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Bayesian Statistics and Data Analysis
Lecture 5

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Thanks to Aki Vehtari, Aalto University

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It's all about expectations

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

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

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

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

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Monte Carlo

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  - Inverse CDF works for 1D

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  - Laplace, Variational*, EP* (Ch 4, 13*, next course)

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- Goal in MCMC: Construct a transition distribution with $p(\theta|y)$ as the stationary distribution

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Markov chain Monte Carlo (MCMC)

- Produce draws $\theta^{(t)}$ given $\theta^{(t-1)}$ from a Markov chain, with stationary distribution $p(\theta|y)$

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

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Markov chain Monte Carlo (MCMC)

- 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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- Chain has to be initialized with some starting point θ_0
- Transition distribution $T_t(\theta_t|\theta_{t-1})$ (may depend on t)
- Choose a transition distribution so the stationary distribution of the Markov chain is $p(\theta|y)$

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Gibbs sampling

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

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

- Will converge (in total variation) to $p(\theta|y)$ as $T \to \infty$

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- j can be multiple (blocked) parameters
- 1D sampling ($|j| = 1$) is generally easy

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- Related to the (stochastic) EM algorithm

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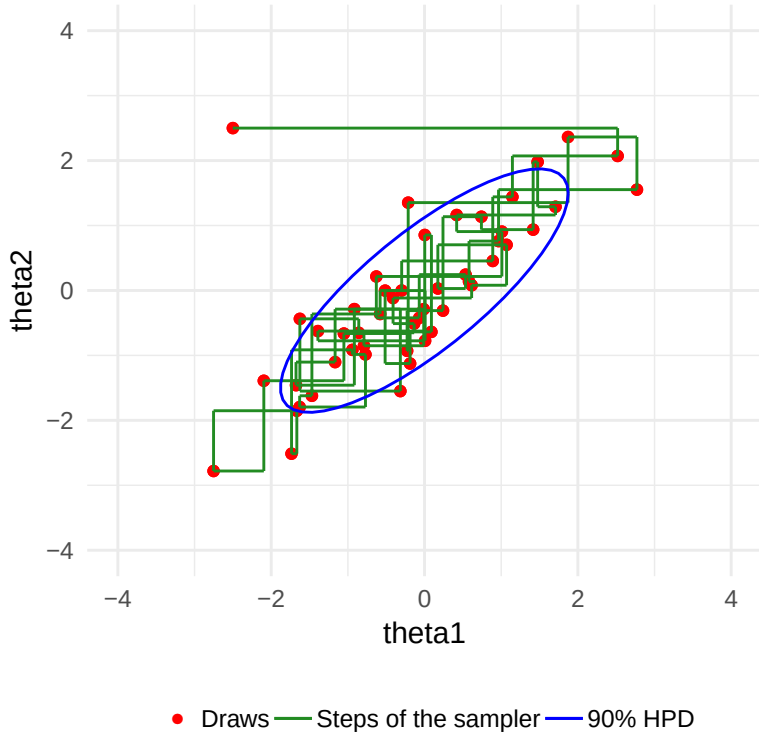
- Monte Carlo recap
- Markov Chain Monte Carlo (MCMC)
  - Gibbs sampling
  - Metropolis-Hastings

Gibbs sampling



demo

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- For not so easy conditionals, use e.g. inverse-CDF
- Several parameters can be updated in blocks (*blocking*)
- Slow if parameters are highly dependent in the posterior...

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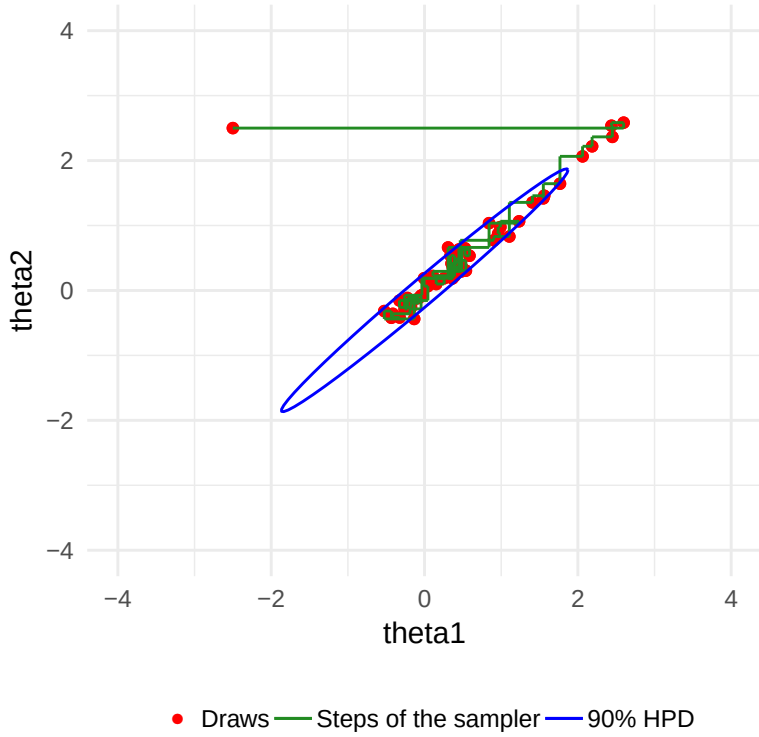

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Sampling conditional vs joint

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

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Sampling conditional vs joint

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

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The Metropolis algorithm

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

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

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

     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
  - step c is executed by generating a random number from $\mathcal{U}(0, 1)$
  - $p(\theta^*|y)$ 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!

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Metropolis algorithm

- Example: one bivariate observation (y_1, y_2)
  - bivariate normal distribution with unknown mean and known covariance

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

  - proposal distribution $J_t(\theta^*|\theta_{t-1}) = \mathcal{N}(\theta^*|\theta_{t-1}, \sigma_p^2)$

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Why Metropolis algorithm works

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

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- Theoretically
  1. Prove that simulated series is a Markov chain which has unique stationary distribution
  2. Prove that this stationary distribution is the desired target distribution

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Why Metropolis algorithm works

1. Prove that simulated series is a Markov chain which has unique stationary distribution
   a) irreducible

   b) aperiodic

   c) recurrent / not transient

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   c) recurrent / not transient
      = probability to return to a state i is 1 as $T \to \infty$
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Why Metropolis algorithm works

2. Prove that this stationary distribution is the desired target distribution $p(\theta|y)$
   - consider starting algorithm at time $t-1$ with a draw $\theta_{t-1} \sim p(\theta|y)$

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     which is the same as the probability of transition from θ_a to θ_b, since we have required that $J_t(\cdot|\cdot)$ is symmetric

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2. Prove that this stationary distribution is the desired target distribution $p(\theta|y)$
   - consider starting algorithm at time $t-1$ with a draw $\theta_{t-1} \sim p(\theta|y)$
   - consider any two such points θ_a and θ_b drawn from $p(\theta|y)$ and labeled so that $p(\theta_b|y) \geq p(\theta_a|y)$
   - the unconditional probability density of a transition from θ_a to θ_b is

$$p(\theta_{t-1} = \theta_a, \theta_t = \theta_b) = p(\theta_a|y) J_t(\theta_b|\theta_a),$$

   - the unconditional probability density of a transition from θ_b to θ_a is

$$\begin{aligned} p(\theta_t = \theta_a, \theta_{t-1} = \theta_b) &= p(\theta_b|y) J_t(\theta_a|\theta_b) \left(\frac{p(\theta_a|y)}{p(\theta_b|y)} \right) \\ &= p(\theta_a|y) J_t(\theta_a|\theta_b), \end{aligned}$$

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

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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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Metropolis-Hastings algorithm

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

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    $\rightarrow$ many steps accepted, but the chain moves slowly due to small steps
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demo

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  demo
- Generic rule for rejection rate is 60-90%

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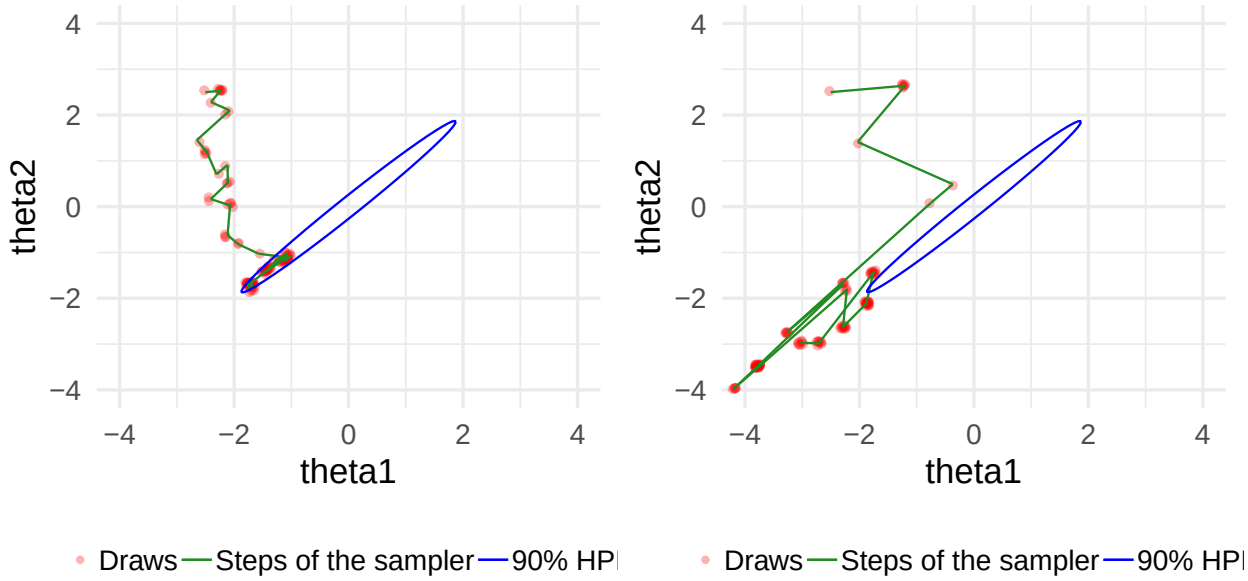
Gibbs sampling as a special case

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

Metropolis

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



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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
    - Demo http://elevanth.org/blog/2017/11/28/build-a-better-markov-chain/

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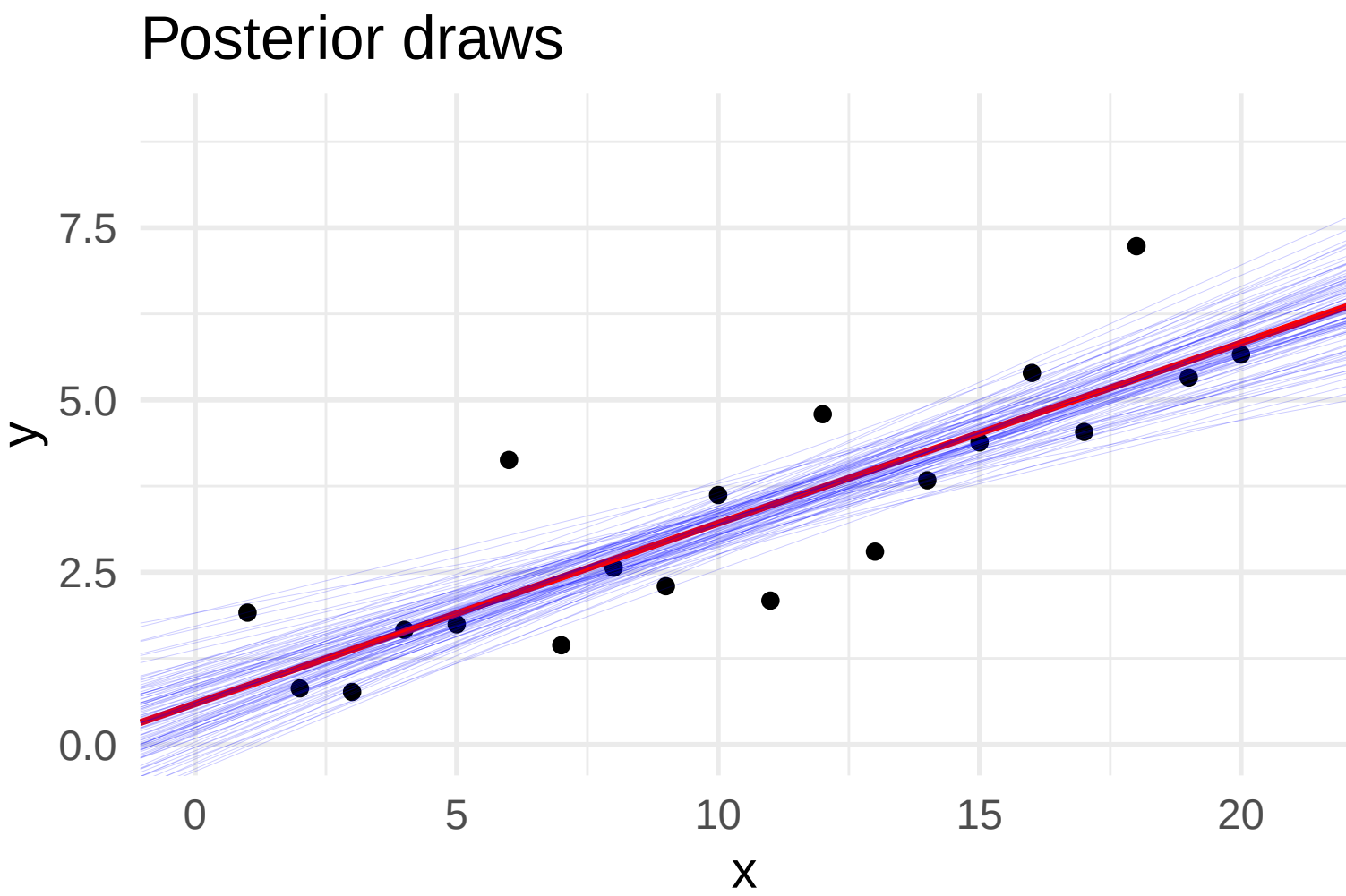
- Monte Carlo recap
- Markov Chain Monte Carlo (MCMC)
  - Gibbs sampling
  - Metropolis-Hastings

Example of uncertainty in modeling



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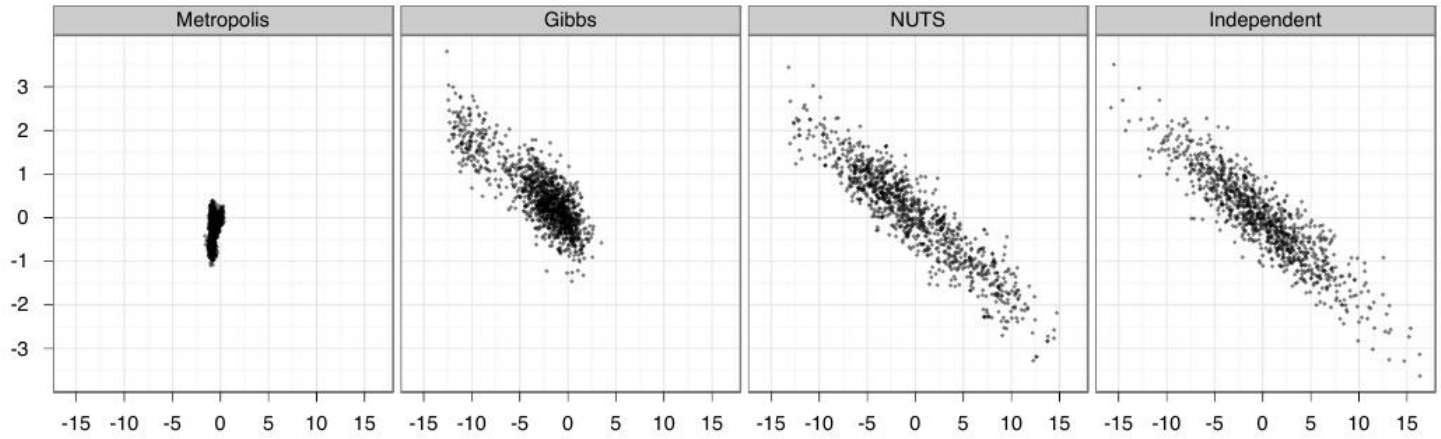
HMC / NUTS

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)



Source: Jonah Gabry

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Warm-up and convergence diagnostics

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

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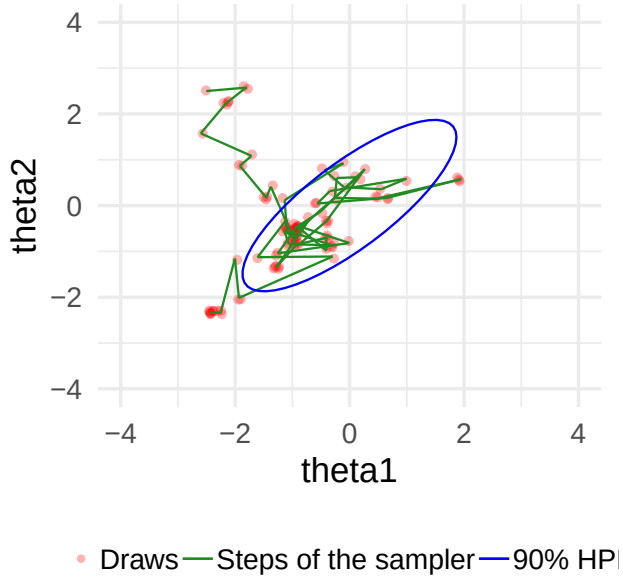

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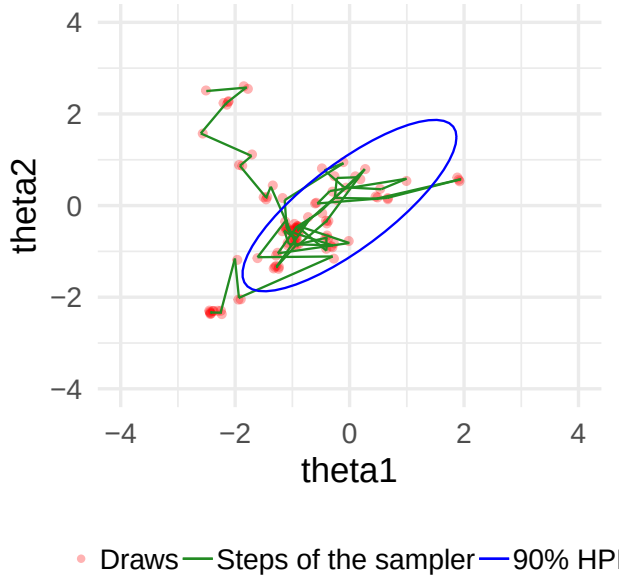

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  - warm-up may include also phase for adapting algorithm parameters

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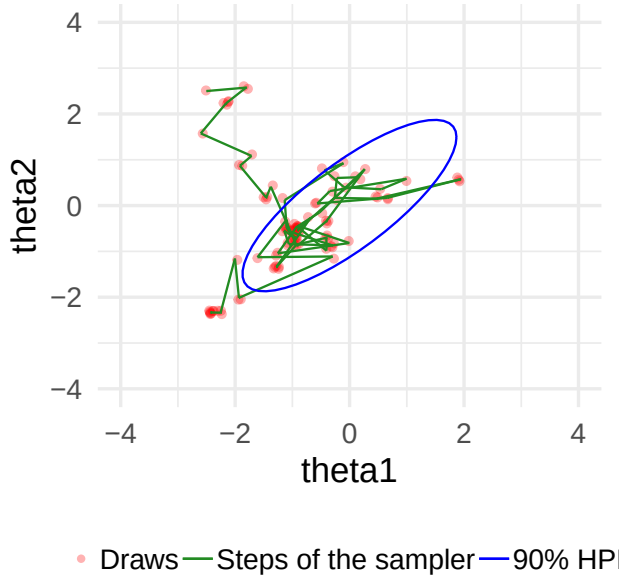

- Warm-up = remove draws from the beginning of the chain
  - warm-up may include also phase for adapting algorithm parameters
- Convergence diagnostics
  - Do we get samples from the target distribution?

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MCMC draws are dependent

- Monte Carlo estimates still valid (central limit theorem holds)

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

- Estimation of Monte Carlo error is more difficult
  - evaluation of *effective* sample size

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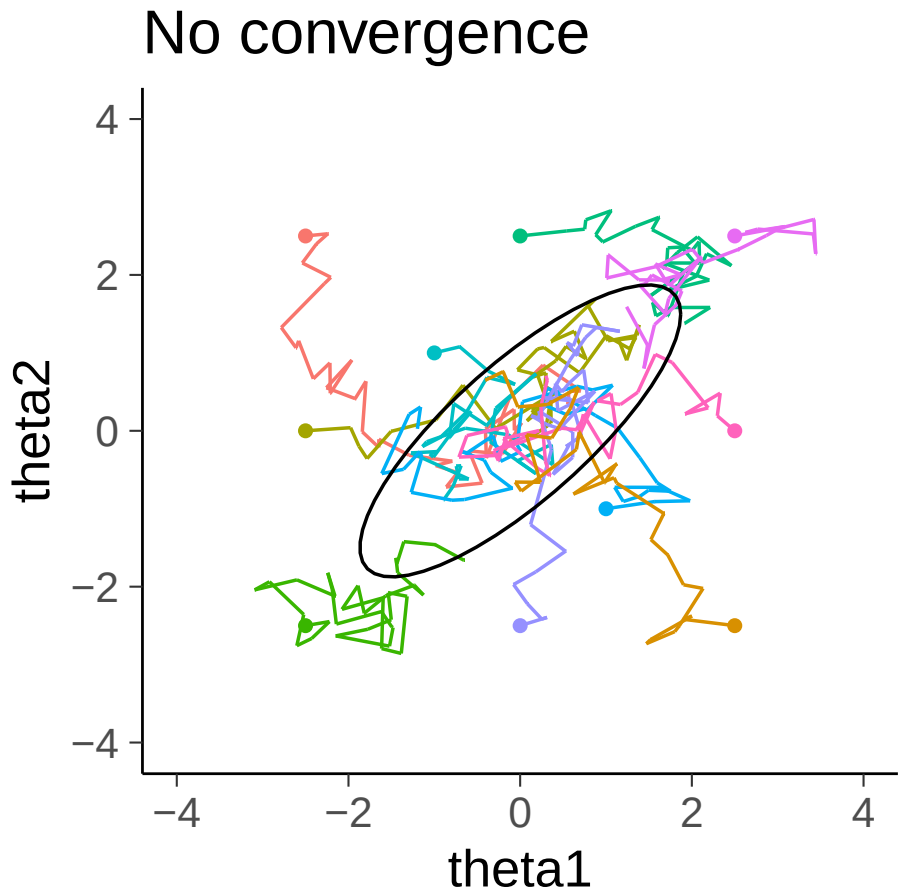
Several chains

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



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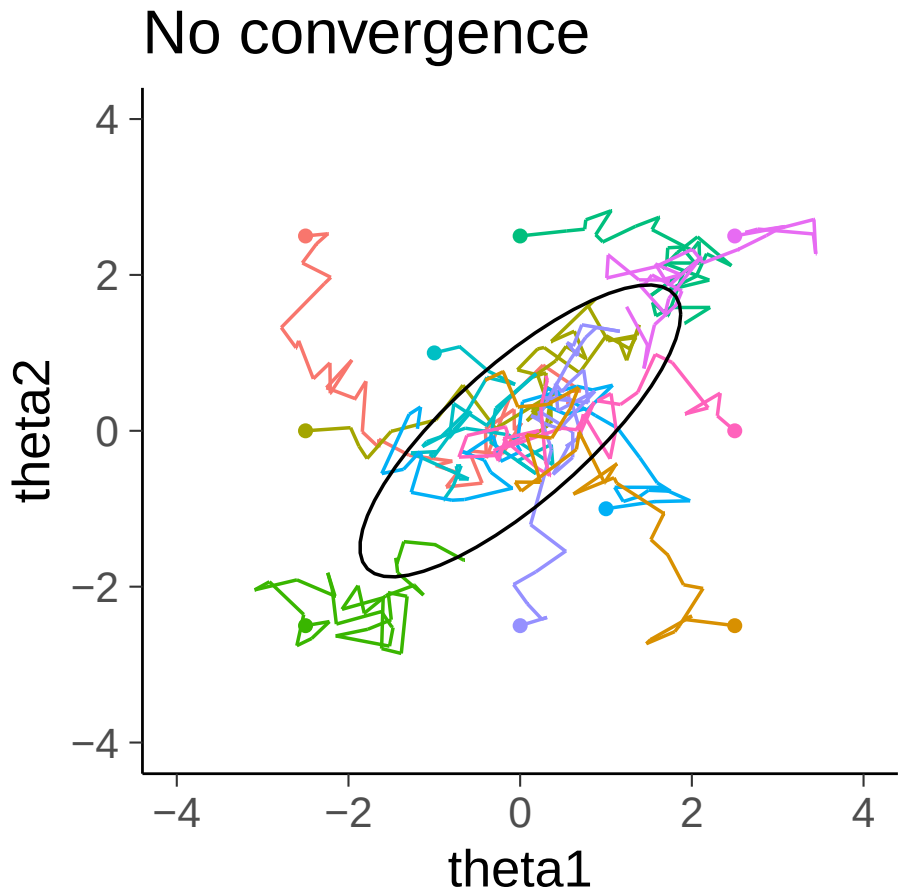

- Remove draws from the beginning of the chains and run chains long enough so that it is not possible to distinguish where each chain started and the chains are well mixed

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- Monte Carlo recap
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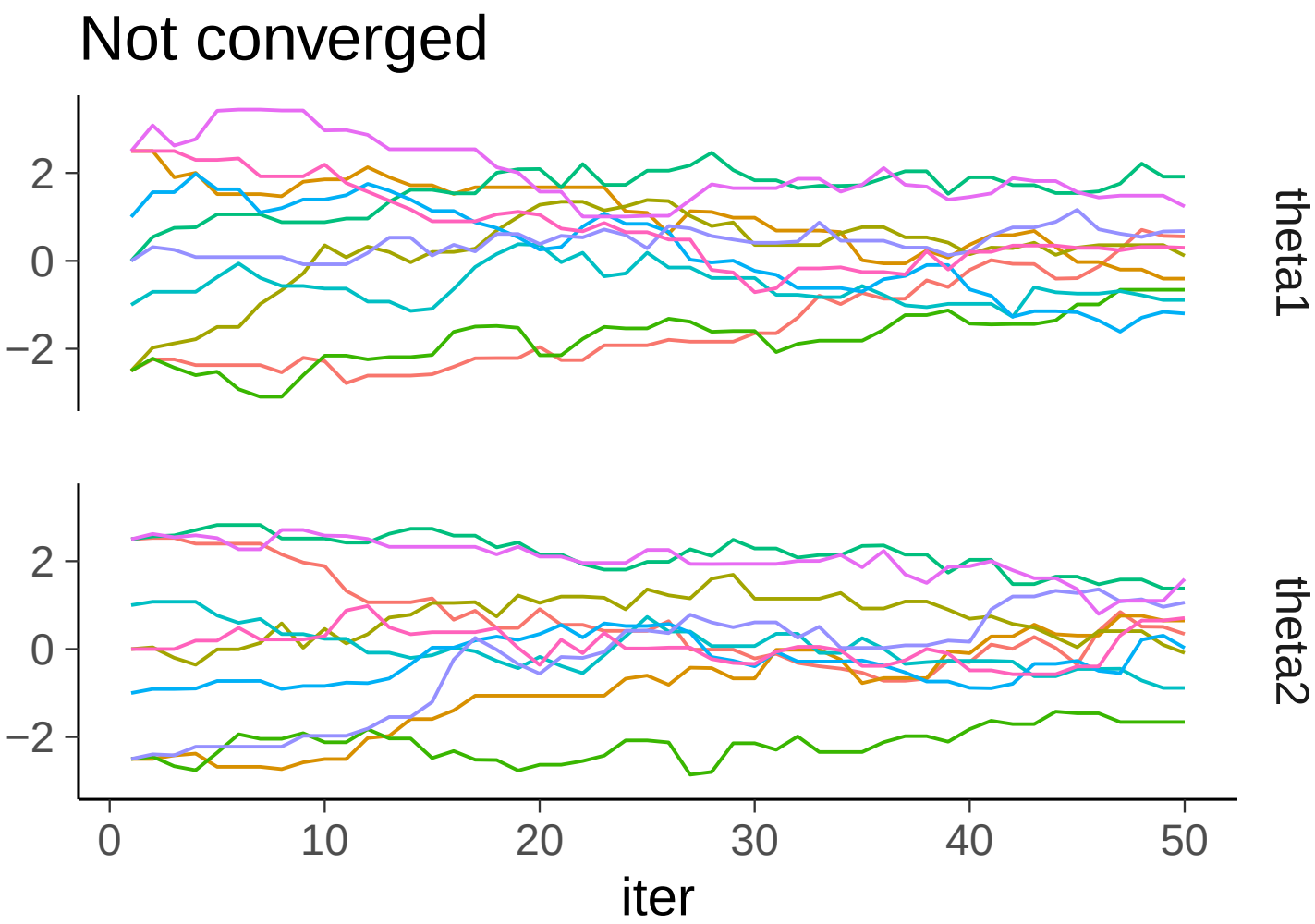
Several chains



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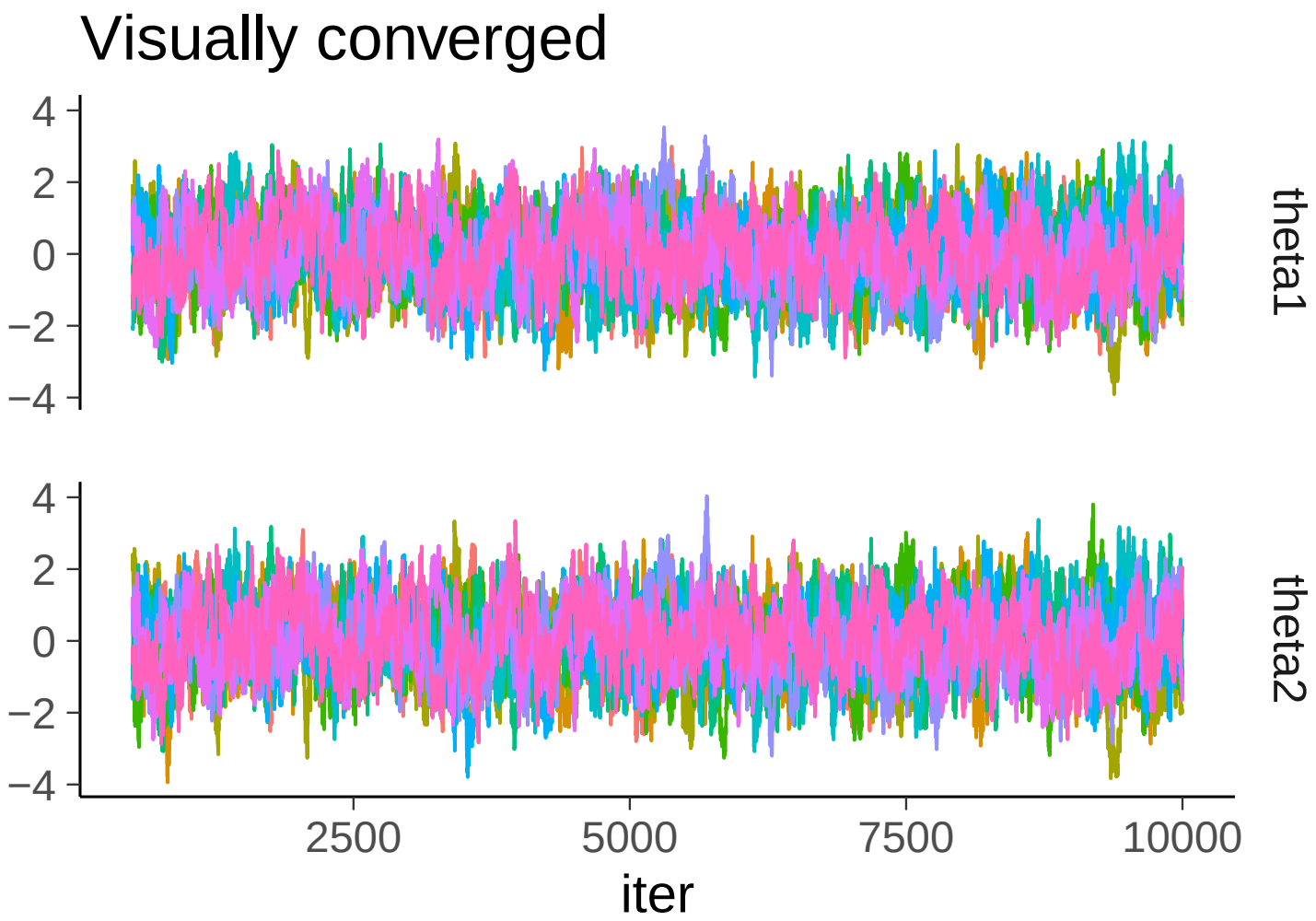

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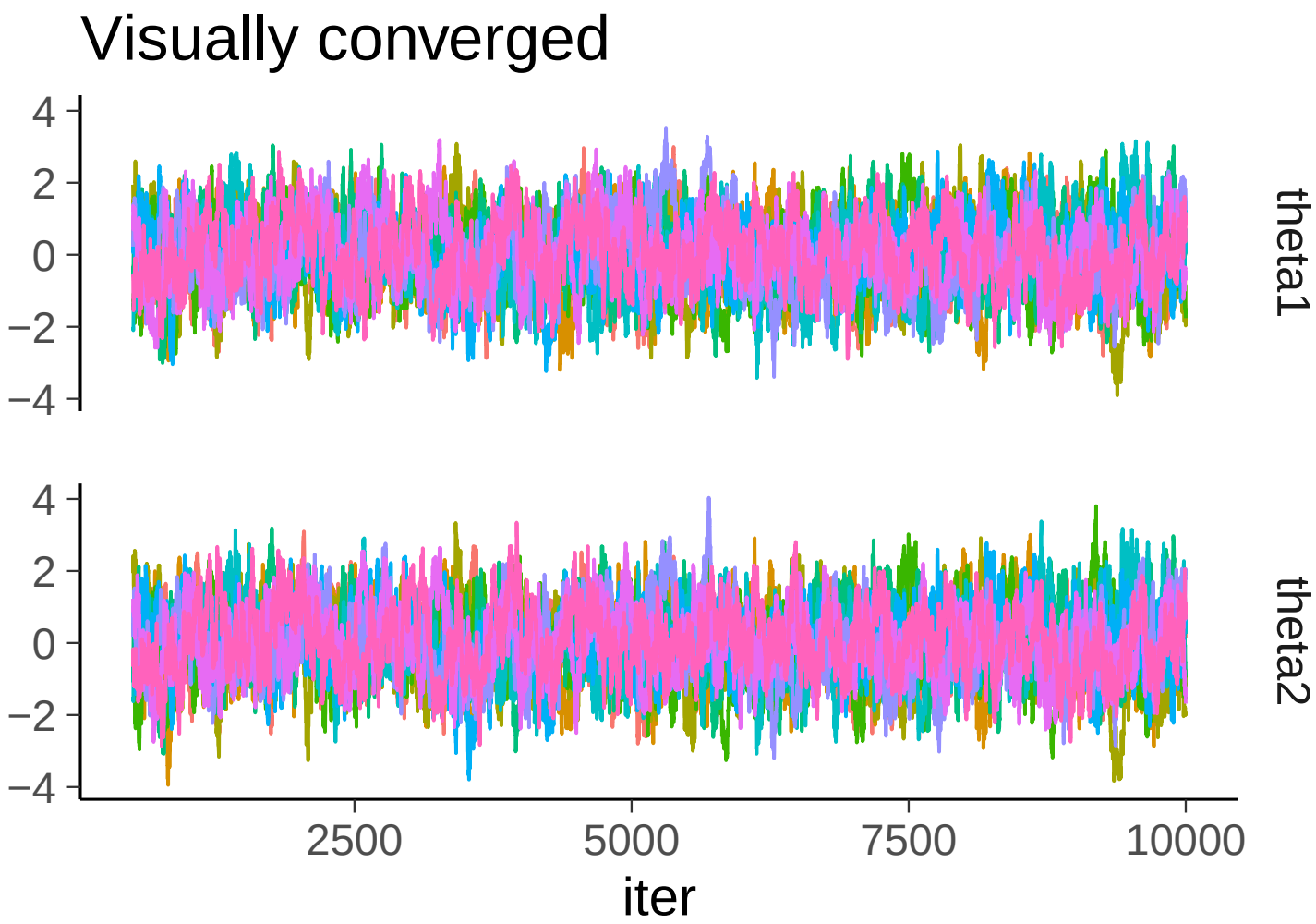

Visual convergence check is not sufficient

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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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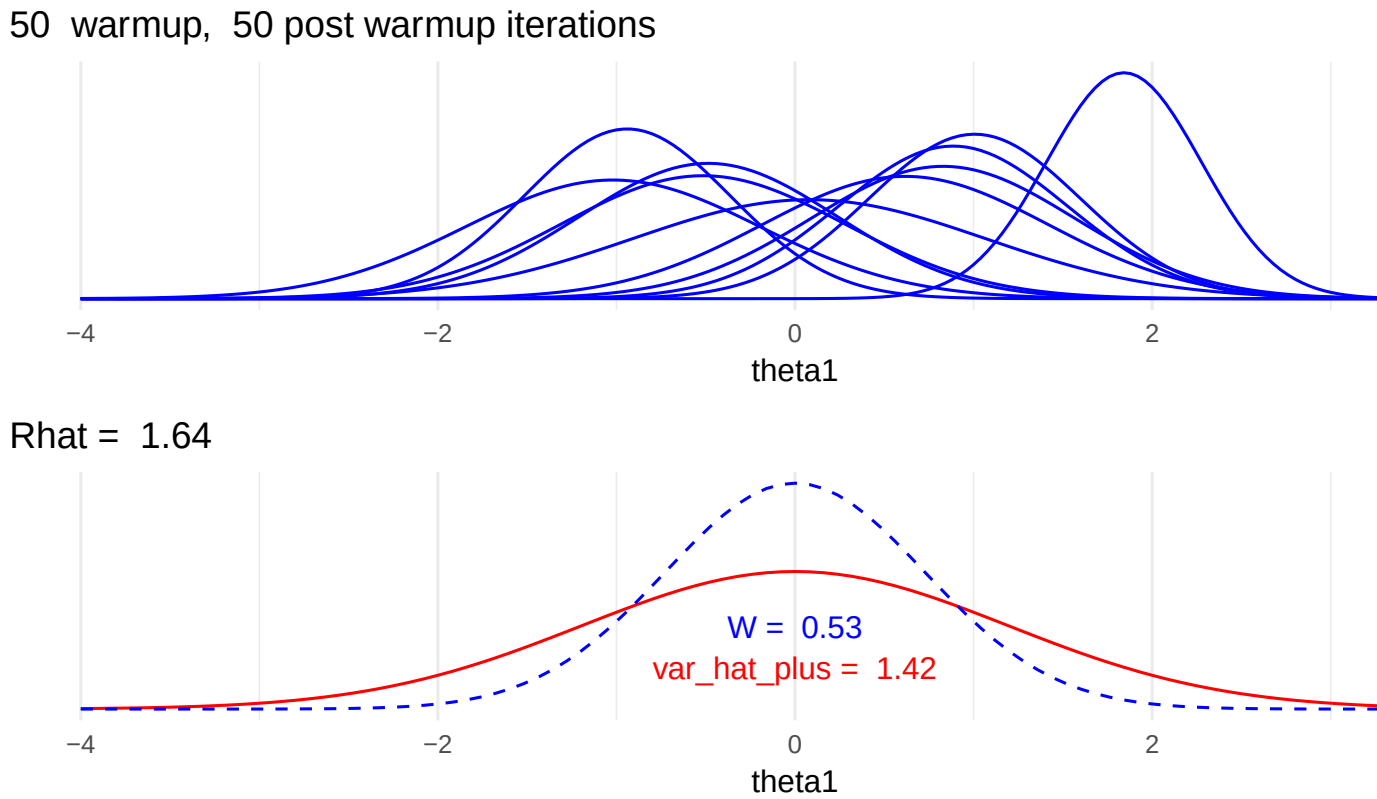

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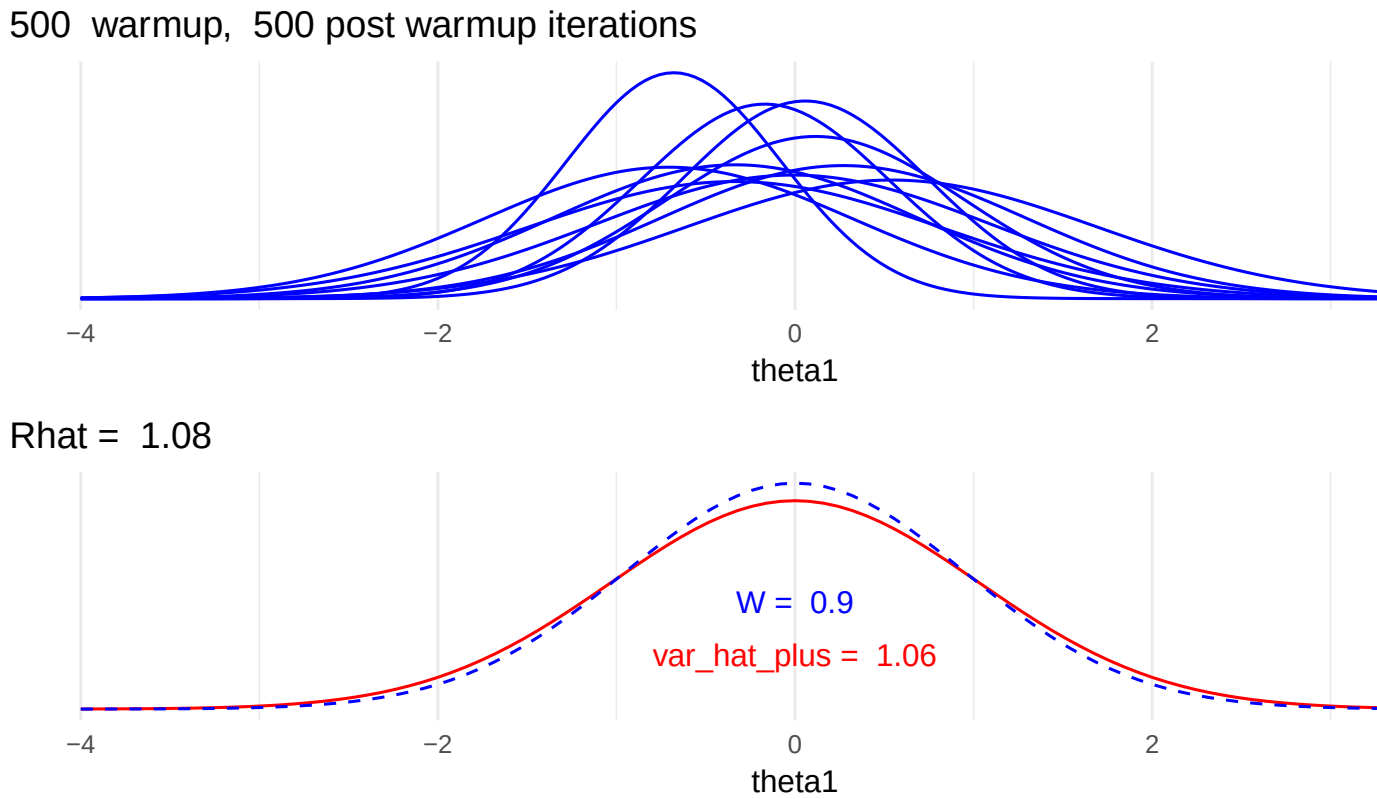

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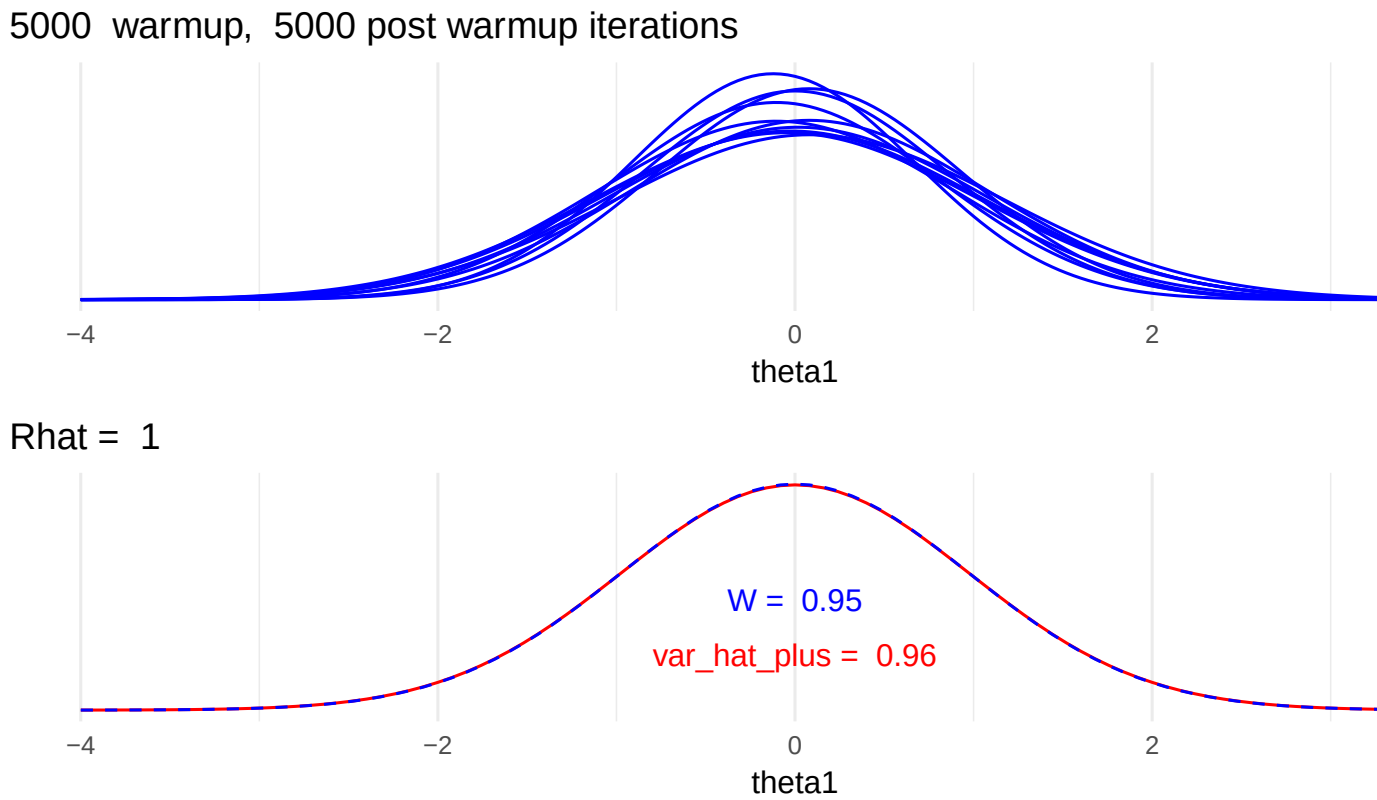

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- M chains, each having N draws (with new R-hat notation)

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- Within chains variance W

$$W = \frac{1}{M}\sum_{m=1}^{M} s_m^2, \text{ where } s_m^2 = \frac{1}{N-1}\sum_{n=1}^{N}(\theta_{nm} - \bar{\theta}_{.m})^2$$

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

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

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- Given finite N, W *underestimates* marginal posterior variance
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- As $\widehat{\mathrm{var}}^{+}(\theta|y)$ overestimates and W underestimates, compute

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

$\widehat{R}$

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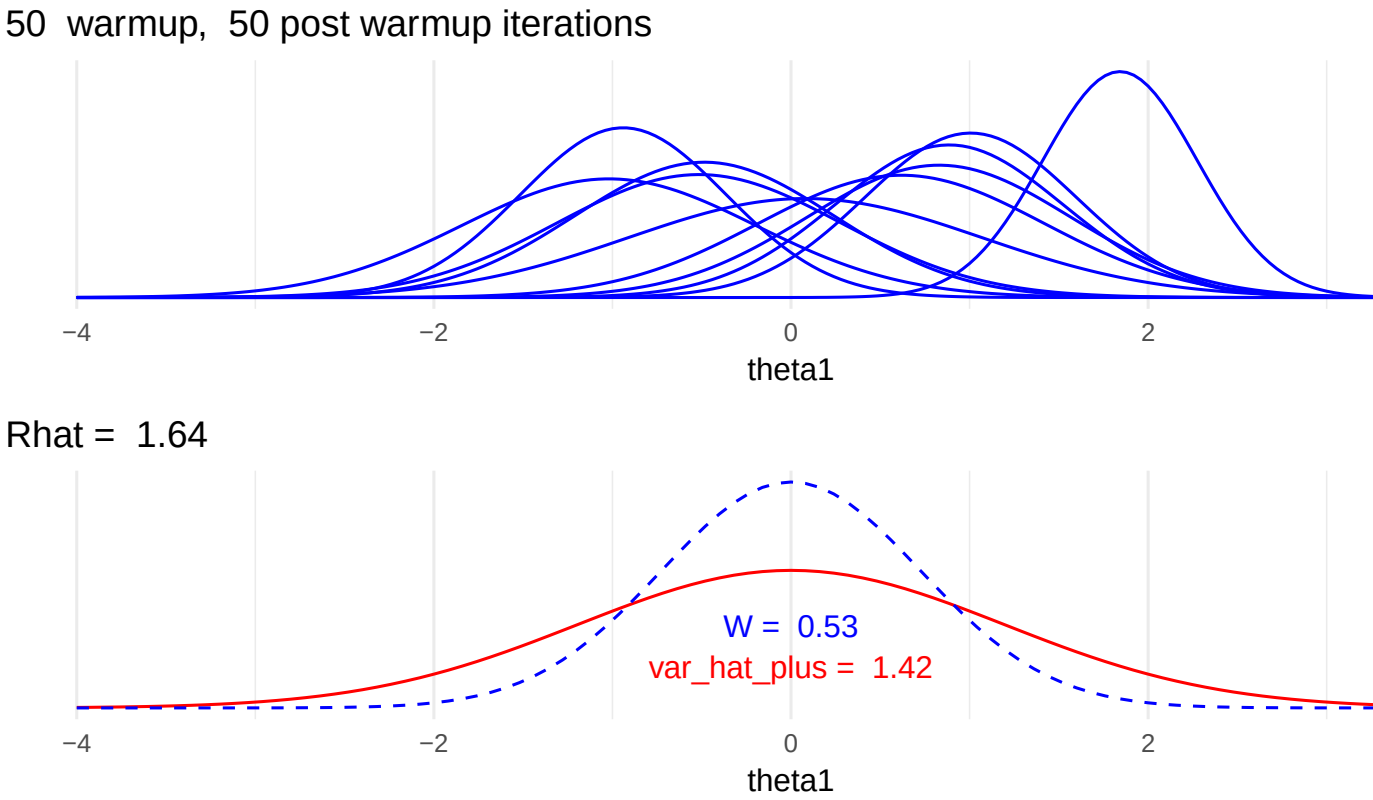

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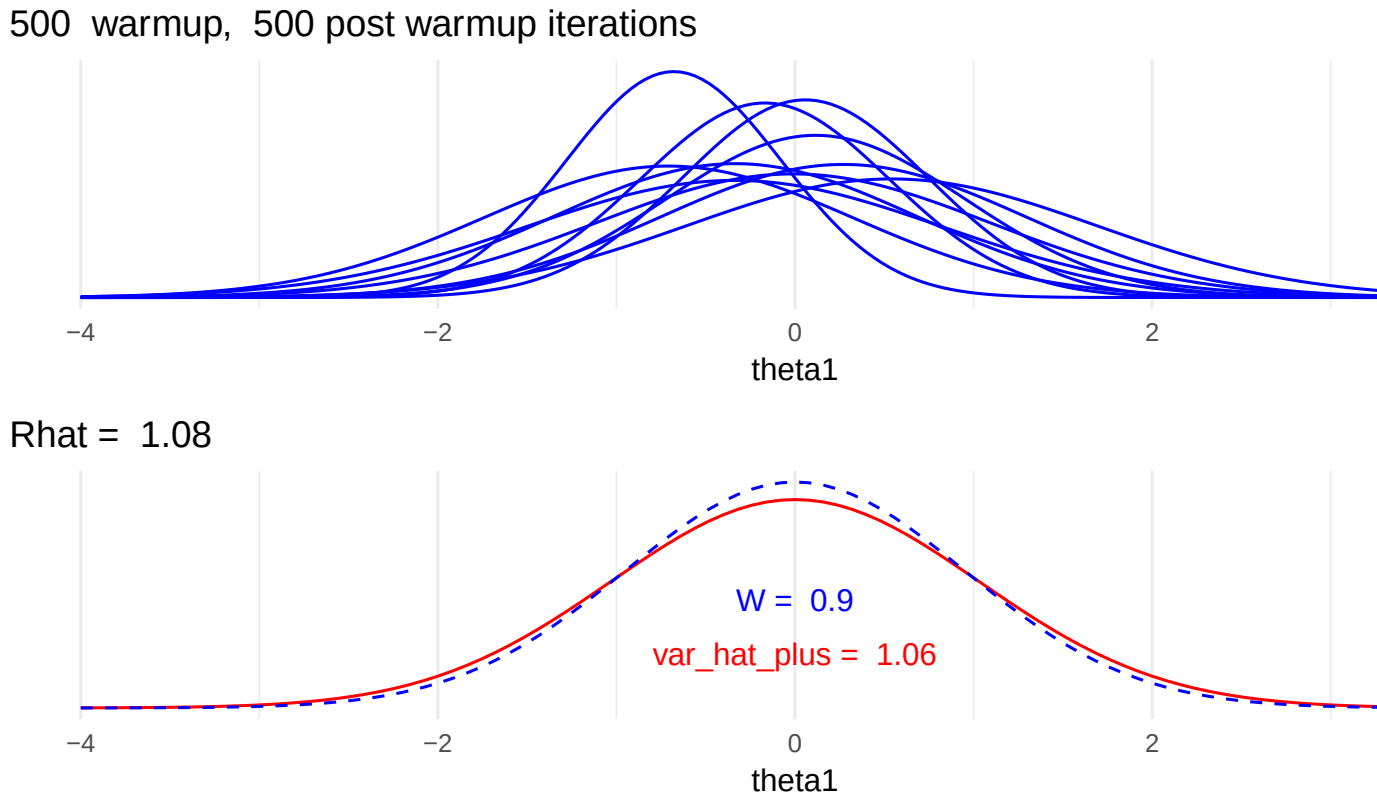

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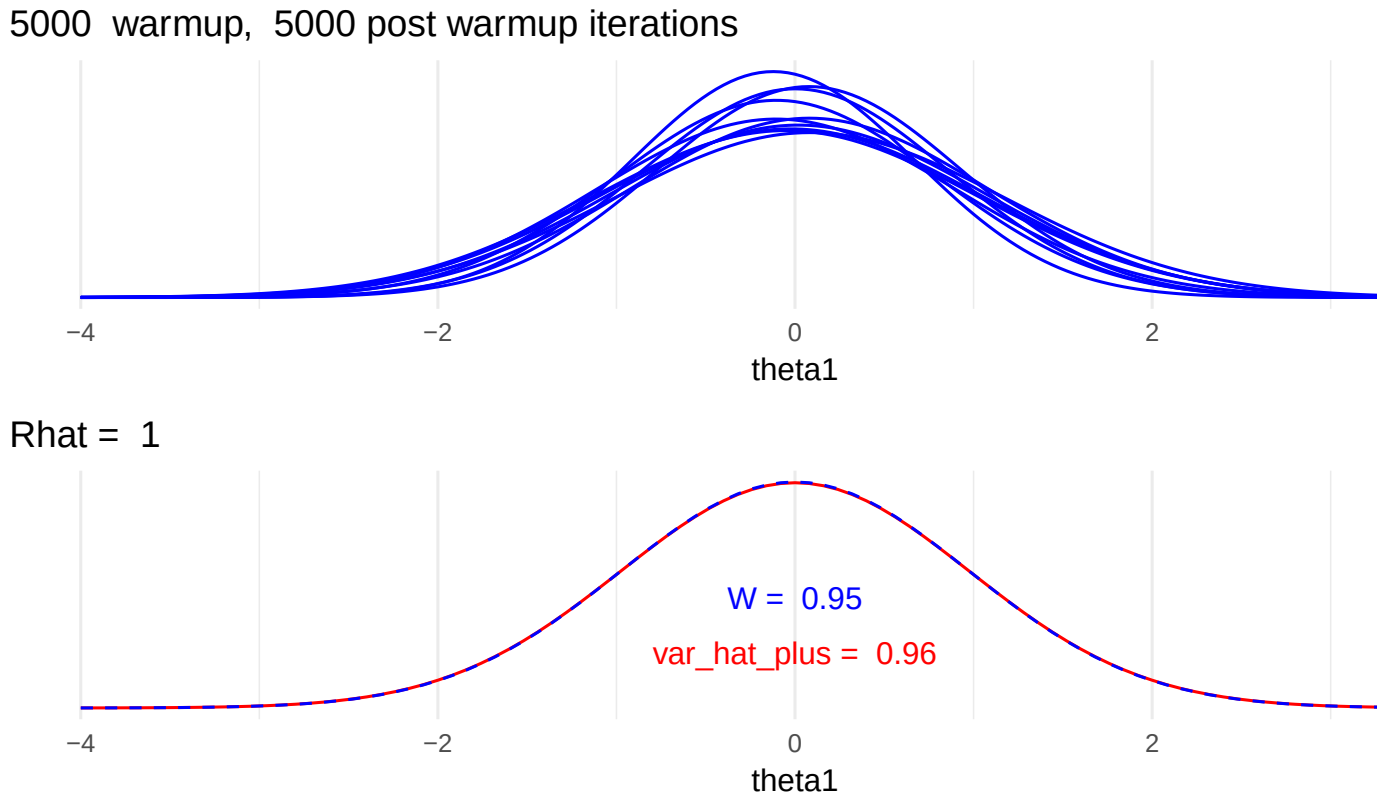

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- Estimates how much the scale of ψ could reduce if $N \to \infty$
- $\widehat{R} \to 1$, when $N \to \infty$
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- If $\widehat{R}$ close to 1, it is still possible that chains have not converged
  - if starting points were not overdispersed
  - distribution far from normal (especially if infinite variance)
  - just by chance when N is finite

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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 θ_{nm} $\quad (n = 1, \ldots, N; m = 1, \ldots, M)$
  - compare means and variances of the split chains

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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 R-hat for assessing convergence of MCMC. Bayesian Analysis, doi:10.1214/20-BA1221. https://projecteuclid.org/euclid.ba/1593828229.

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- Notation updated compared to BDA3

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Time series analysis

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

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- Monte Carlo recap
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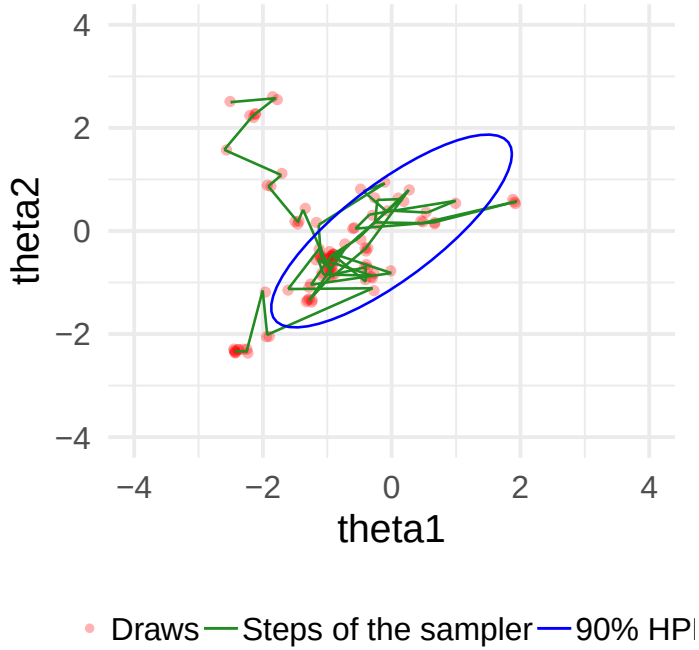
Auto correlation



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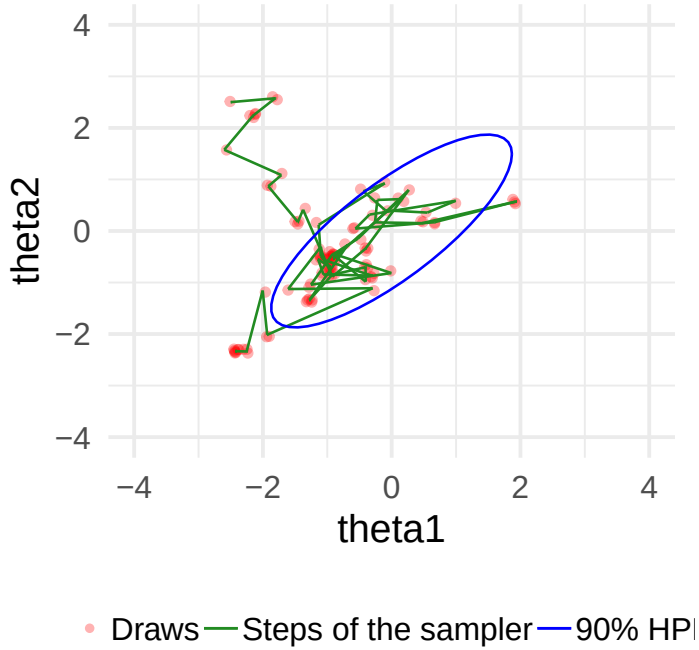

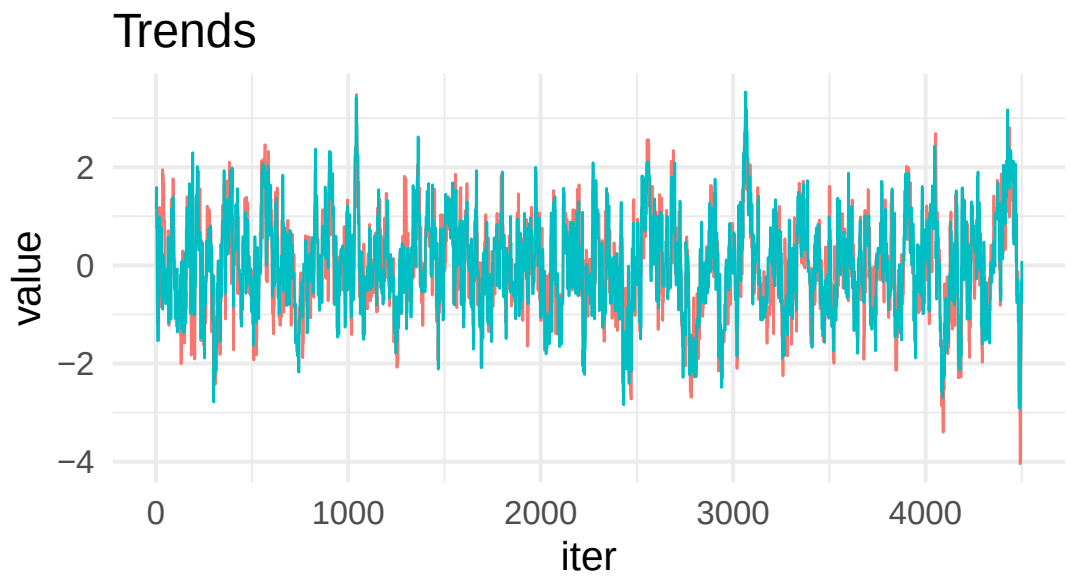

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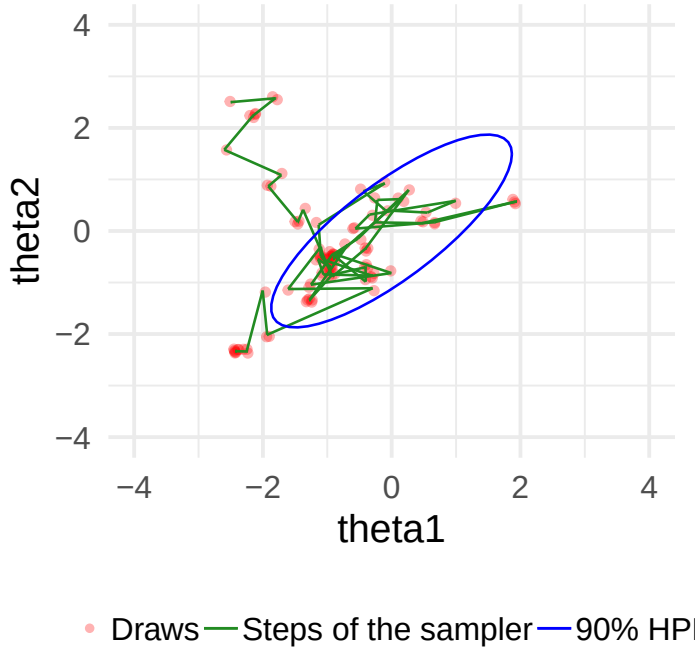

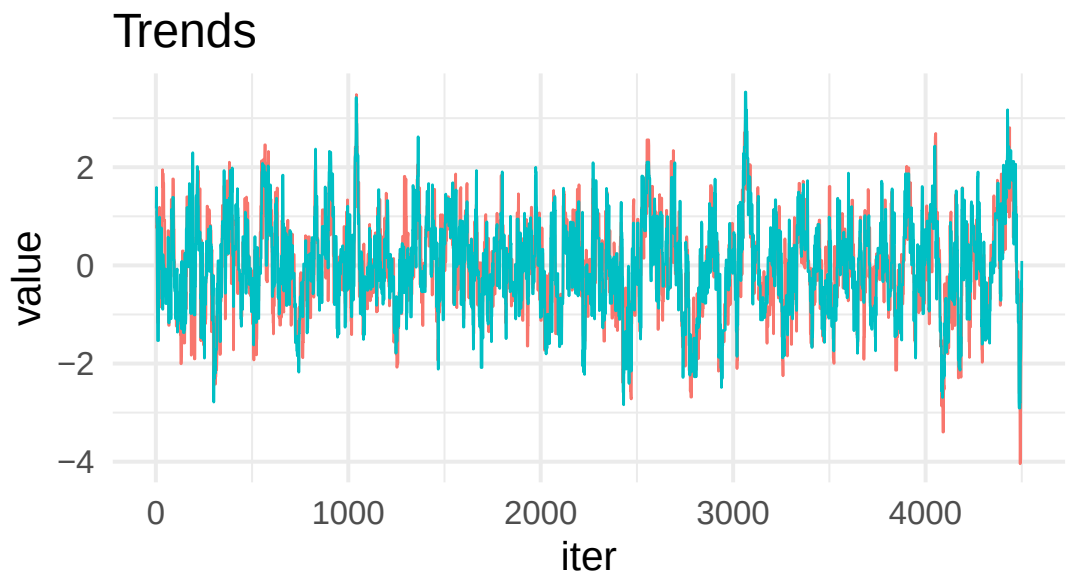

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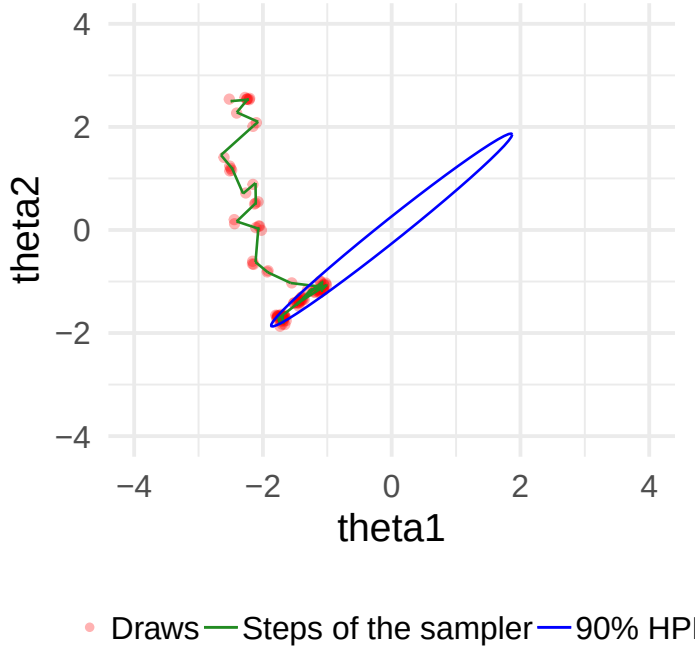

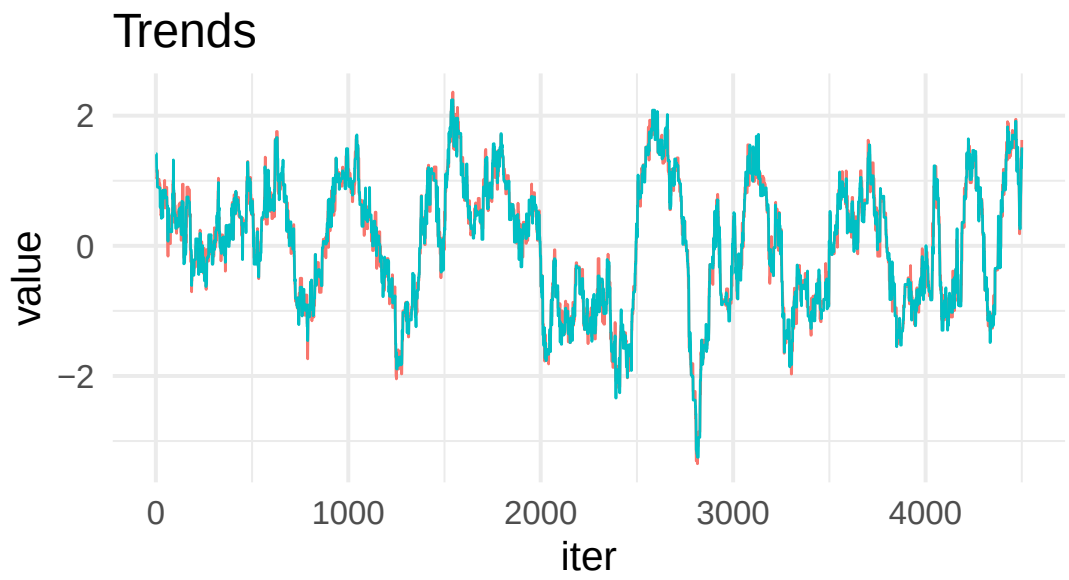

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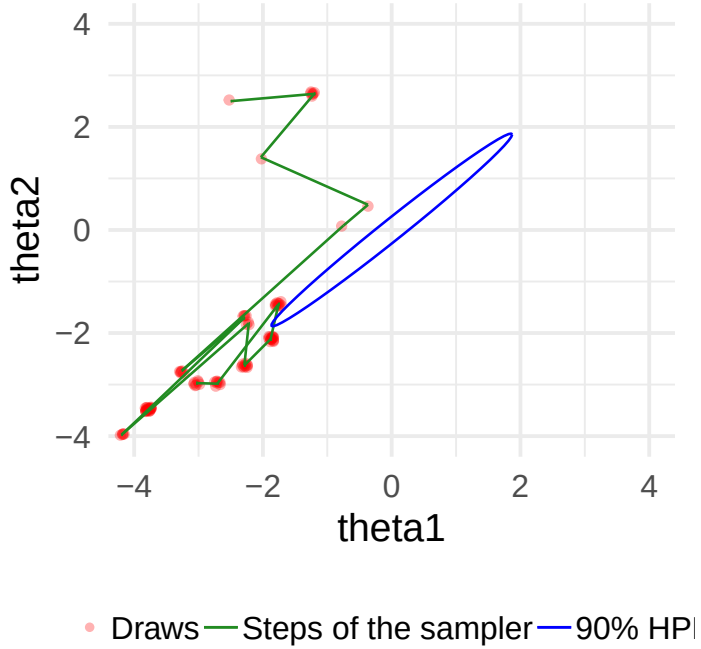

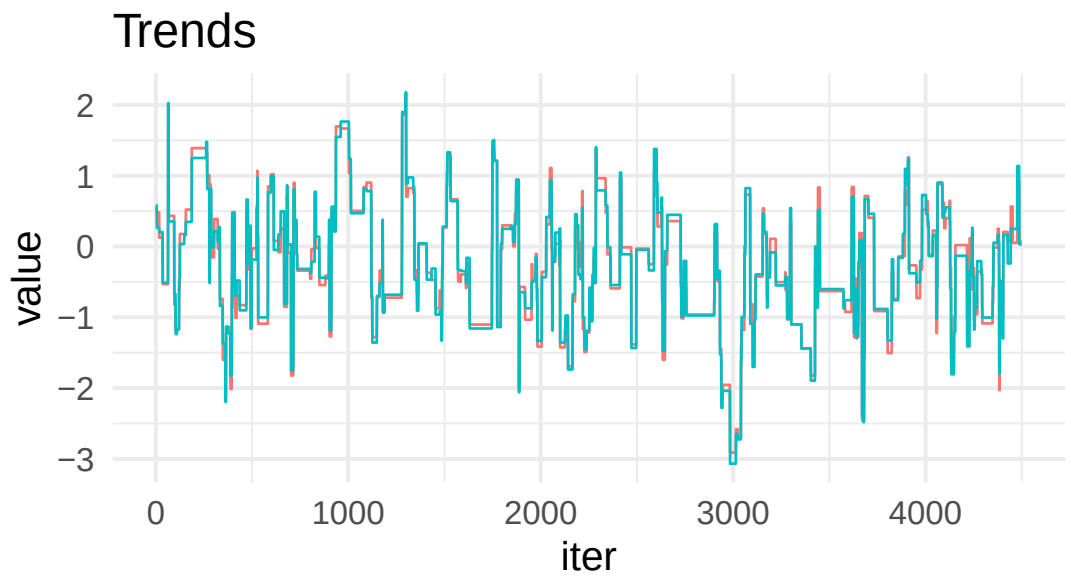

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Time series analysis

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

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

where $S_{E_{\max}} = S/\tau$, and τ is sum of autocorrelations

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

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Time series analysis

- Estimation of the autocorrelation using several chains

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

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- BDA3 has slightly different and less accurate equation. The above equation is used in Stan 2.18+
- Compared to a method which computes the autocorrelation from a single chain, the multi-chain estimate has smaller variance

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Time series analysis

- Estimation of τ

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

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

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- As τ is estimated from a finite number of draws, it's expectation is overoptimistic
  - if $\hat{\tau} > MN/20$ then the estimate is unreliable

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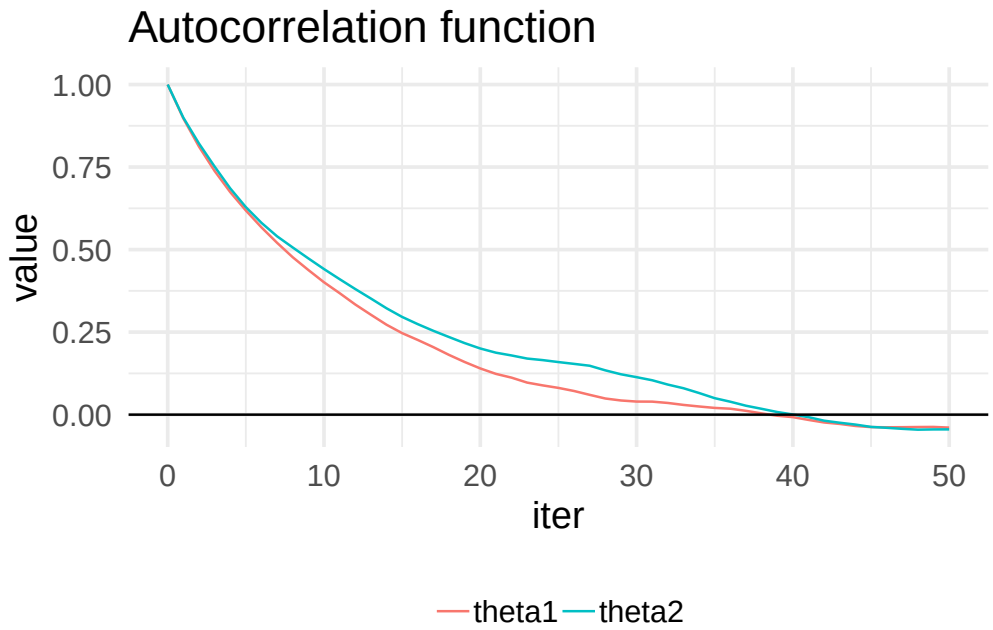
  - let $\Gamma_m = \rho_{2m} + \rho_{2m+1}$, which is sum of two consequent autocorrelations
  - Γ_m is positive, decreasing and convex function of m
- Initial positive sequence estimator (Geyer's IPSE)
  - Choose the largest m so, that all values of the sequence $\hat{\Gamma}_1, \ldots, \hat{\Gamma}_m$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



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Effective sample size

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

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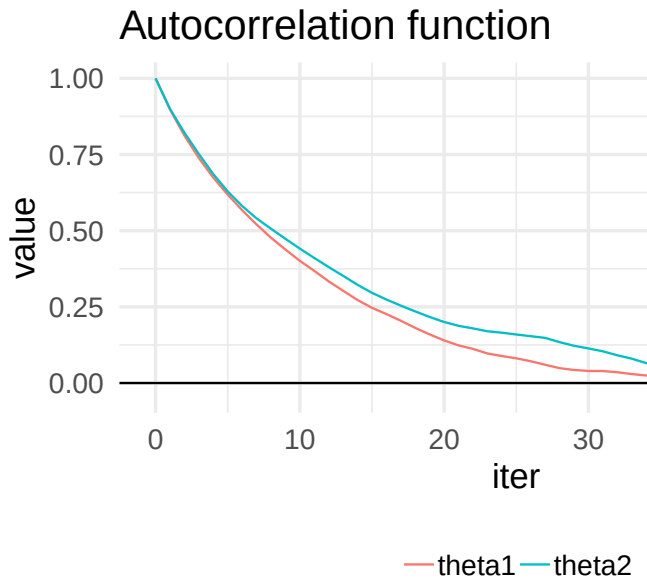

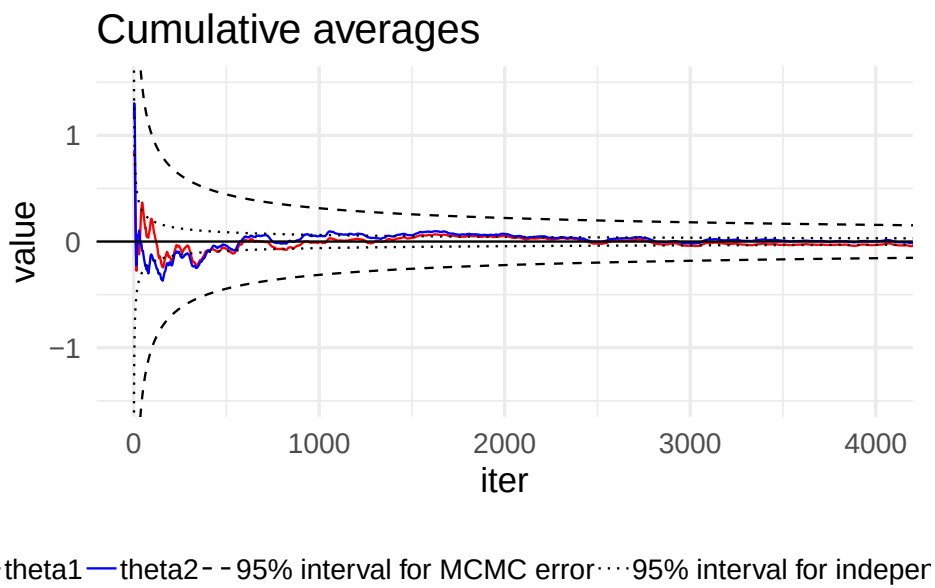

$$\hat{\tau} = 1 + 2\sum_{t=1}^{T} \hat{\rho}_t$$

$$\approx 24$$

Effective sample size

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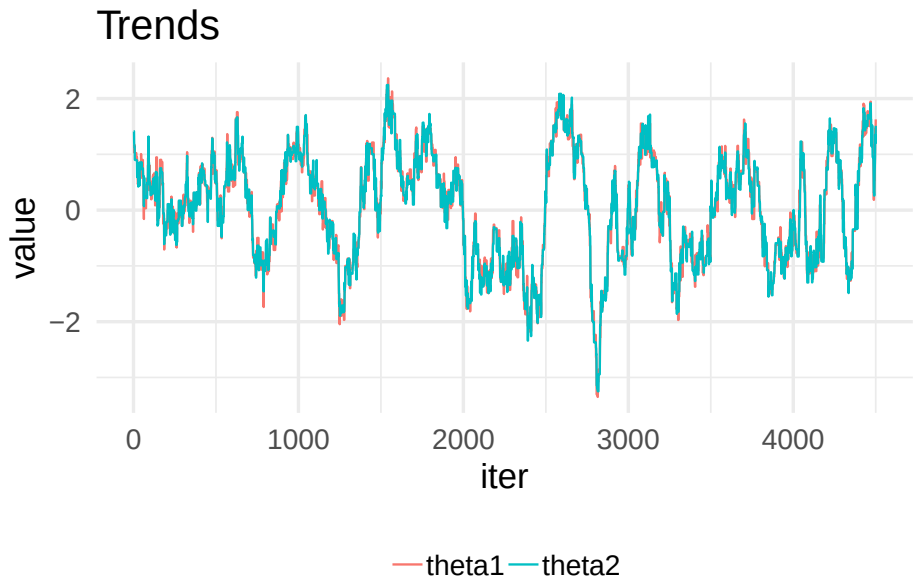

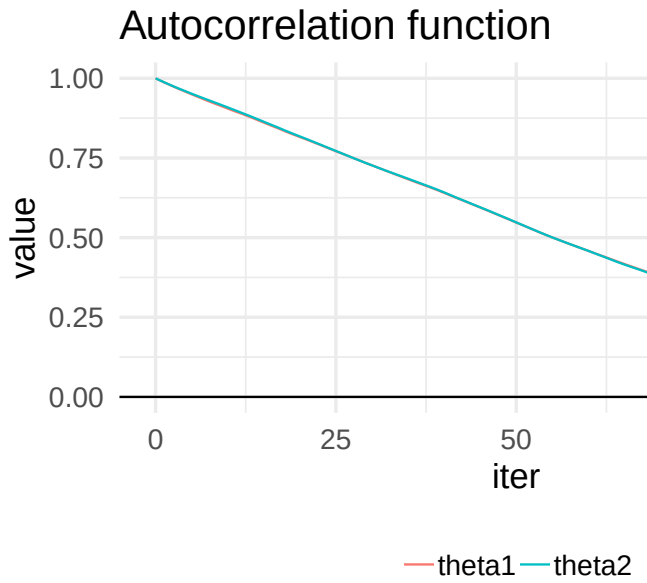

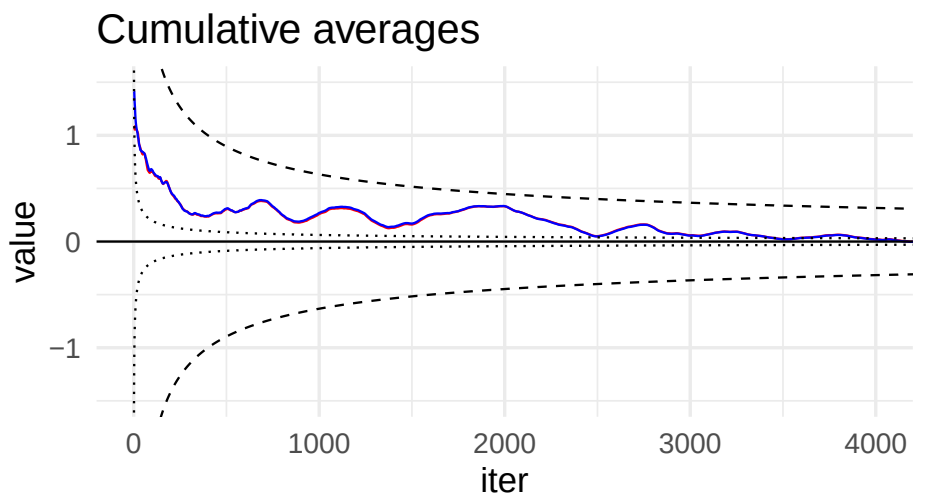

$$\hat{\tau} = 1 + 2\sum_{t=1}^{T} \hat{\rho}_t$$

$$\approx 104$$

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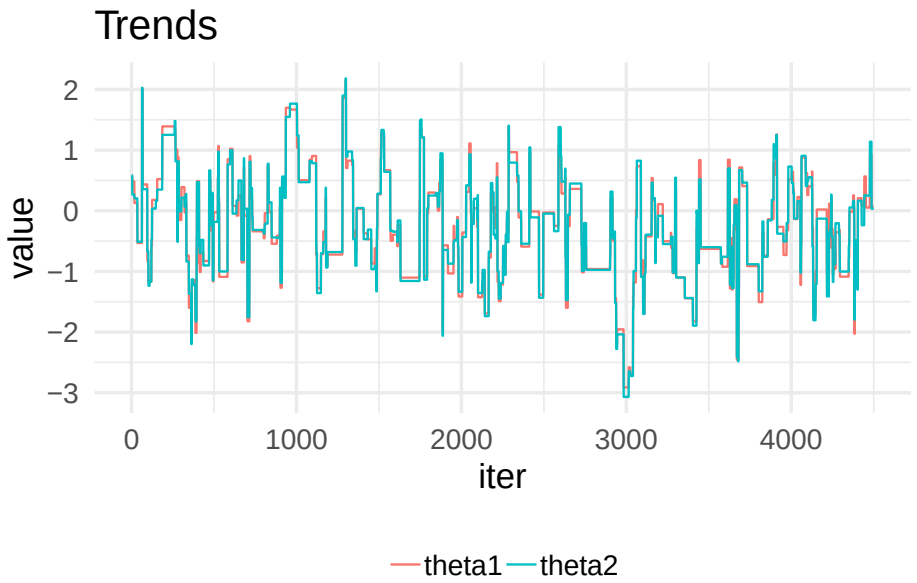

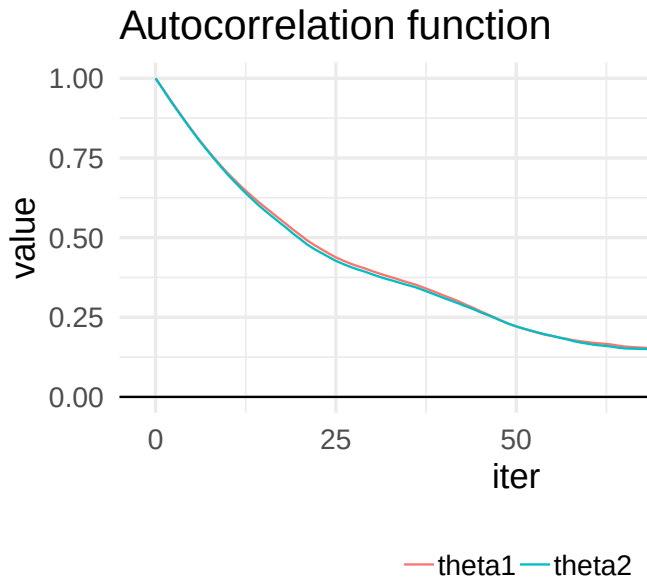

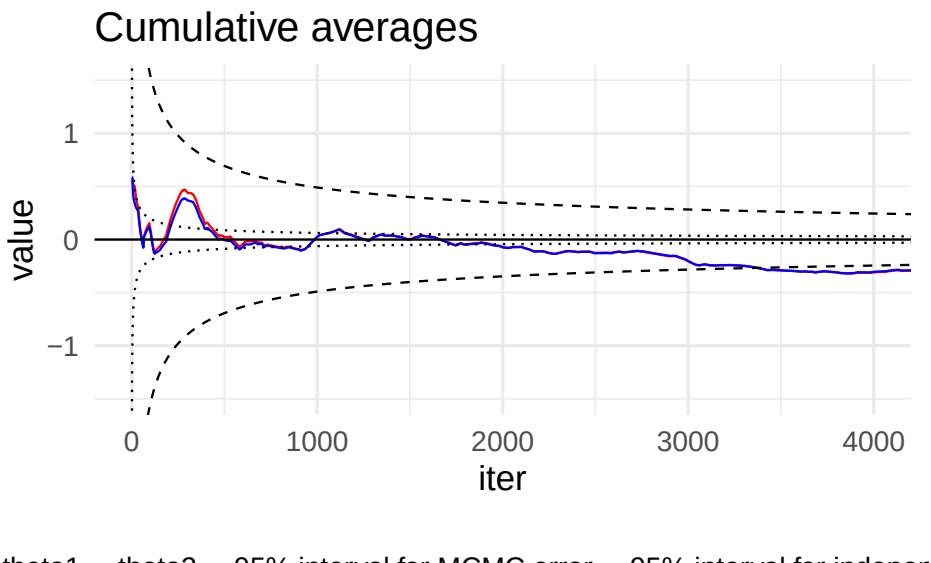

$$\hat{\tau} = 1 + 2\sum_{t=1}^{T} \hat{\rho}_t$$

$$\approx 63$$

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Problematic distributions

- Nonlinear dependencies
  - optimal proposal depends on location

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- Long-tailed with non-finite variance and mean
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