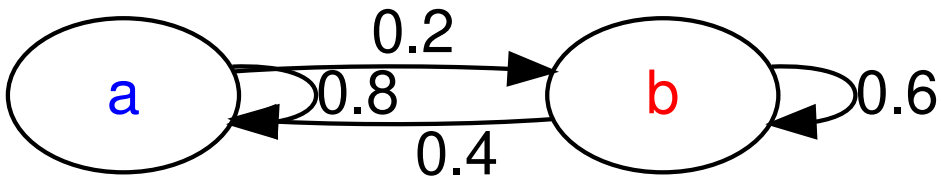

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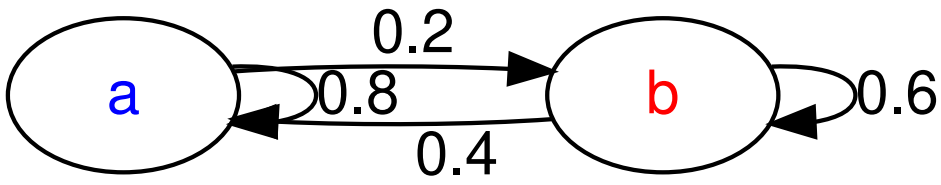

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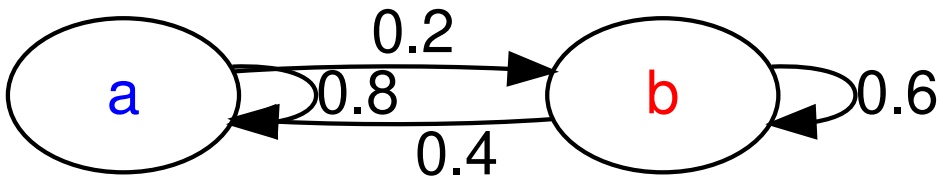

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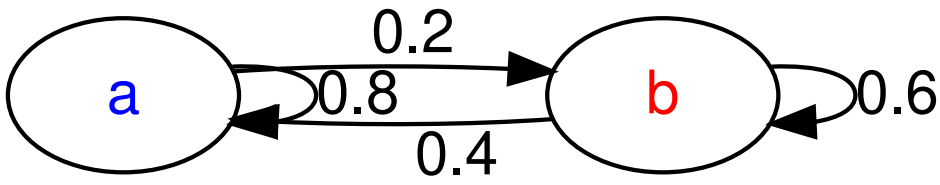

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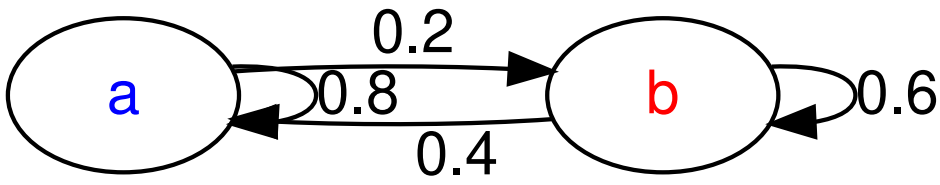

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- From A^s we get $p(\text{a}) = 0.67$ and $p(\text{b}) = 0.33$

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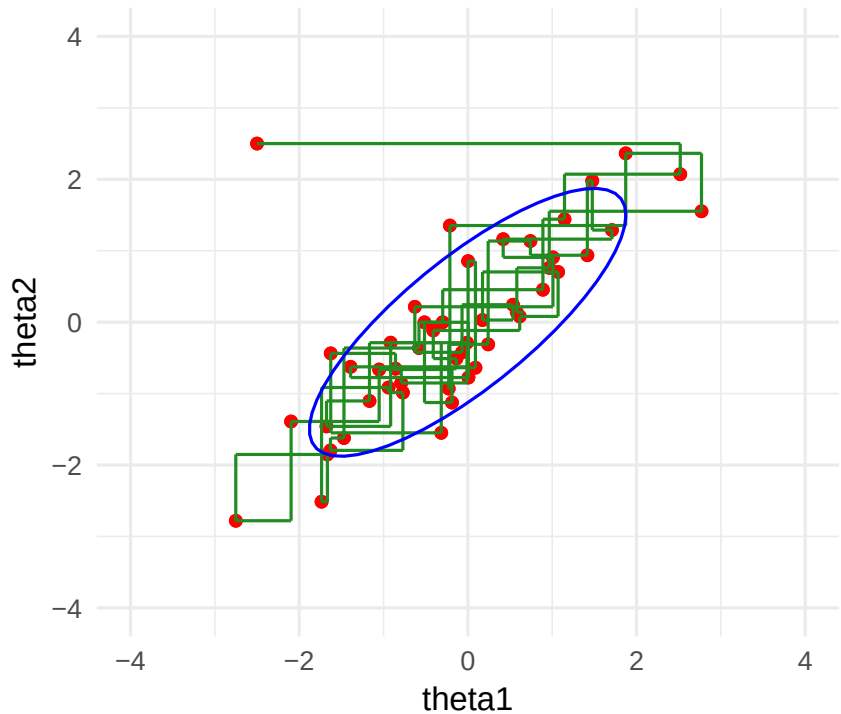

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  - \- draws are dependent
  - \- construction of efficient Markov chains is not always easy

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- Set of random variables $\theta^1, \theta^2, \ldots$, 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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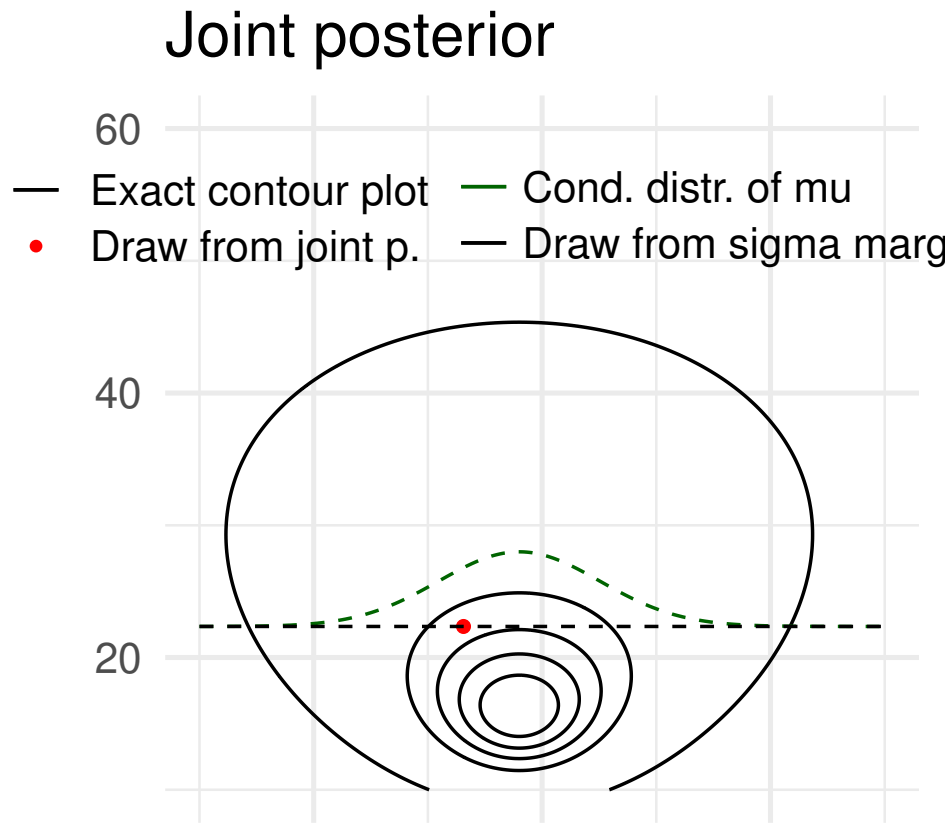

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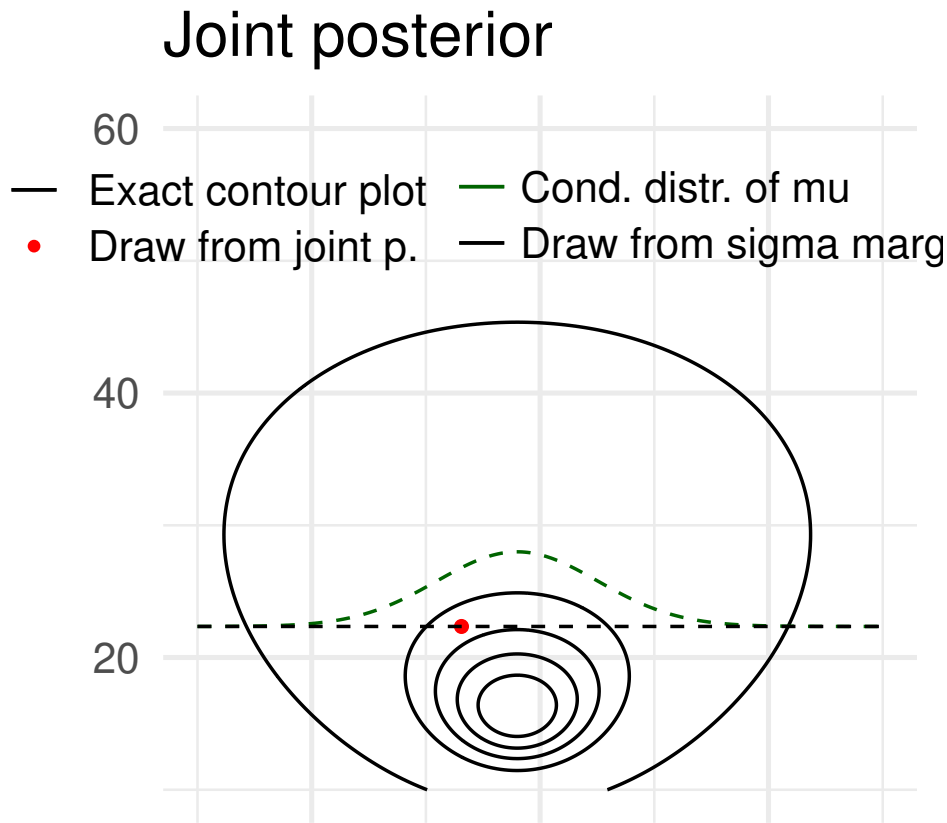

  - 1D is easy even if no conjugate prior and analytic posterior

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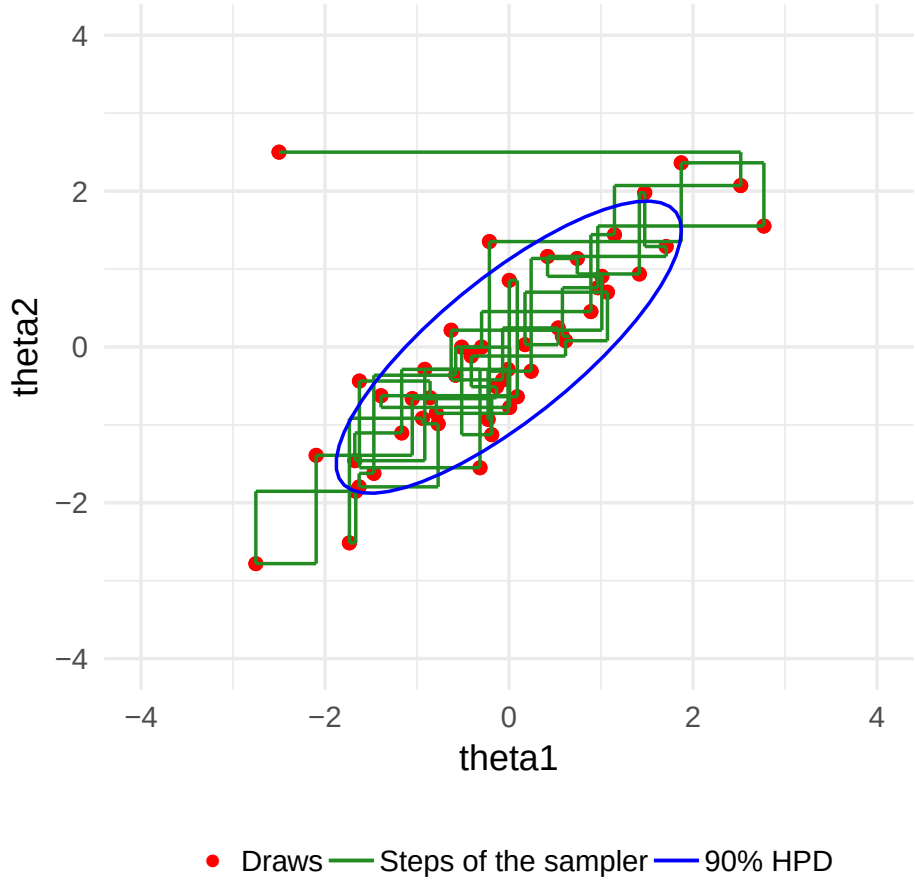

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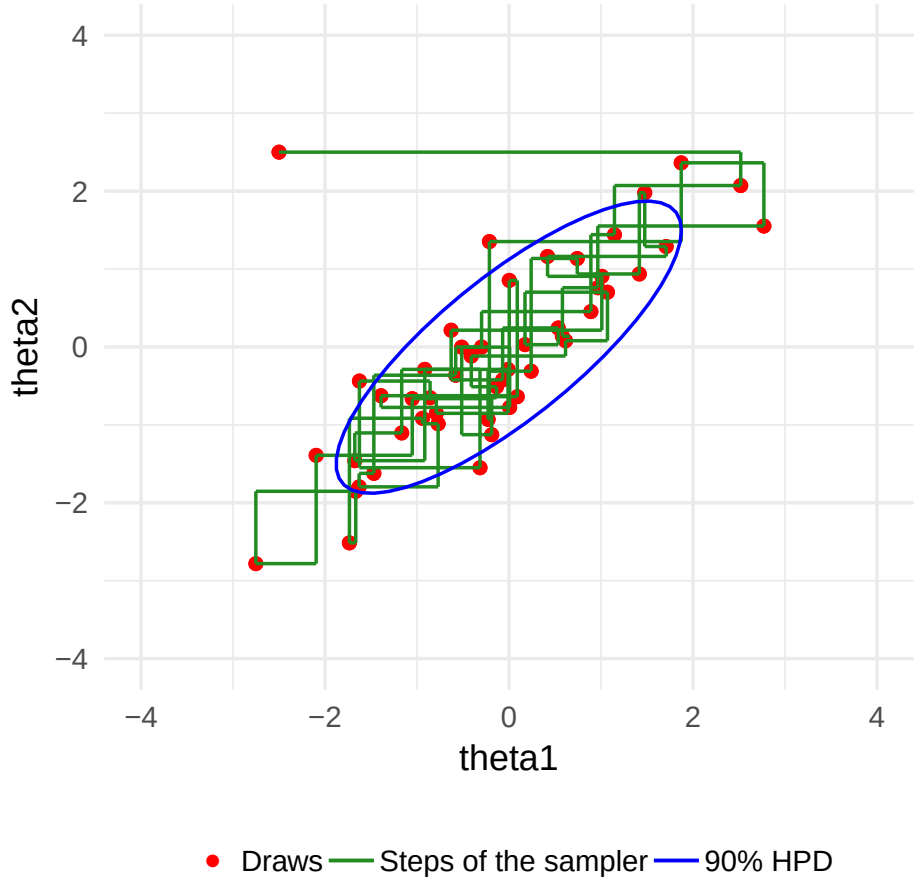

- Basic algorithm

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

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

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- For not so easy conditionals, use e.g. inverse-CDF

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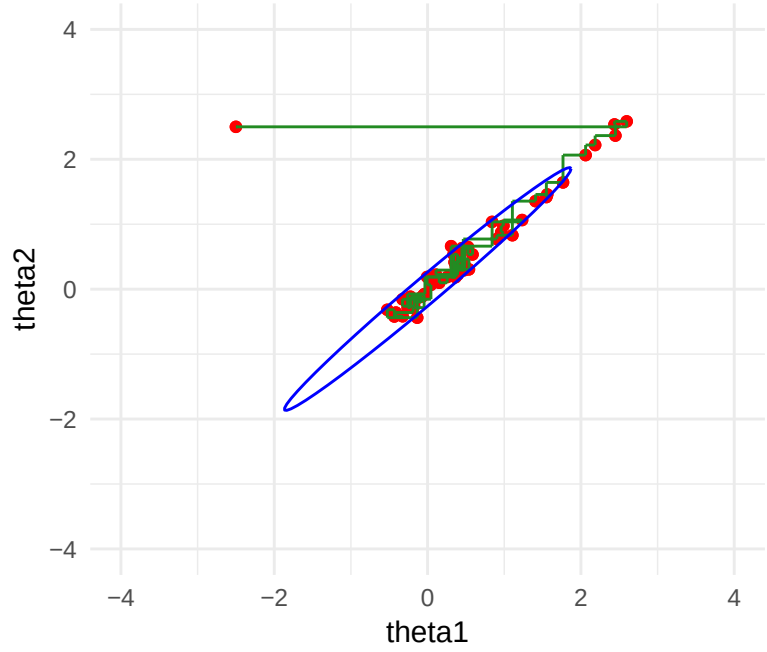
- Slow if parameters are highly dependent in the posterior
  - demo11_1 continues



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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

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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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Metropolis algorithm

- Example: one bivariate observation (y_1, y_2)
  - bivariate normal distribution with unknown mean and known covariance
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- More examples https://chi-feng.github.io/mcmc-demo/

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   which is the same as the probability of transition from θ_a to θ_b, since we have required that $J_t(\cdot \mid \cdot)$ is symmetric
   - since their joint distribution is symmetric, θ^{t-1} and θ^t have the same marginal distributions, and so $p(\theta \mid y)$ 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

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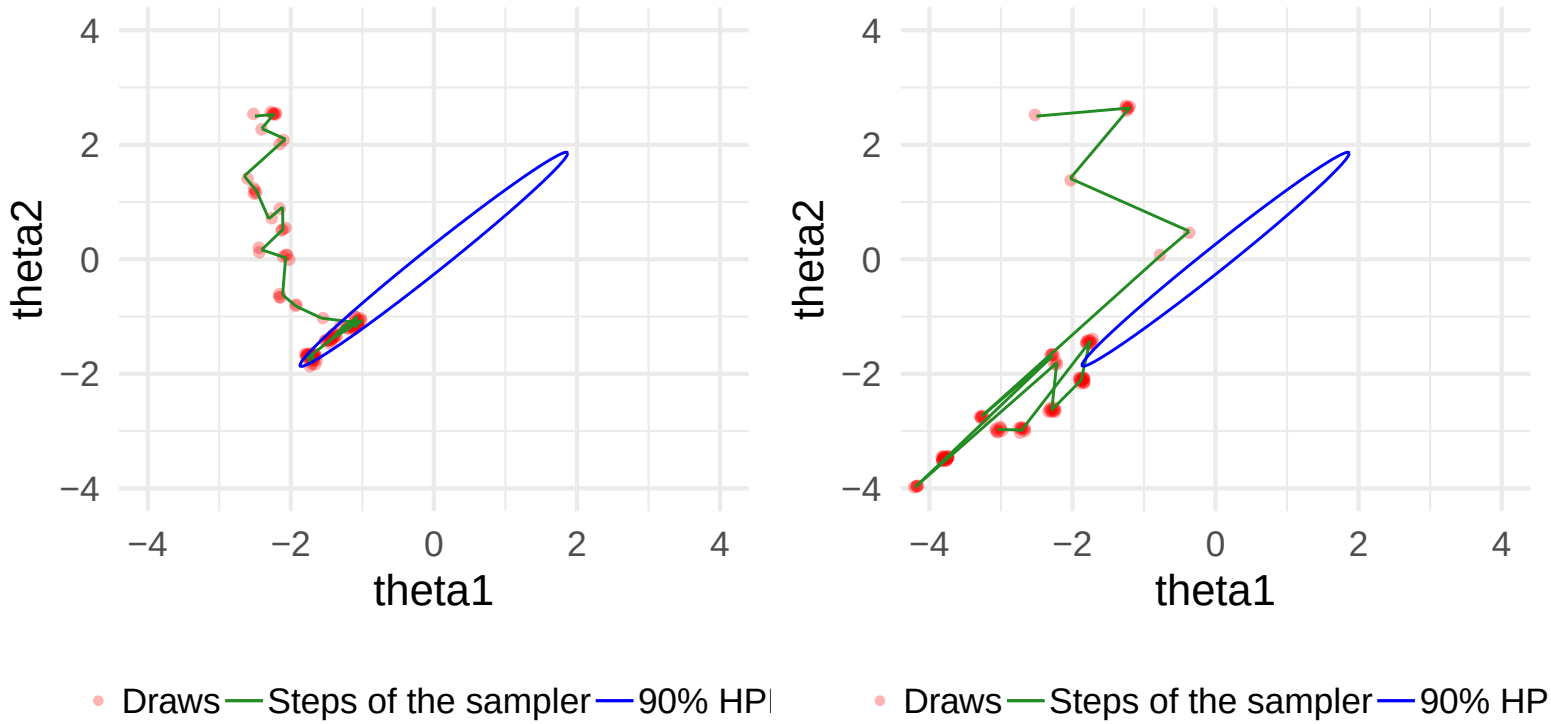
- Generic rule for rejection rate is 60-90% (but depends on dimensionality and a specific algorithm variation)

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



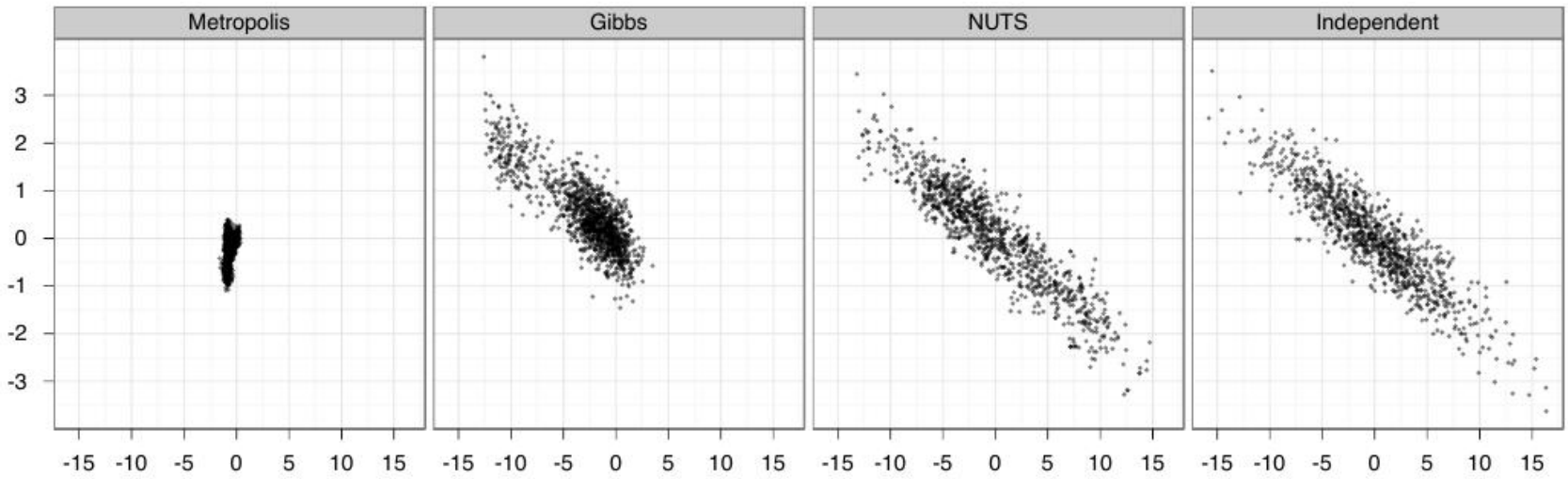
Dynamic Hamiltonian Monte Carlo and NUTS

- 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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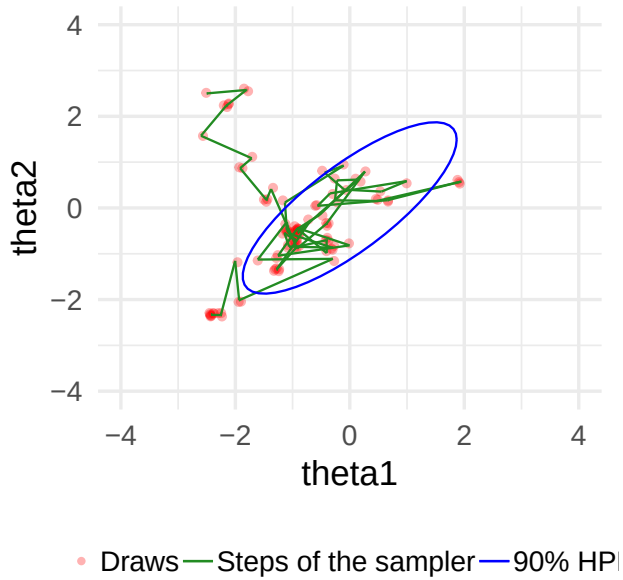

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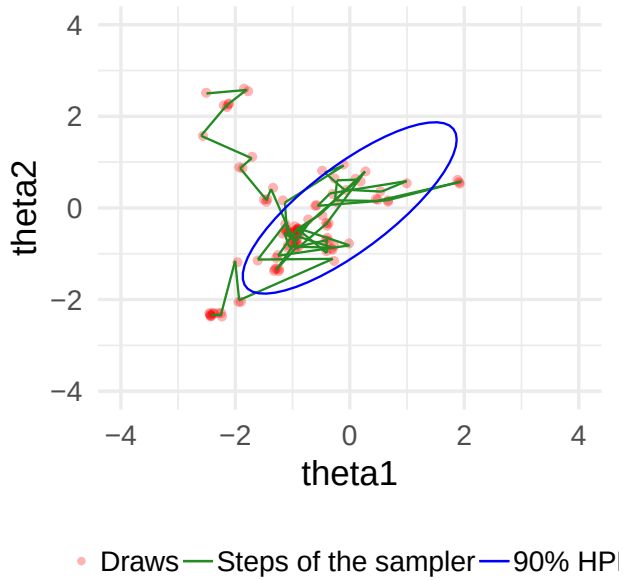

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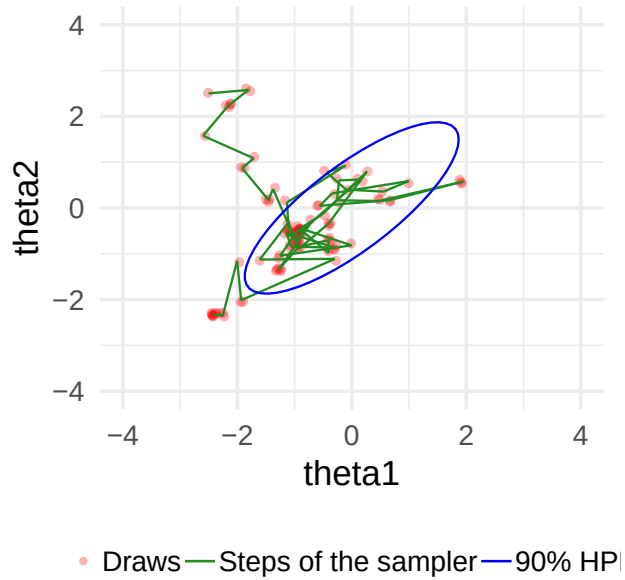

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- Convergence diagnostics
  - Is the sample representative of the target distribution?

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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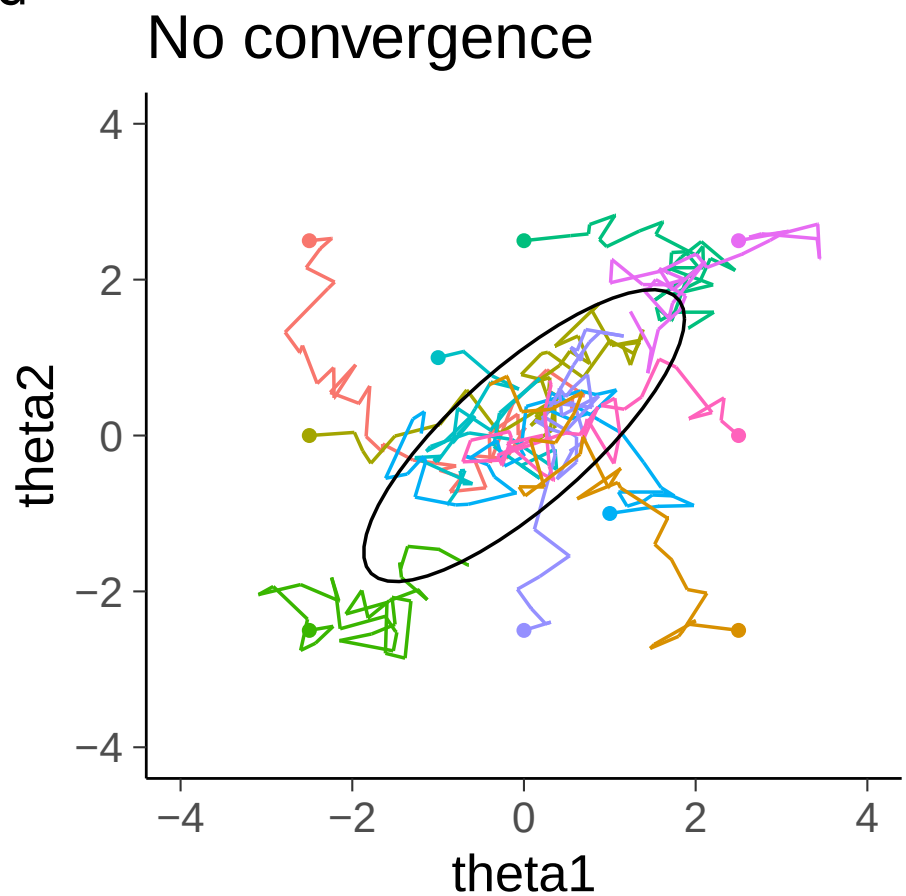
  - given finite variance, the distribution of the expectation approaches normal distribution with variance $\sigma_\theta^2/\text{ESS}$

Several chains

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



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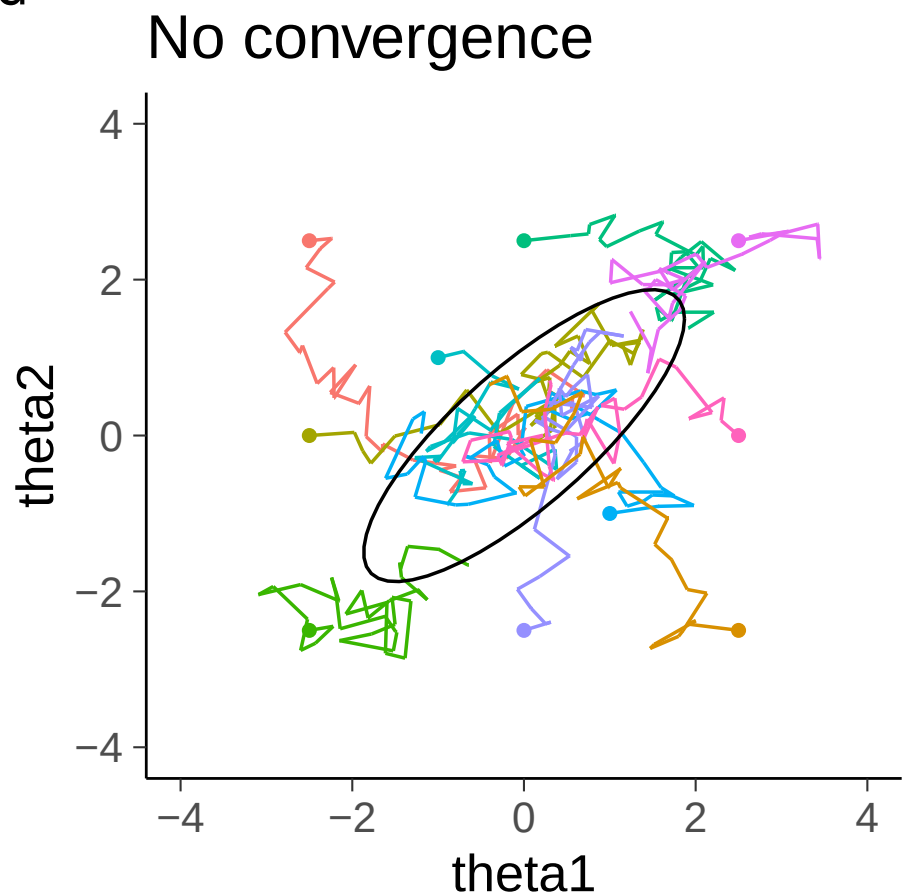

- Remove draws from the beginning of the chains and run chains long enough so that it is not possible to distinguish where each chain started and the chains are well mixed

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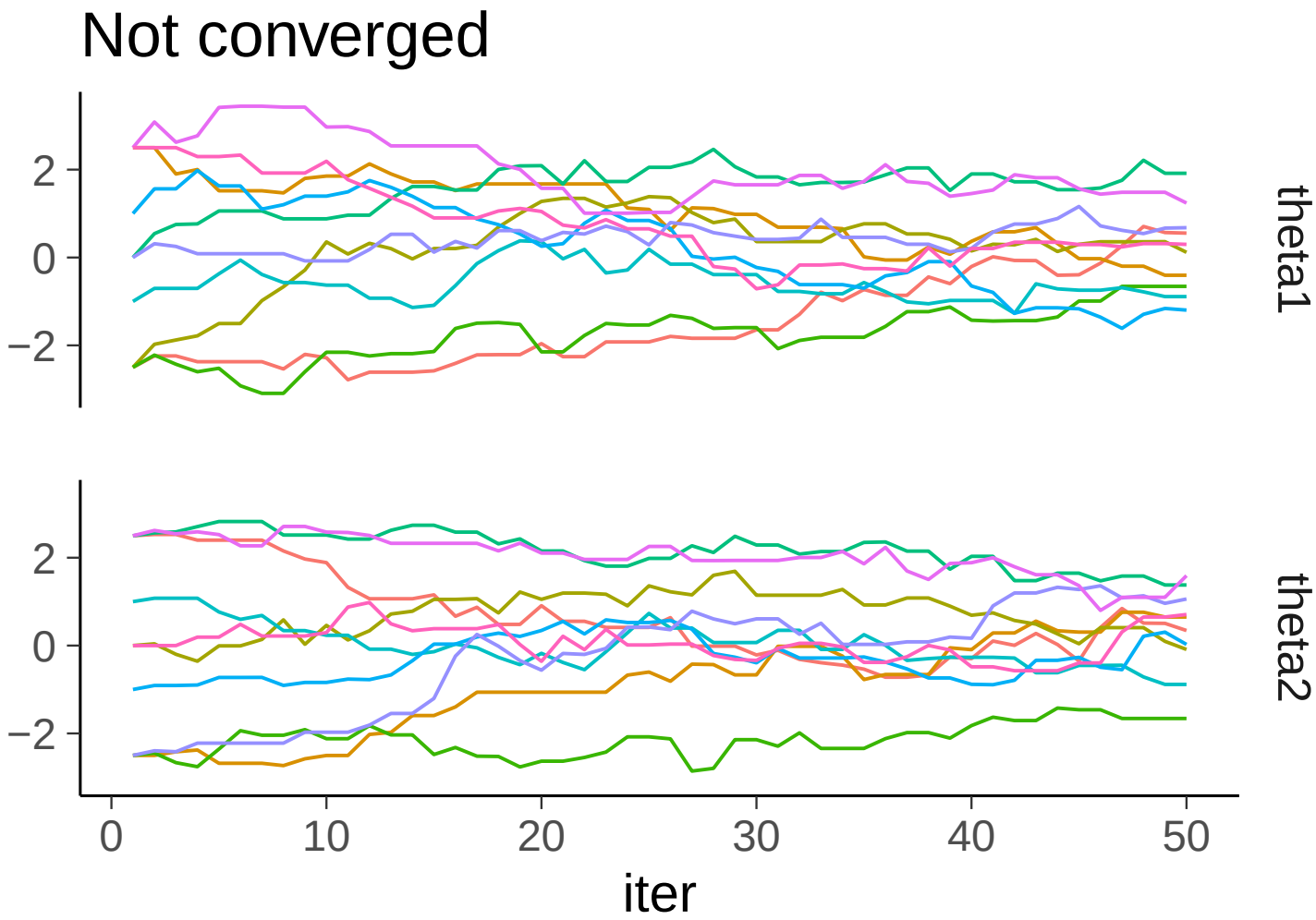

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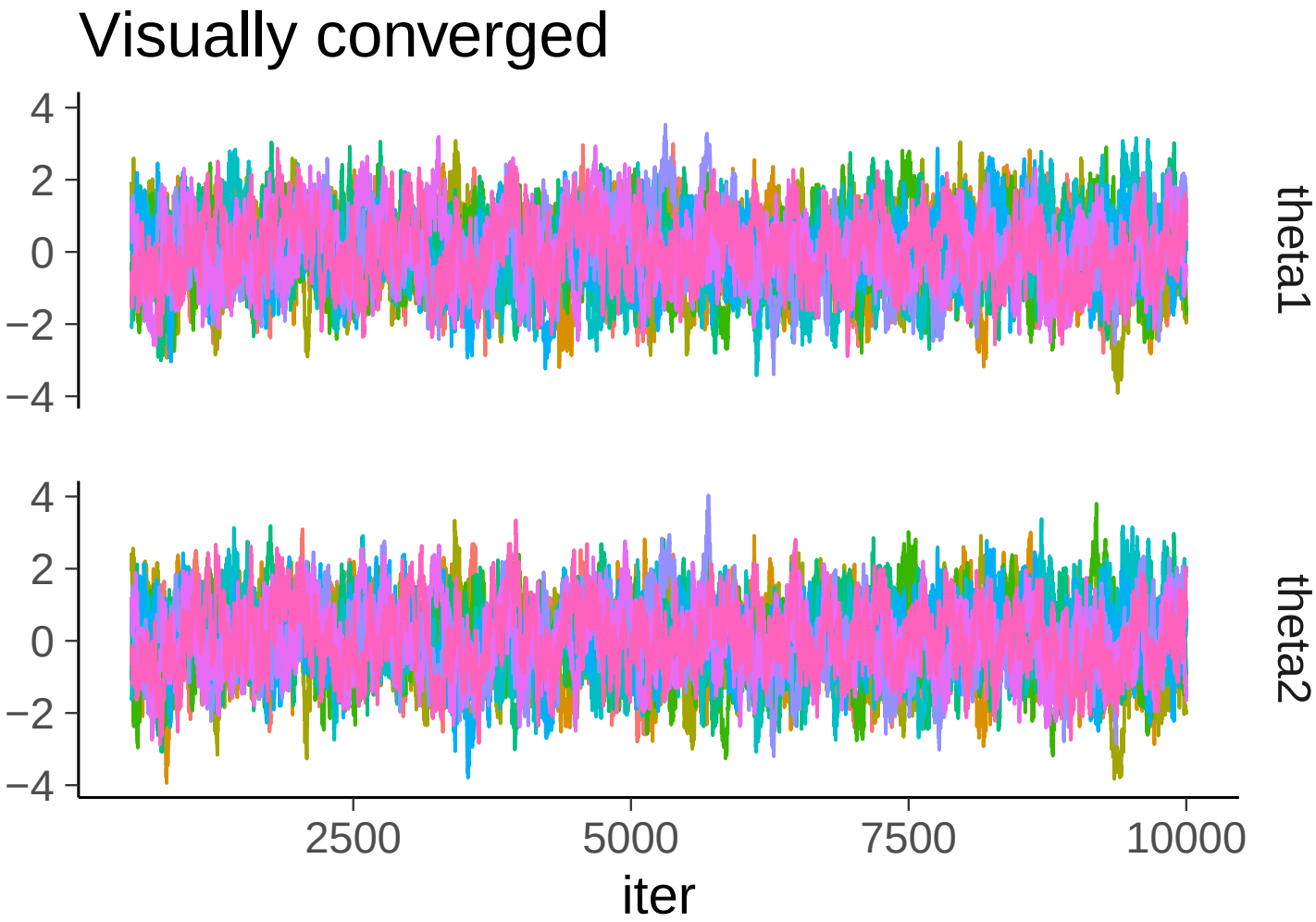

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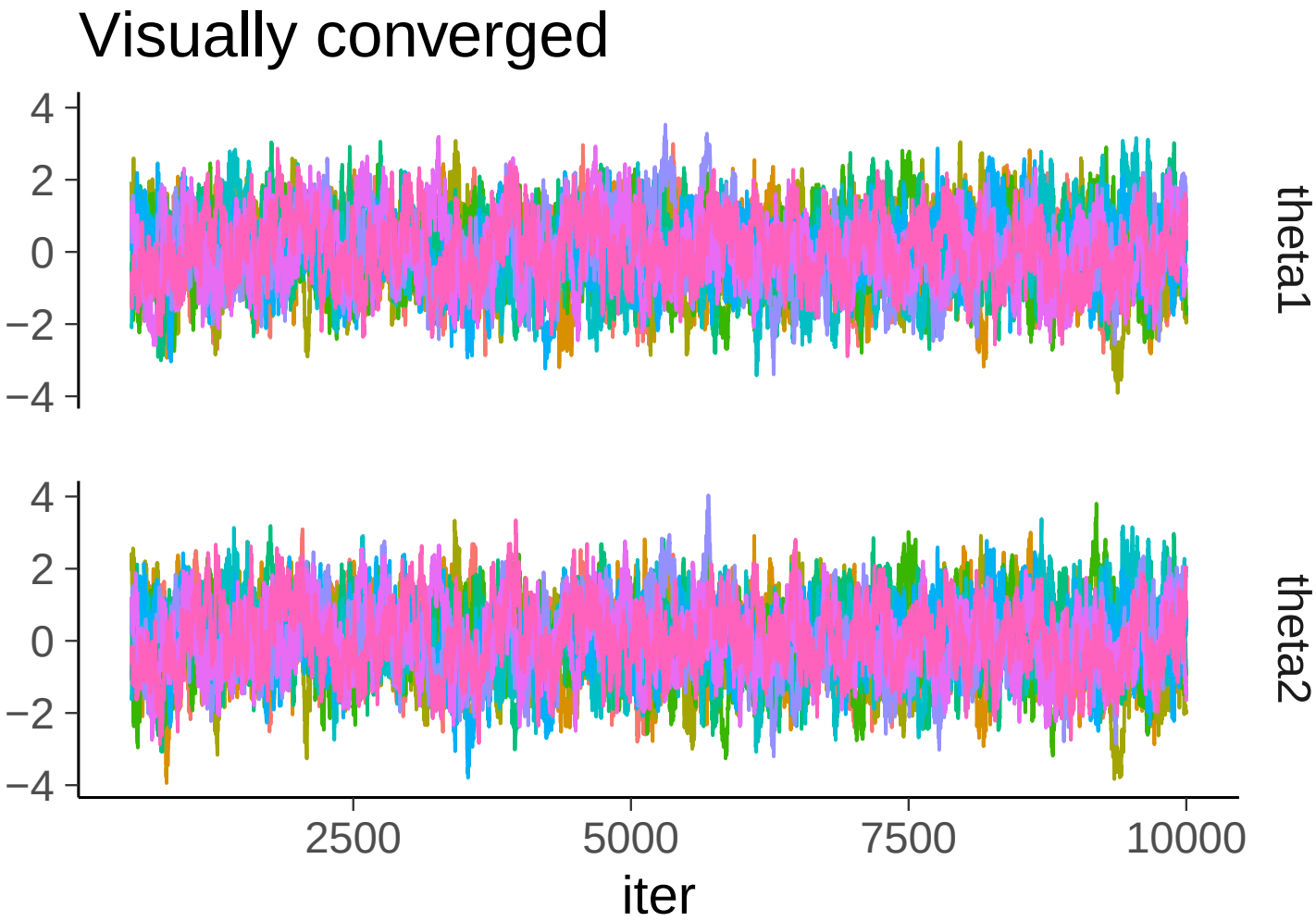

Visual convergence check is not sufficient

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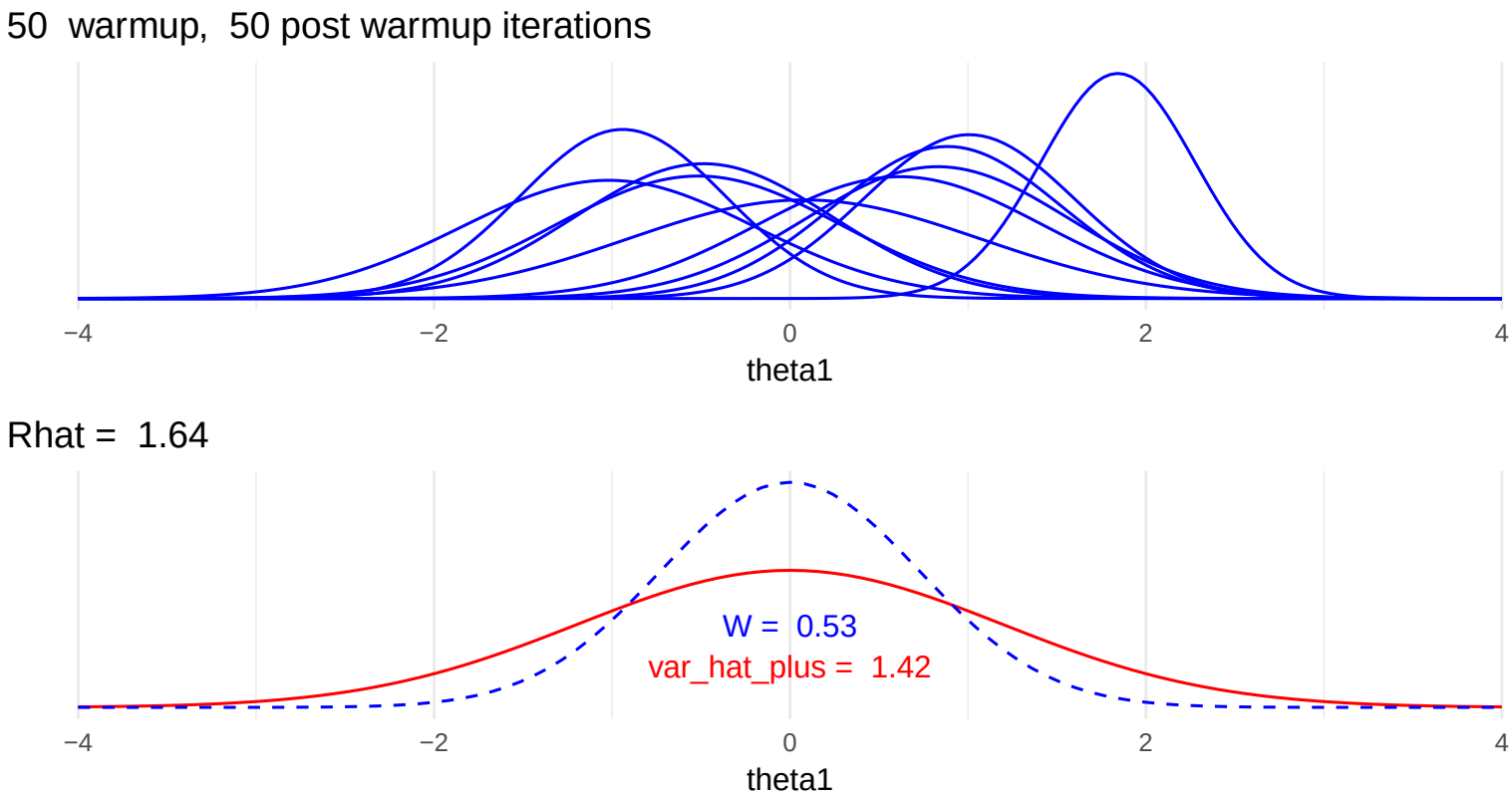

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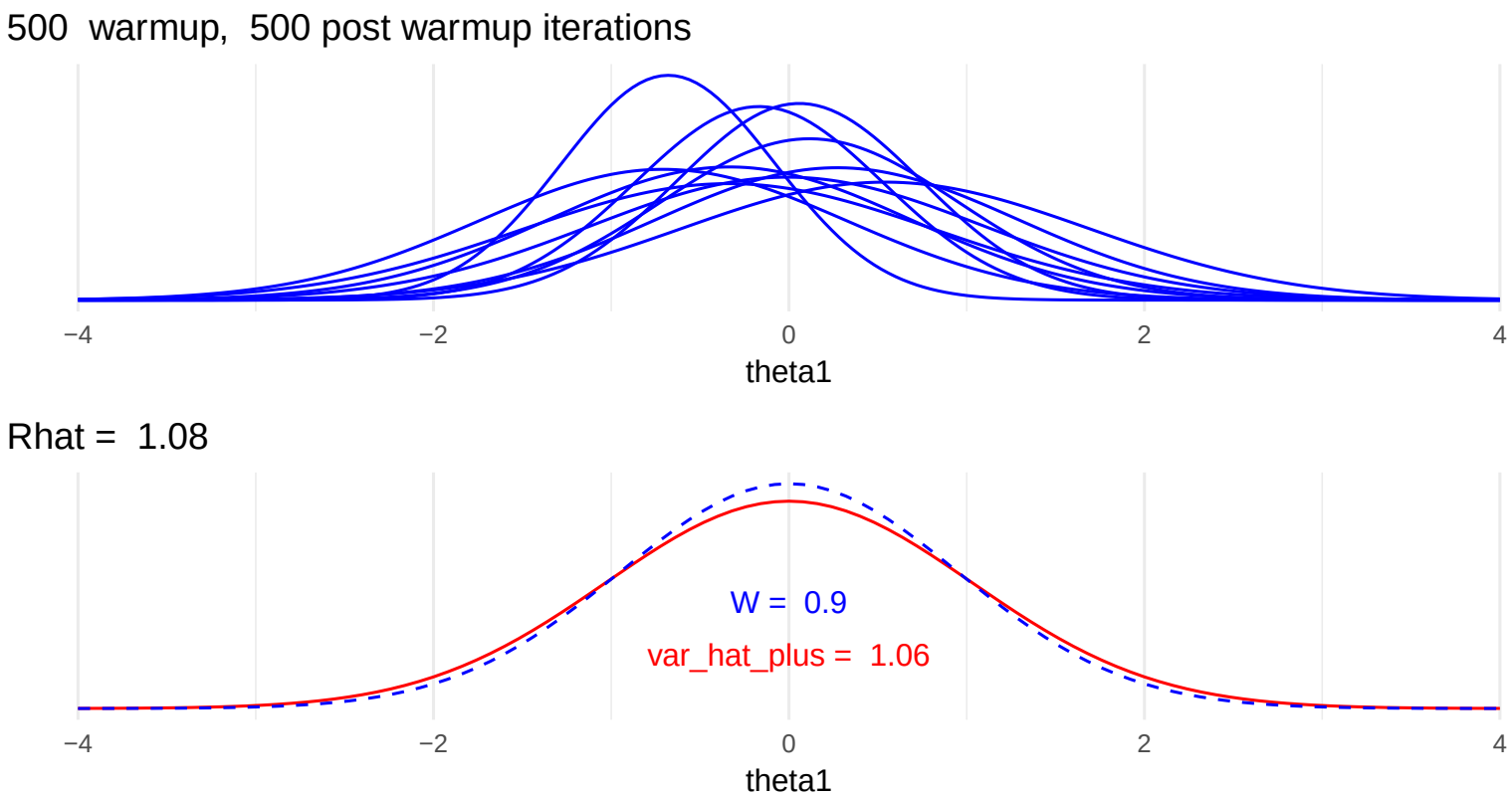

$\widehat{R}$: comparison of within and between variances of the chains

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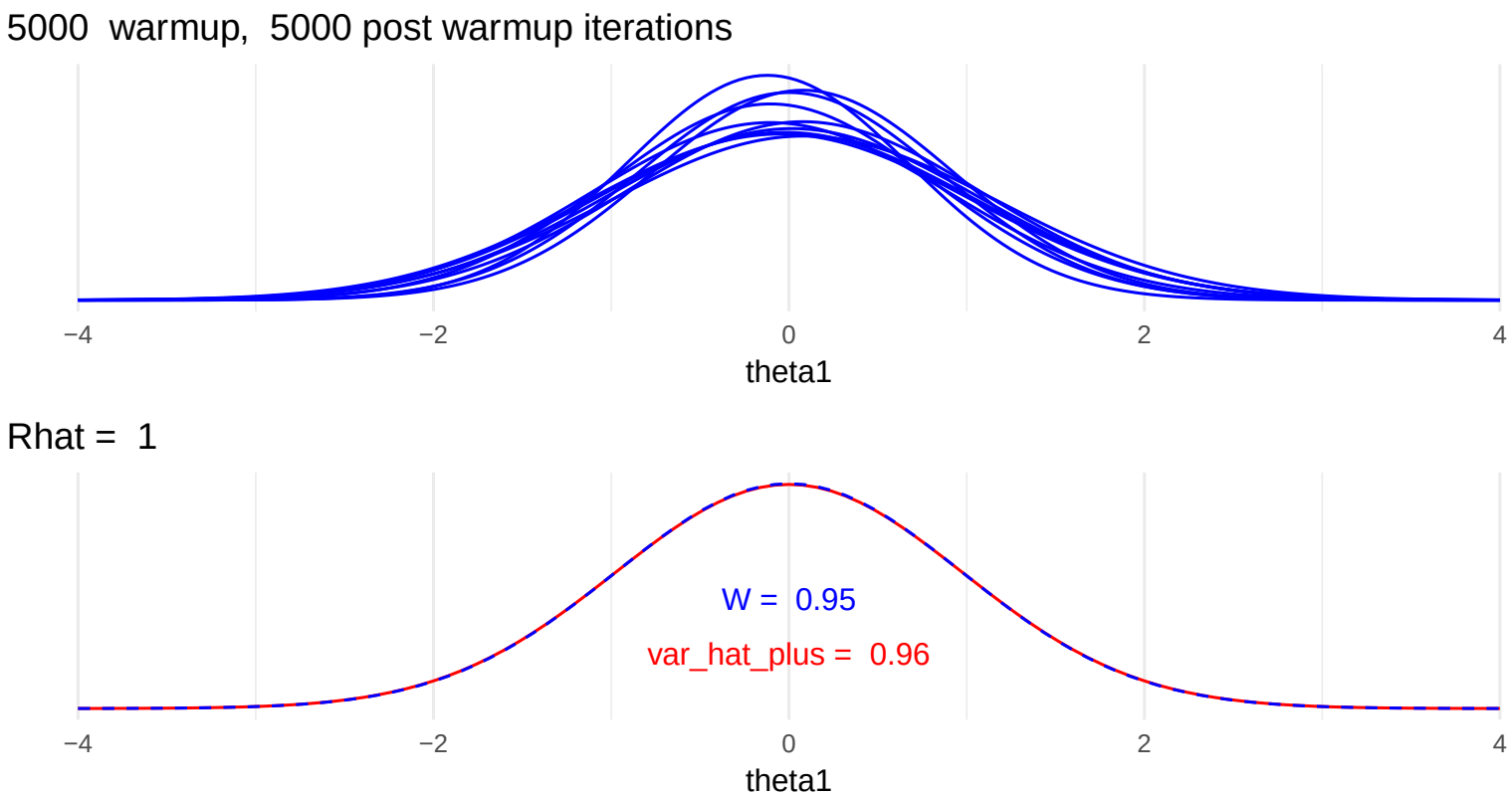

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- Between chains variance B

$$B = \frac{N}{M-1}\sum_{m=1}^{M}(\bar{\theta}_{.m} - \bar{\theta}_{..})^2,$$

$$\text{where } \bar{\theta}_{.m} = \frac{1}{N}\sum_{n=1}^{N}\theta_{nm},\ \bar{\theta}_{..} = \frac{1}{M}\sum_{m=1}^{M}\bar{\theta}_{.m}$$

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

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

- BDA3: $\widehat{R}$ aka *potential scale reduction factor* (PSRF)
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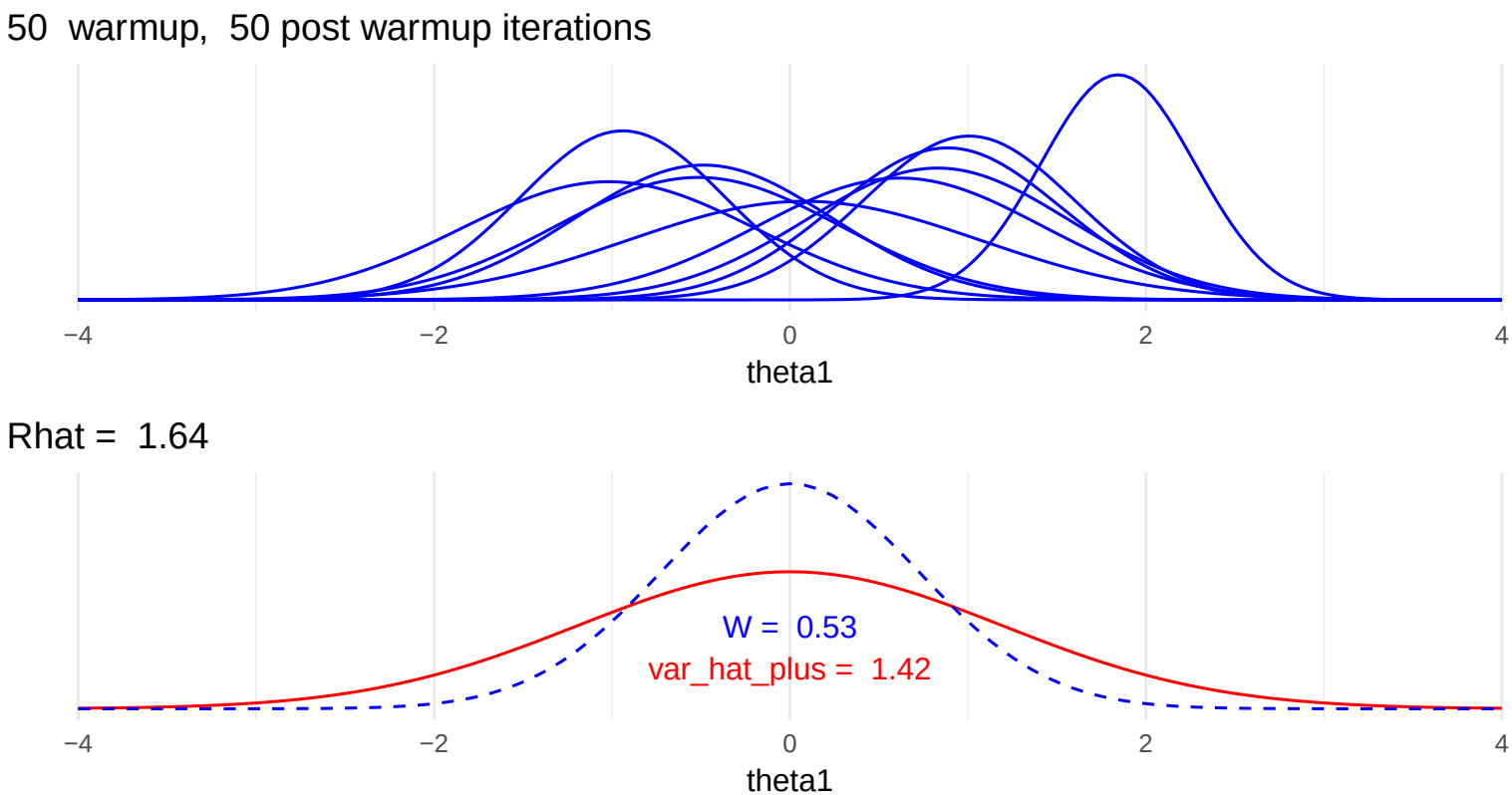

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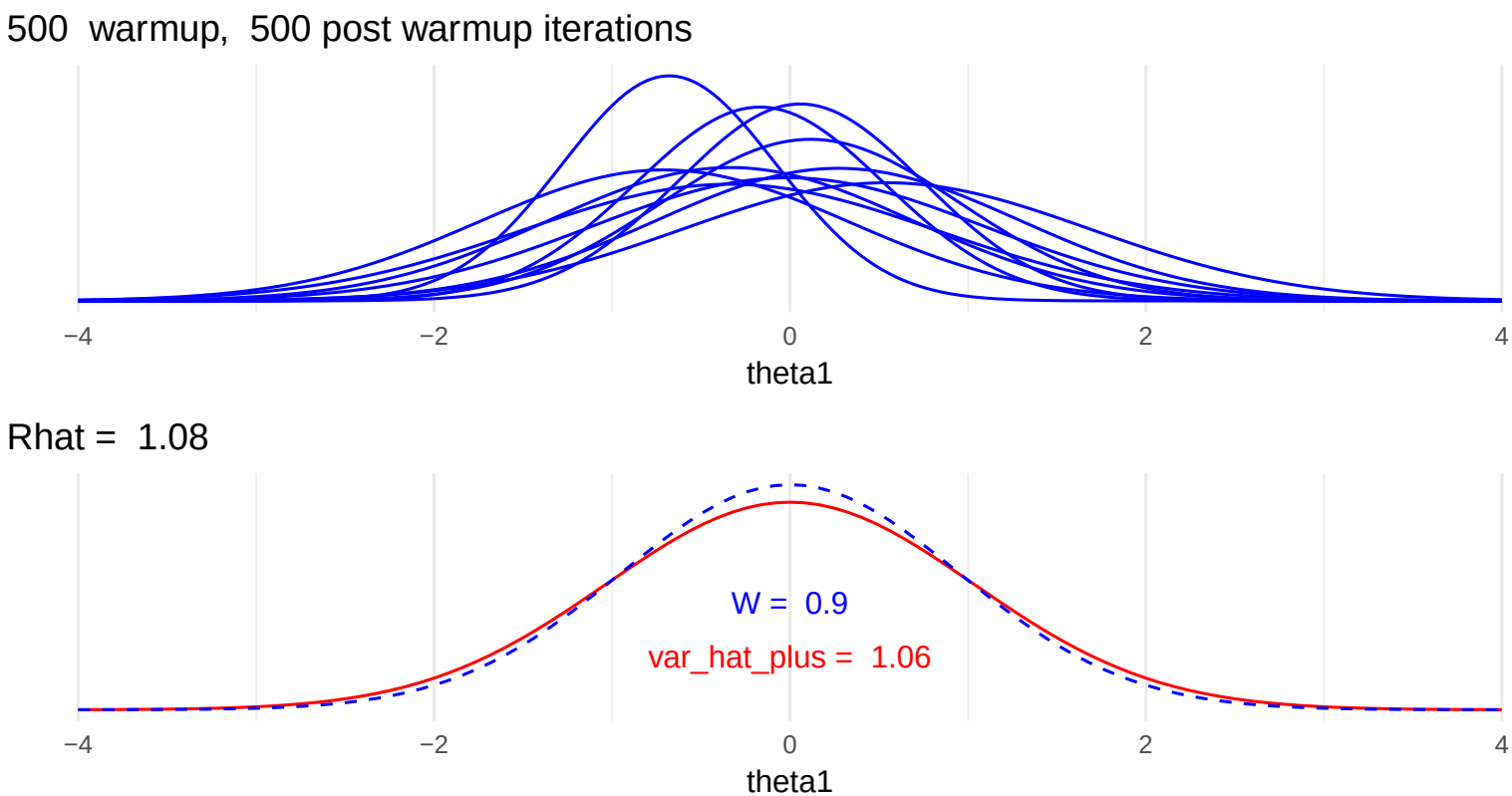

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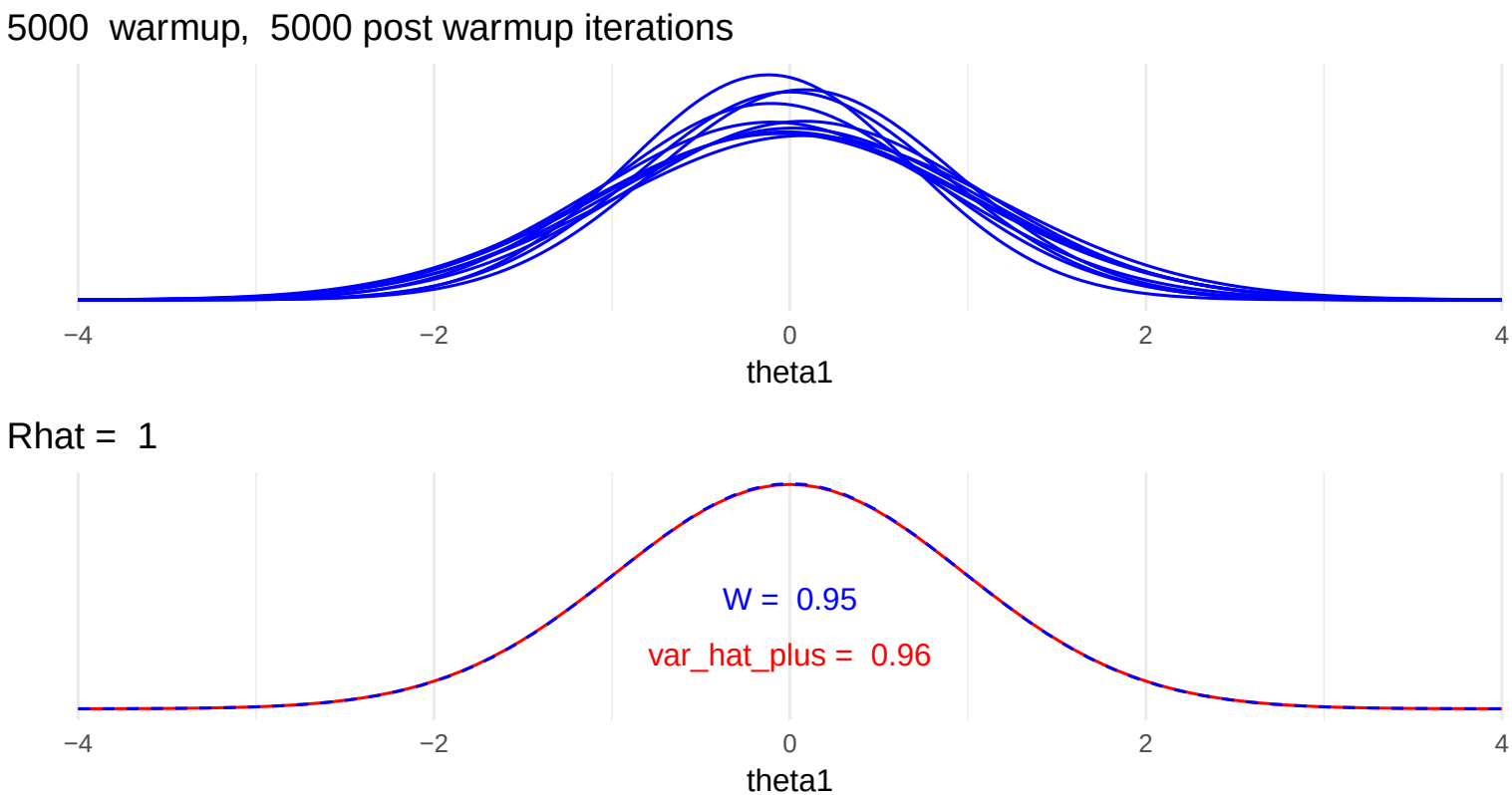

$\widehat{R}$

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

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

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- 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-$\widehat{R}$

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

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- Notation updated compared to BDA3

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$\widehat{R}$ and rank normalized $\widehat{R}$ in `posterior` package

`rhat_basic()` without rank normalization
`rhat()` with rank normalization

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`rhat()` with rank normalization

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

```
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
```

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

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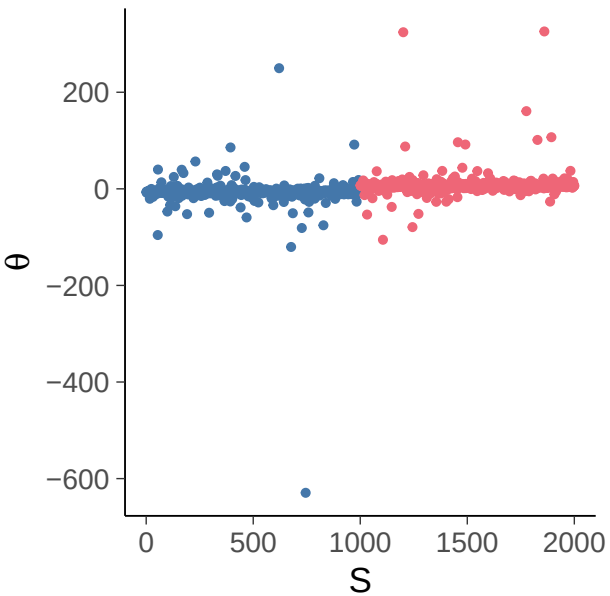
           dim=c(1000, 2, 1))
x <- as_draws_matrix(x)
variables(x) <- "t1_2"
```

```
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 $\widehat{R}$

For example:

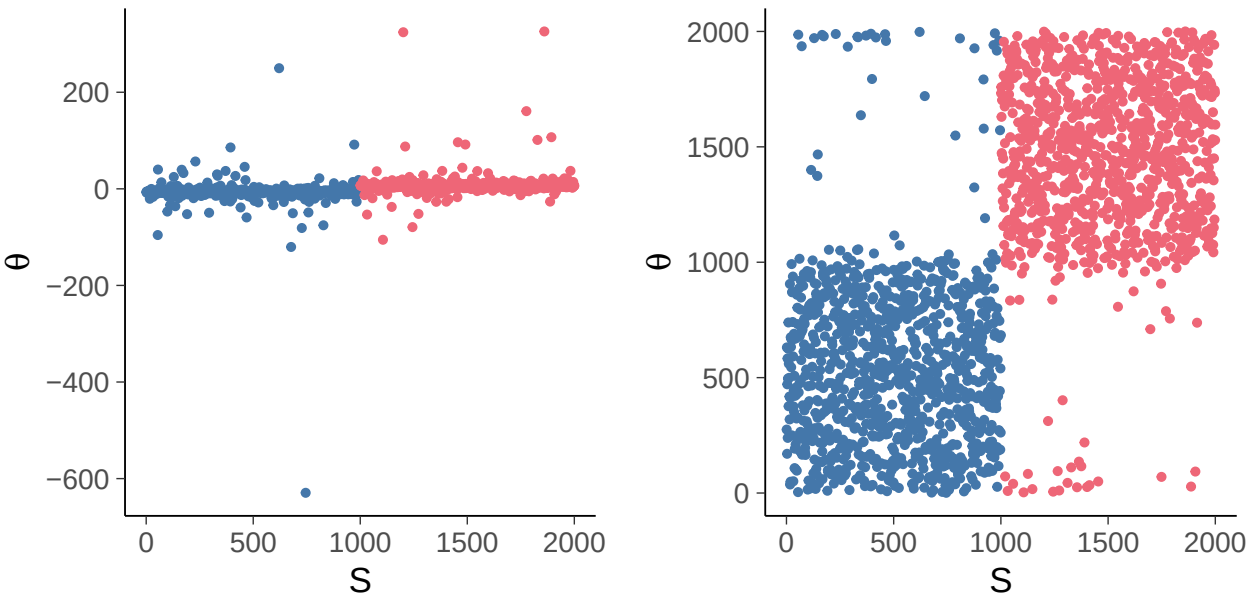
Cauchy mixture



Rank normalized $\widehat{R}$

For example:

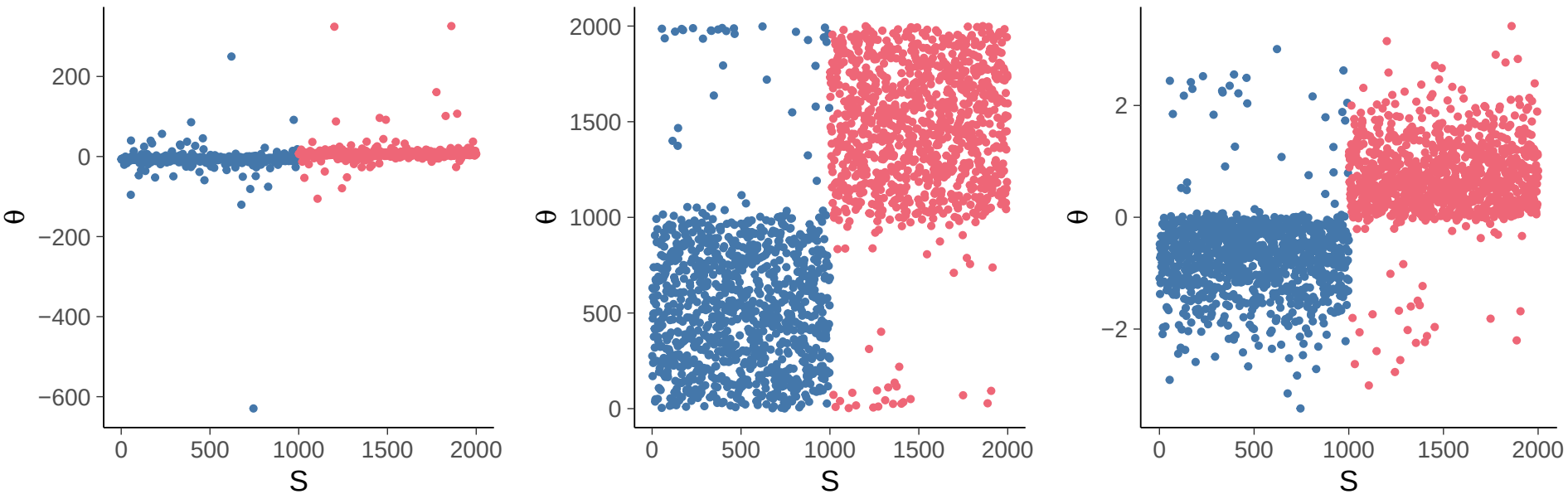
Cauchy mixture $\longrightarrow$ ranks



Rank normalized $\widehat{R}$

For example:

Cauchy mixture → ranks → inverse cdf



$\widehat{R}$ and rank normalized $\widehat{R}$ 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"
```

$\widehat{R}$ and rank normalized $\widehat{R}$ in `posterior` package

`rhat_basic()` without rank normalization
`rhat()` with **folding** and rank normalization

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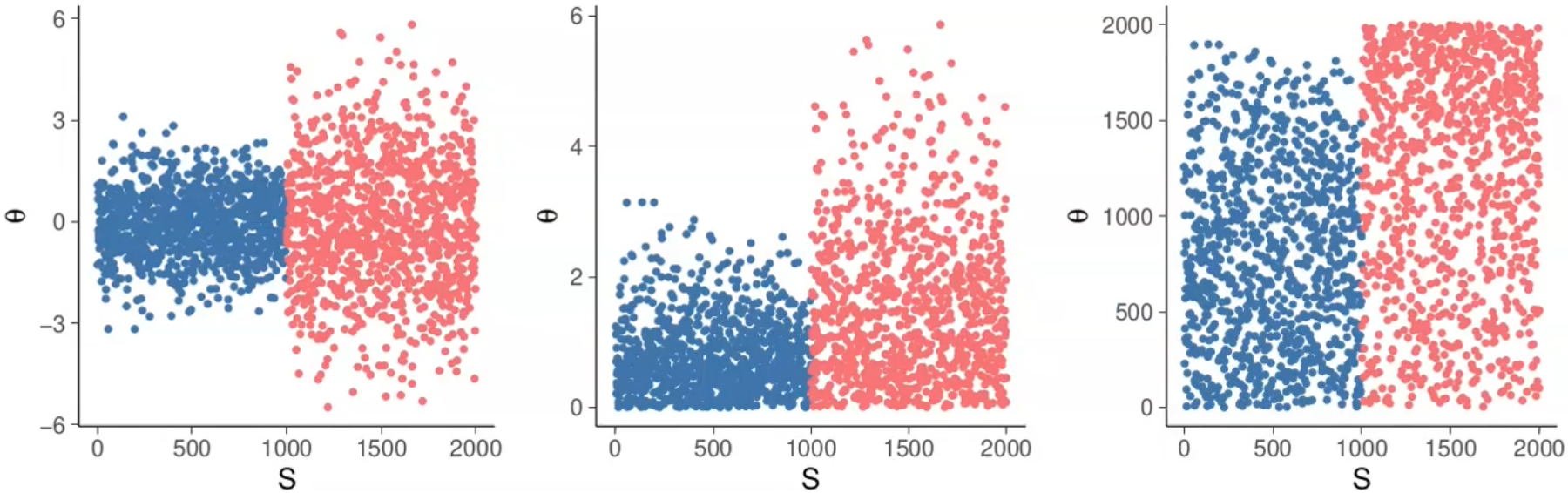
           dim=c(1000, 2, 1))
x <- as_draws_matrix(x)
variables(x) <- "N2v"
```

```
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 $\widehat{R}$ with folding

For example:

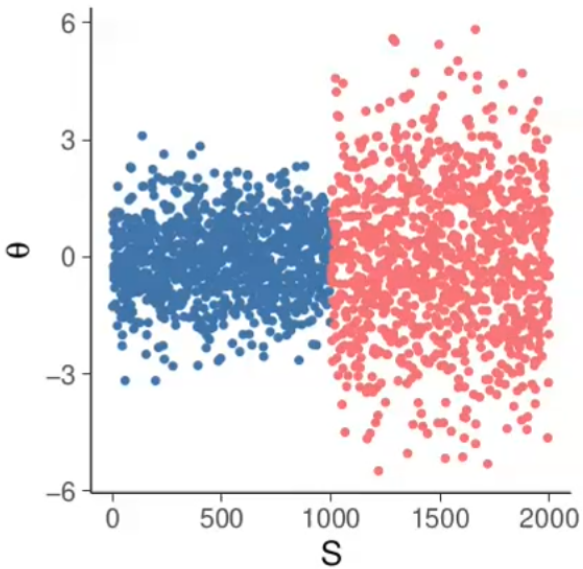
Normal variance mixture $\longrightarrow$ folded $\longrightarrow$ ranks

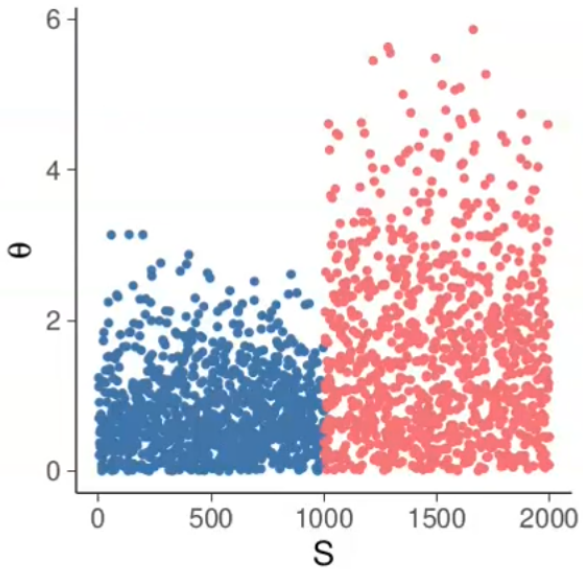


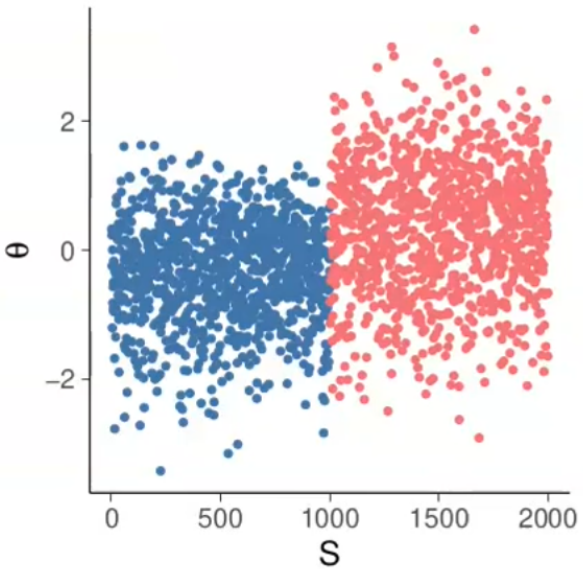
Rank normalized $\widehat{R}$ with folding

For example:

Normal variance mixture $\longrightarrow$ folded $\longrightarrow$ inverse cdf





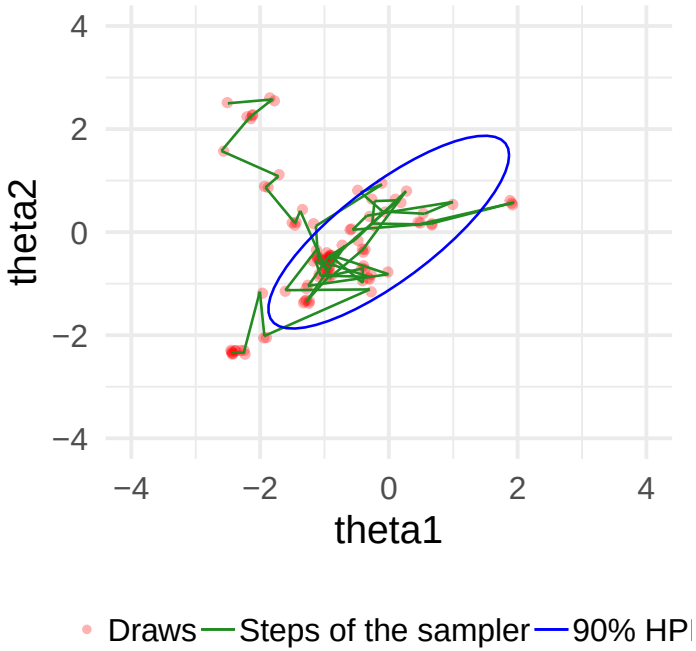


Time series analysis

- 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

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

Autocorrelation



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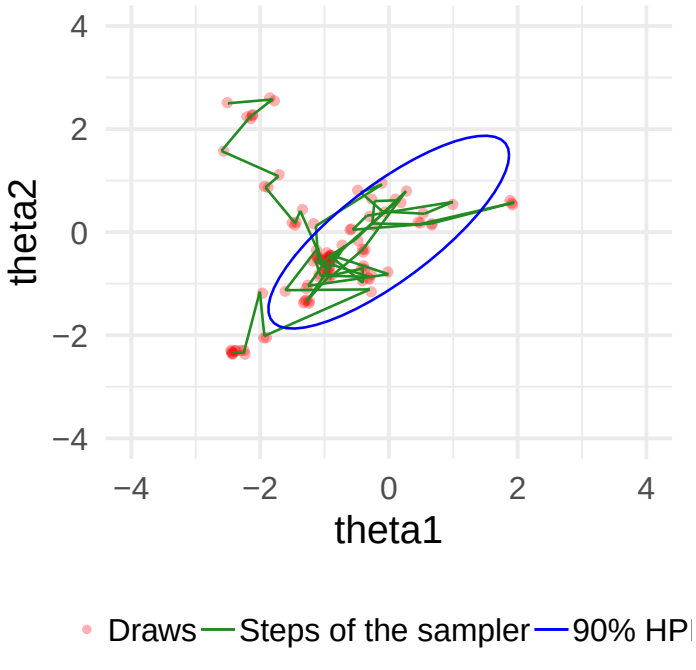

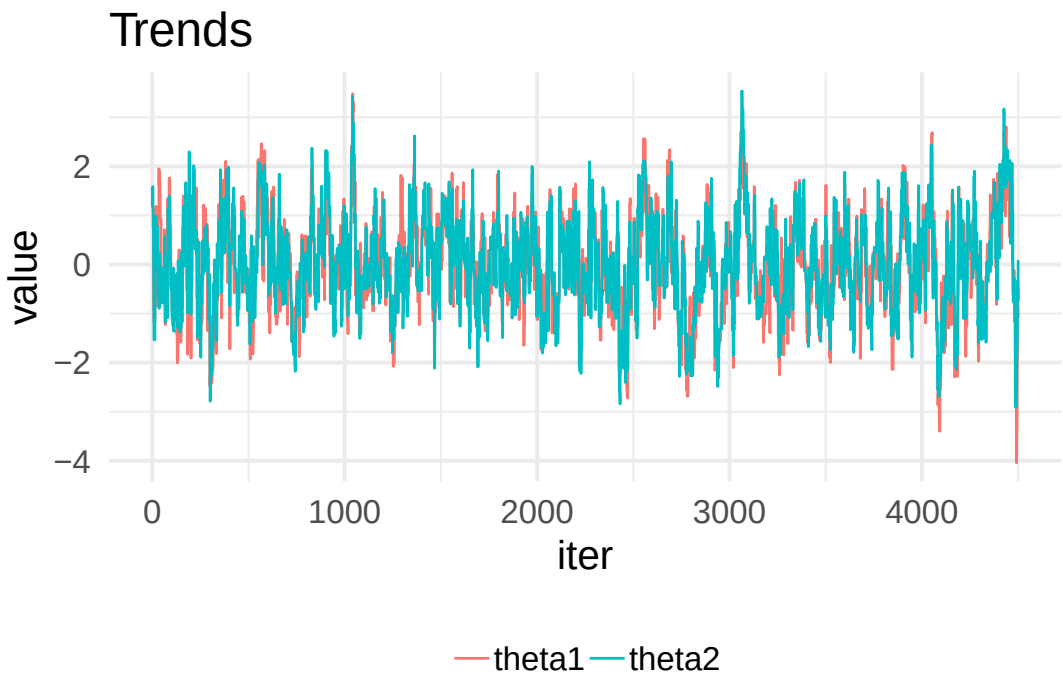

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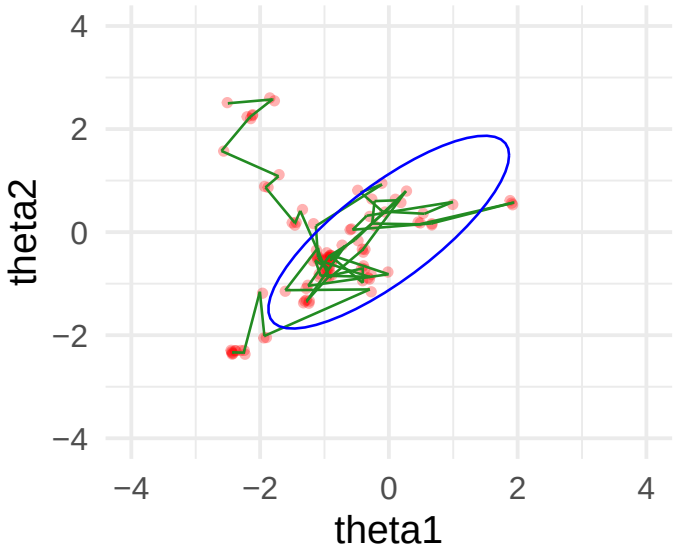
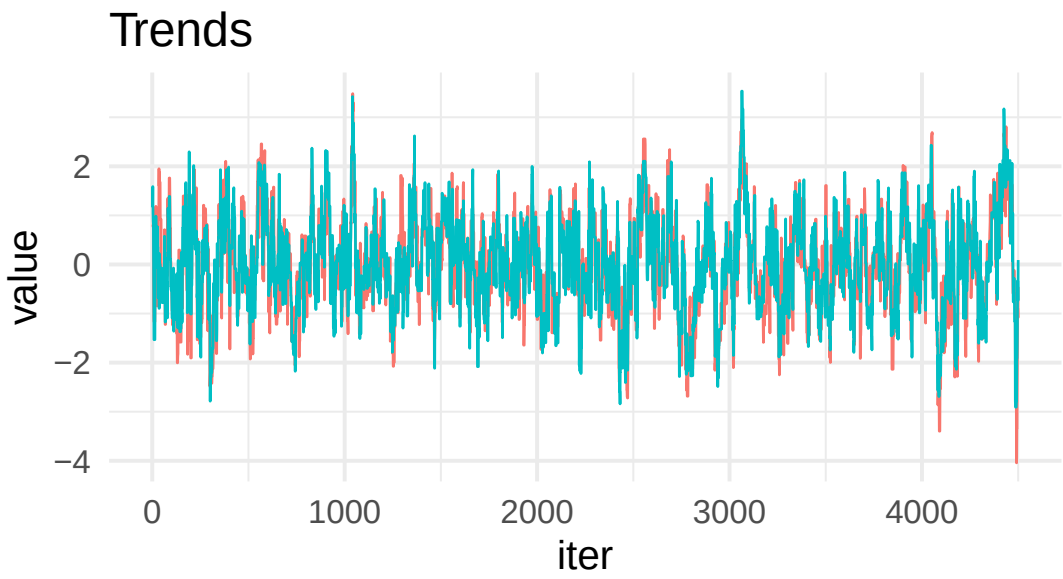
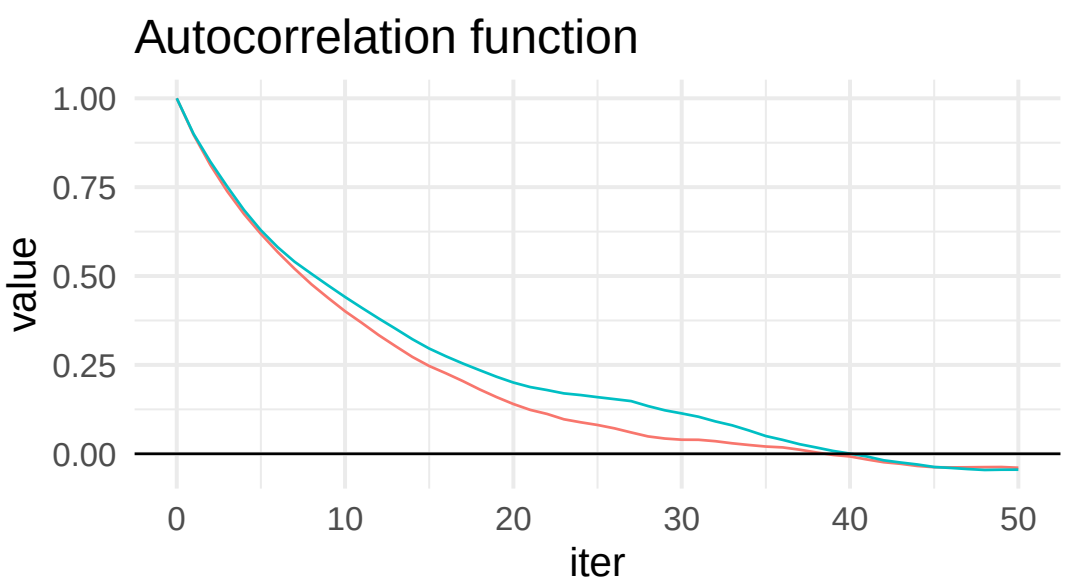


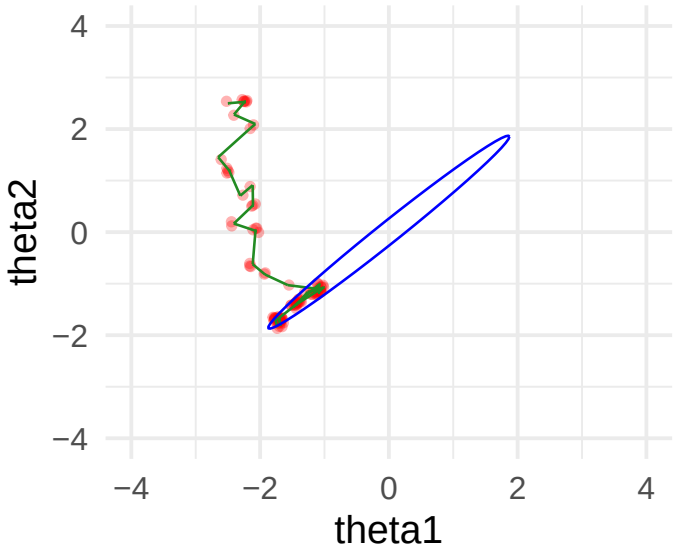


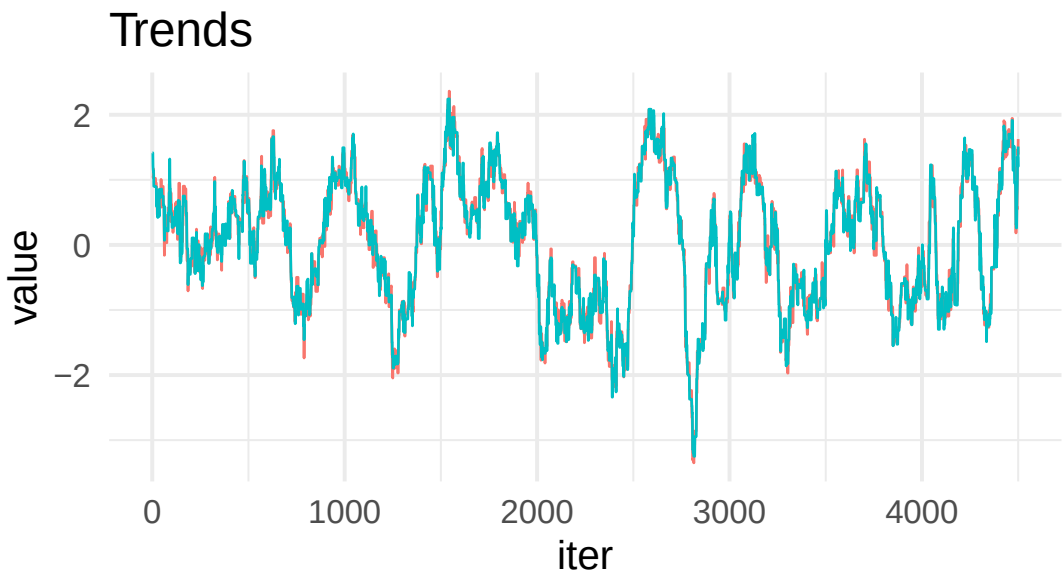
Draws Steps of the sampler 90% HP

theta1 theta2



Autocorrelation (slow mixing due to small step size)





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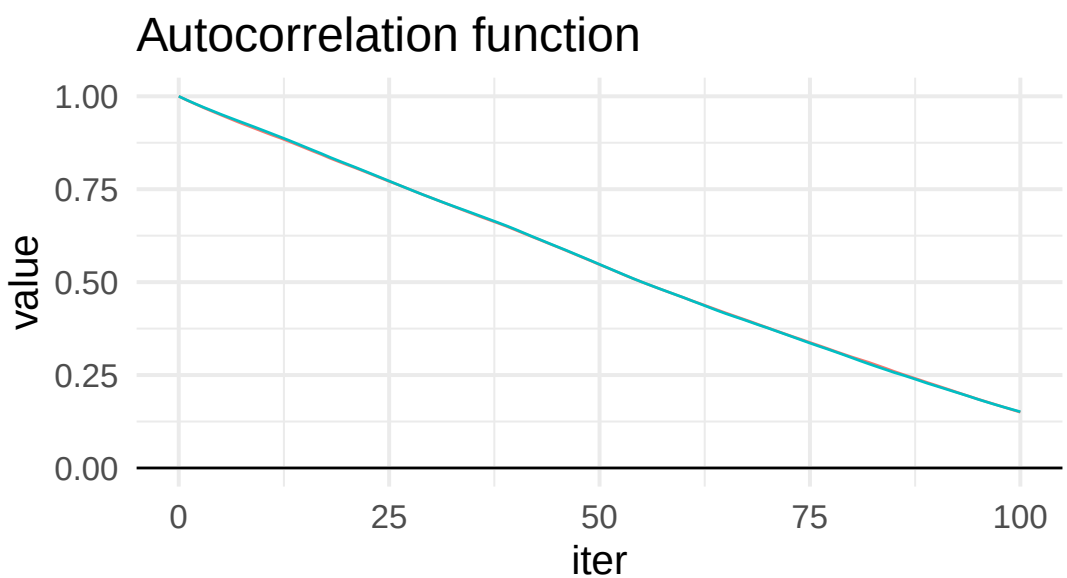
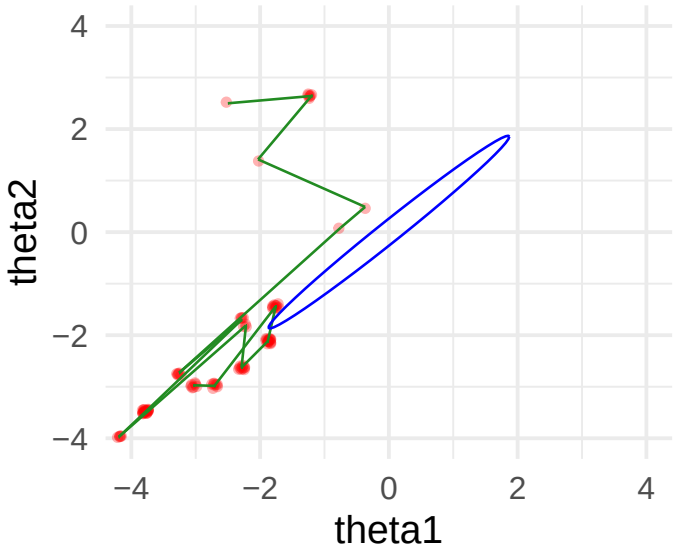
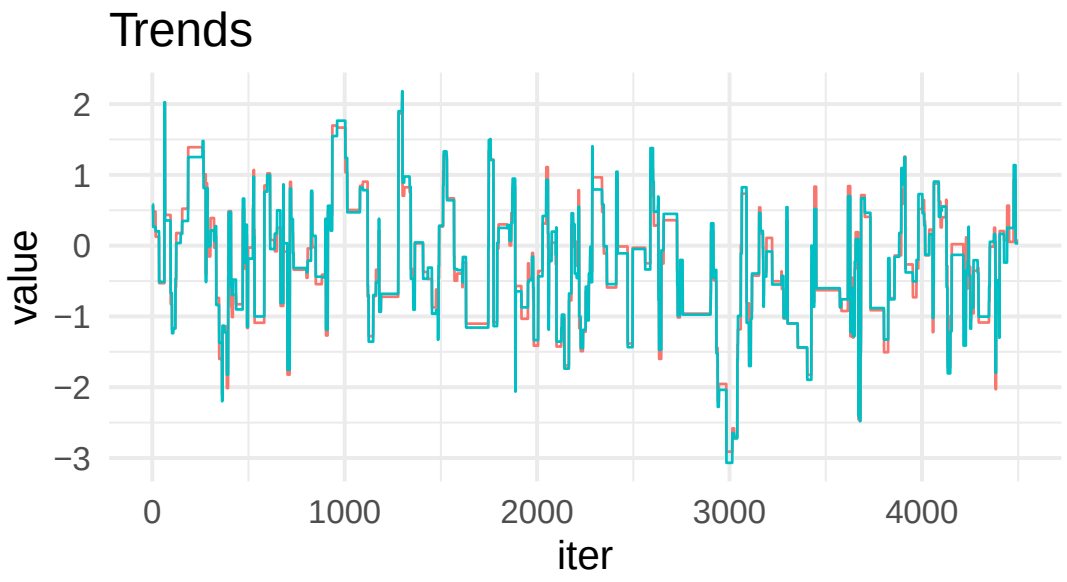


Autocorrelation (slow mixing due to many rejections)





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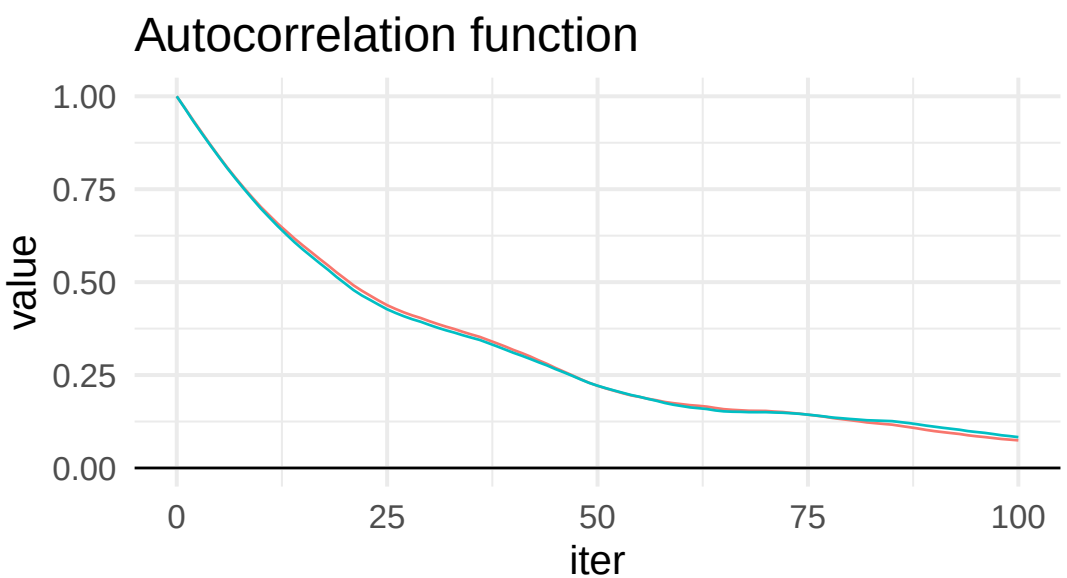
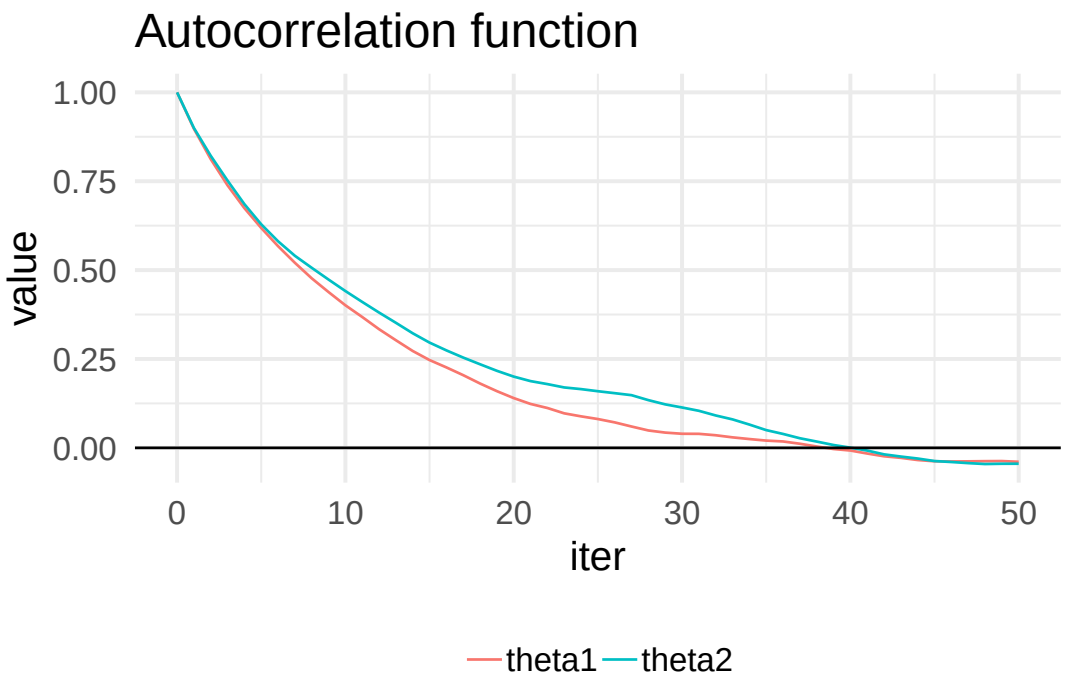


Time series analysis

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

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

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



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  - new $\widehat{R}$ paper $S = NM$ (in BDA3 $N = nm$ and $n_{\mathrm{eff}} = N/\tau$)

Time series analysis

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

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

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

  - τ describes the relative inefficiency due to the dependency
  - new $\widehat{R}$ 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 $\widehat{R}$ paper discusses more about MCSEs for different quantities

Time series analysis

- Estimation of the autocorrelation using several chains

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

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

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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 τ

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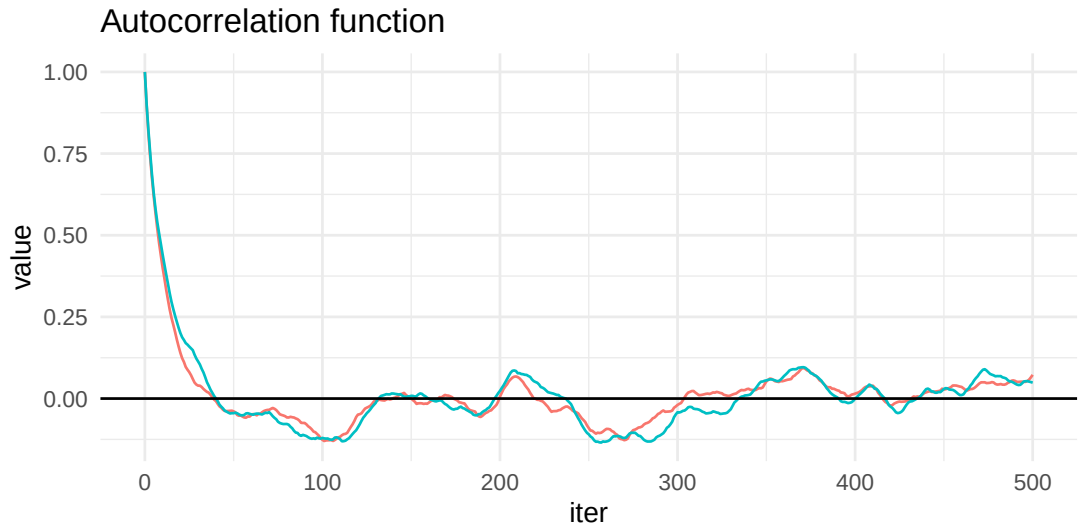

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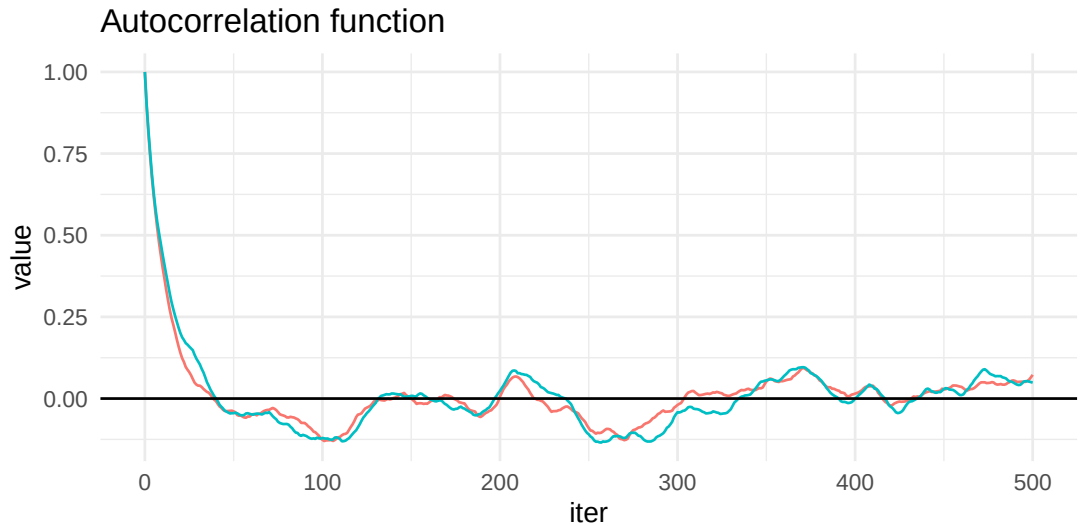

- empirical autocorrelation function is noisy and thus estimate of τ is noisy
- noise is larger for longer lags (less observations)
- less noisy estimate is obtained by truncating

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

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
  - Γ_m is positive, decreasing and convex function of m

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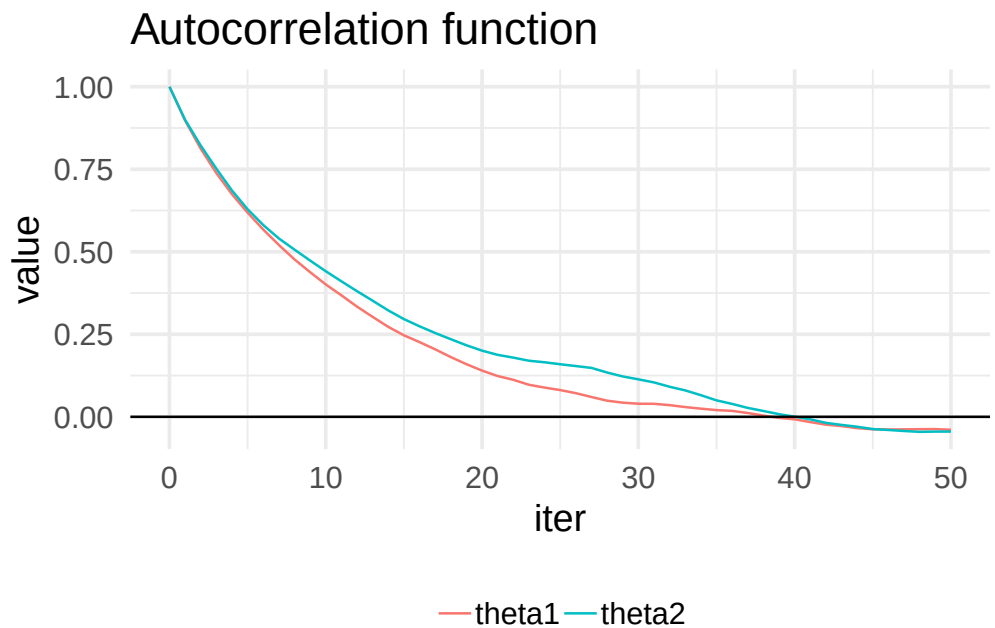
  - let $\Gamma_m = \rho_{2m} + \rho_{2m+1}$, which is sum of two consequent autocorrelations
  - Γ_m is positive, decreasing and convex function of m
- Initial positive sequence estimator (Geyer's IPSE)
  - Choose the largest m so, that all values of the sequence $\hat{\Gamma}_1, \ldots, \hat{\Gamma}_m$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



Effective sample size

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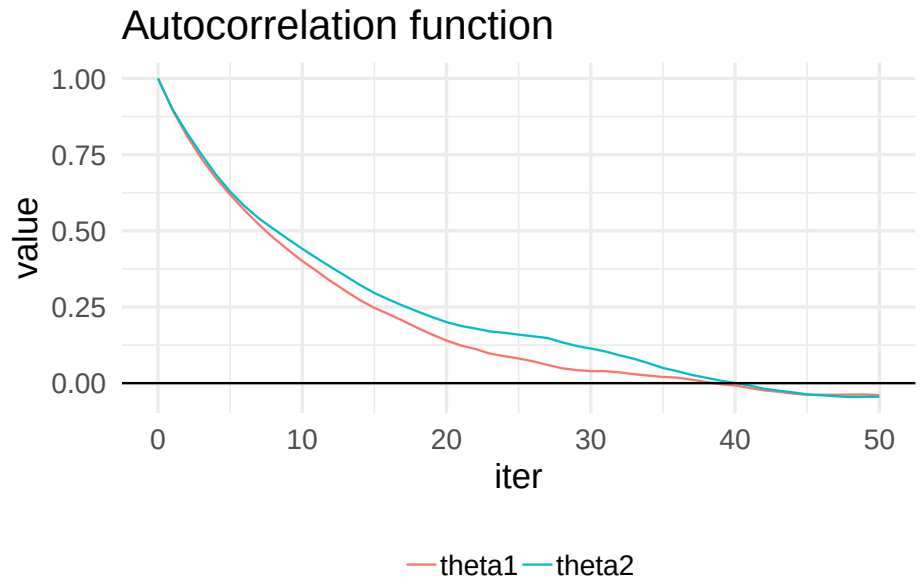

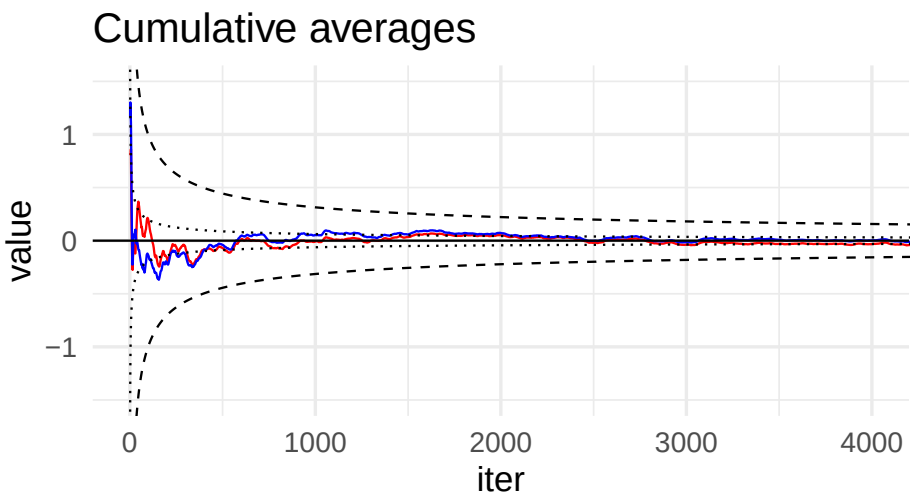

$$\hat{\tau} = 1 + 2\sum_{t=1}^{T} \hat{\rho}_t$$

$$\approx 24$$

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

Effective sample size

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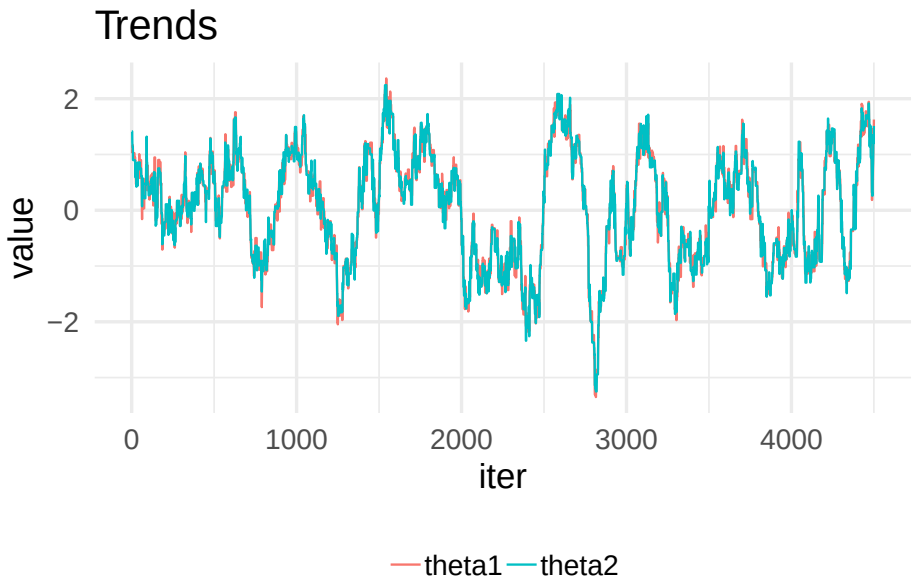

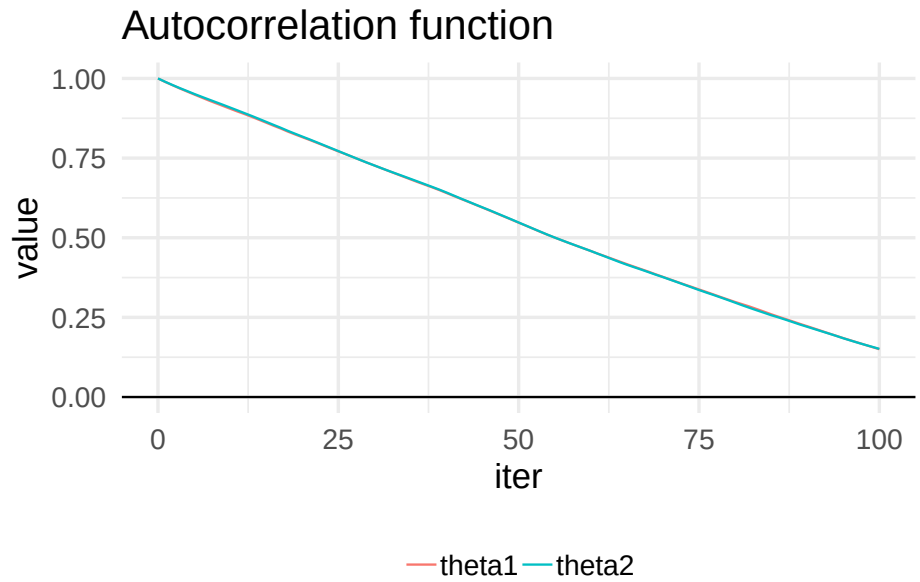

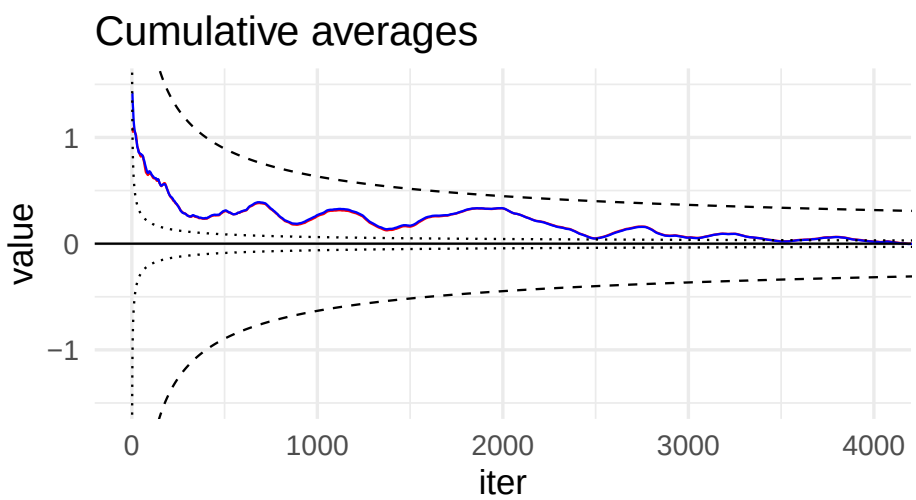

$$\hat{\tau} = 1 + 2\sum_{t=1}^{T} \hat{\rho}_t$$

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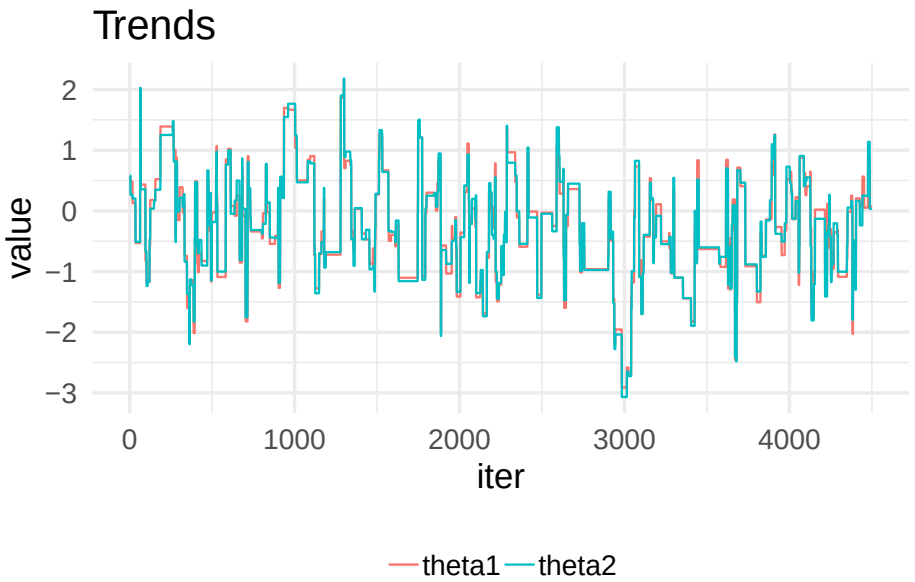

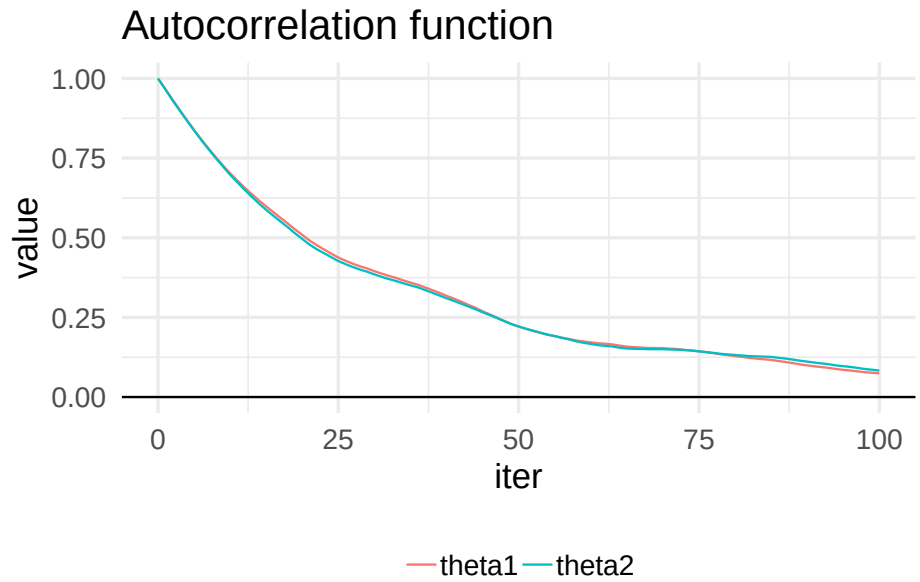

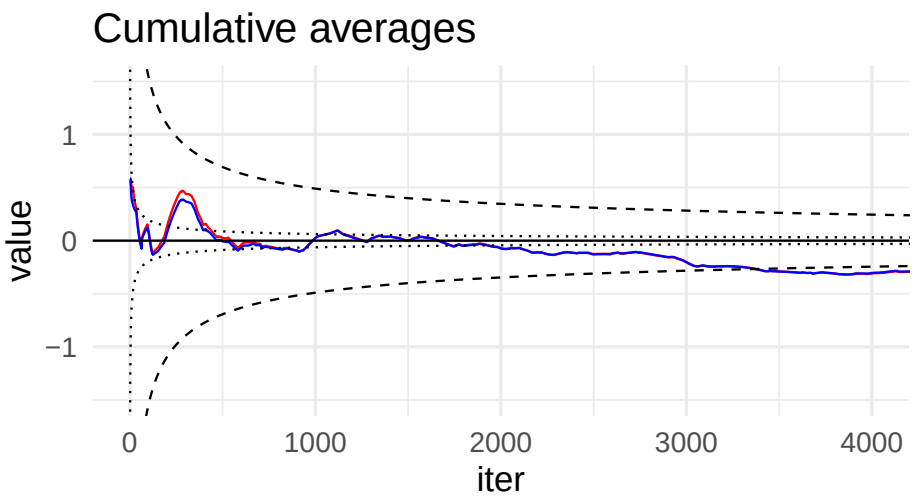

$$\hat{\tau} = 1 + 2\sum_{t=1}^{T} \hat{\rho}_t$$

$$\approx 63$$

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,
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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 $\widehat{R}$ `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:

- $\widehat{R}$, 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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  - `library(bayesplot)`
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- Python
  - see ArviZ package

Problematic distributions

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

Next week: HMC, NUTS, and dynamic HMC

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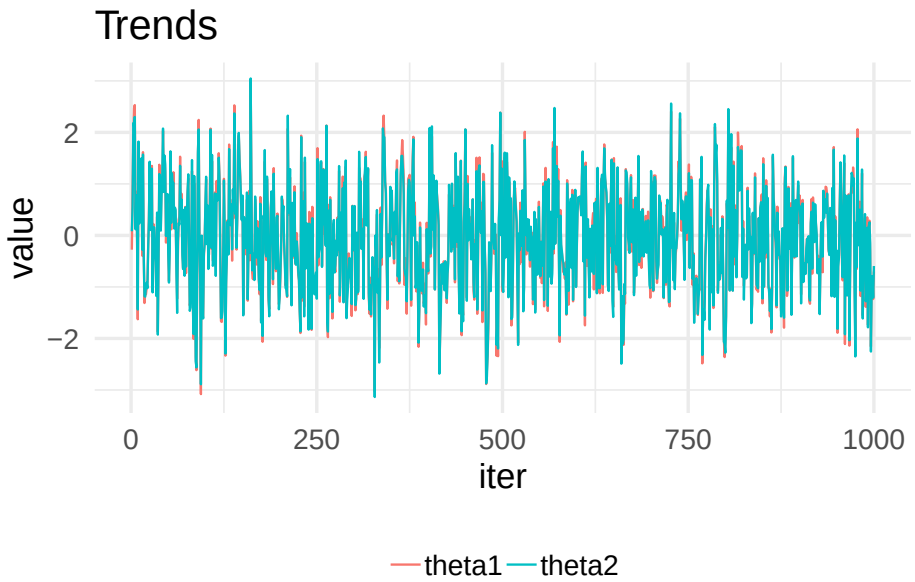

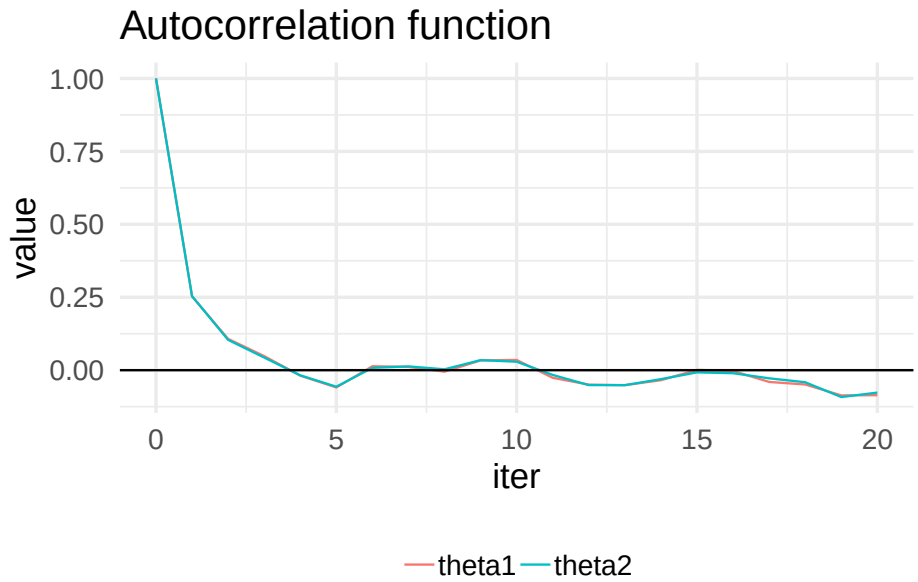

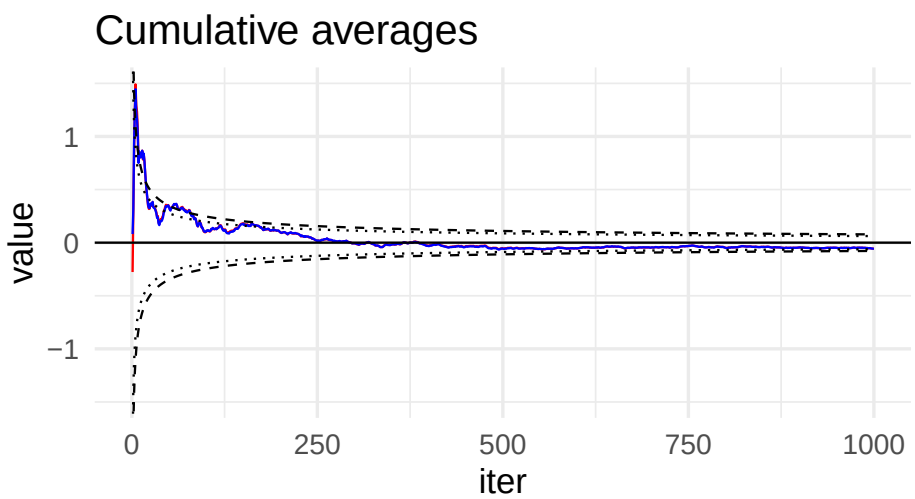

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$$\approx 1.6$$

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

MCMC summary

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