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

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

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 $p(\theta|y)$

Gibbs sampling

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

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

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- Related to the (stochastic) EM algorithm

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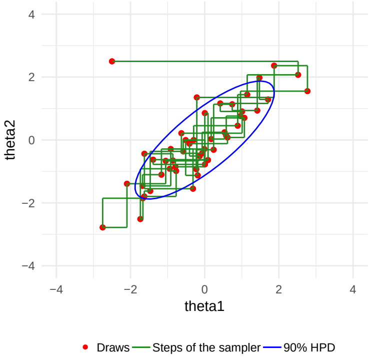

demo

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- Slow if parameters are highly dependent in the posterior...

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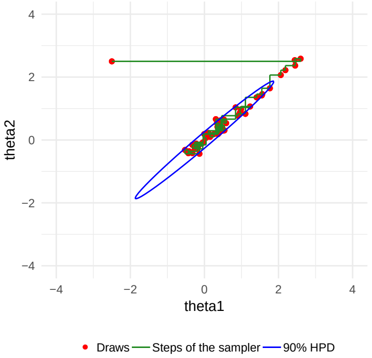

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Sampling conditional vs joint

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

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

The Metropolis algorithm

- Algorithm
  1. starting point θ^0
  2. $t = 1, 2, \ldots$
     (a) pick a proposal θ^* from the 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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     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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  - 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!

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 $J_t(\theta^*|\theta^{t-1}) = \mathcal{N}(\theta^*|\theta^{t-1}, \sigma_p^2)$
- Demo http://elevanth.org/blog/2017/11/28/build-a-better-markov-chain/

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
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  2. Prove that this stationary distribution is the desired target distribution

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   c) recurrent / not transient
      = probability to return to a state i is 1
      - holds for a random walk on any proper distribution (except for trivial exceptions)

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2. Prove that this stationary distribution is the desired target distribution $p(\theta|y)$
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   - 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

Metropolis-Hastings algorithm

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

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Metropolis-Hastings algorithm

- Ideal proposal distribution is the distribution itself
  - $J(\theta^*|\theta) \equiv p(\theta^*|y)$ for all θ
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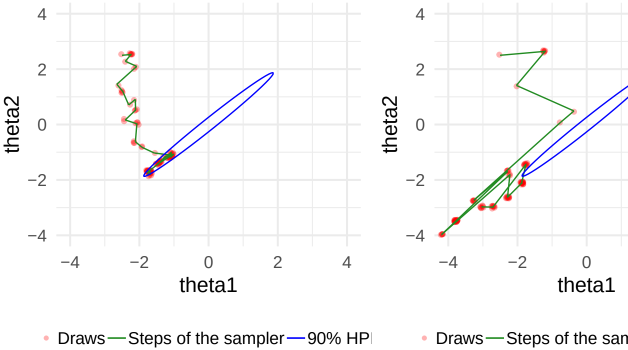
    $\rightarrow$ long steps proposed, but many of those rejected and again chain moves slowly
- Generic rule for rejection rate is 60-90% (but depends on dimensionality and a specific algorithm variation)

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

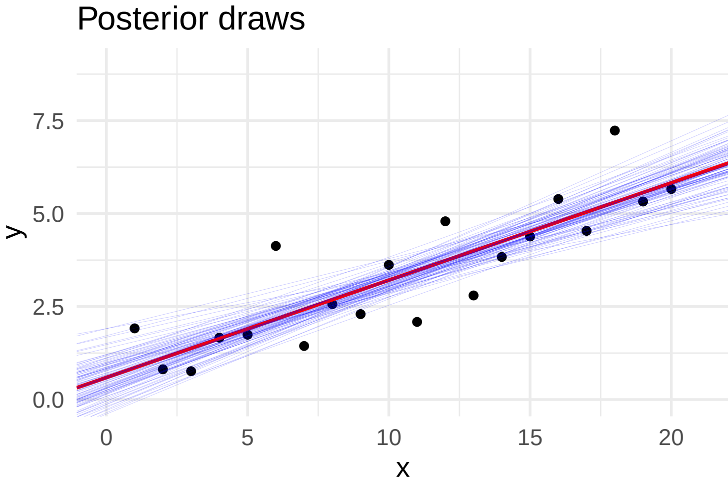
- Usually doesn't scale well to high dimensions
  - if the shape doesn't match the whole distribution, the efficiency drops
  - demo11_2



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

Example of uncertainty in modeling



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- Monte Carlo recap
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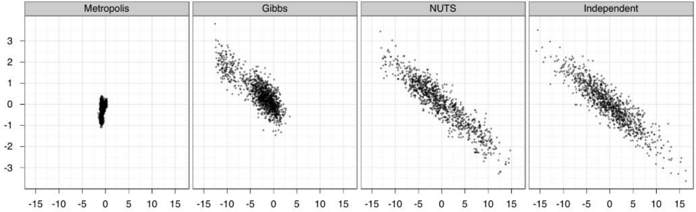
HMC / NUTS

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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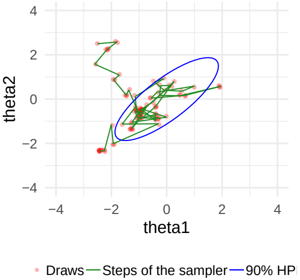

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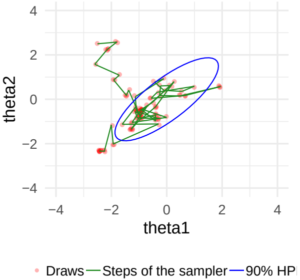

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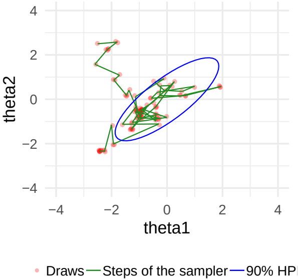


- Warm-up = remove draws from the beginning of the chain
  - warm-up may include also phase for adapting algorithm parameters
- Convergence diagnostics
  - Do we get samples from the target distribution?

MCMC draws are dependent

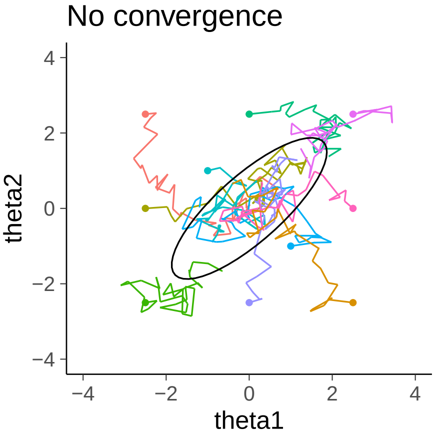
- Monte Carlo estimates still valid (central limit theorem holds)

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

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

Several chains

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



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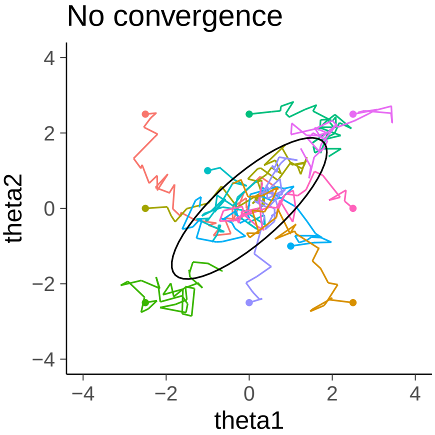

- Remove draws from the beginning of the chains and run chains long enough so that it is not possible to distinguish where each chain started and the chains are well mixed

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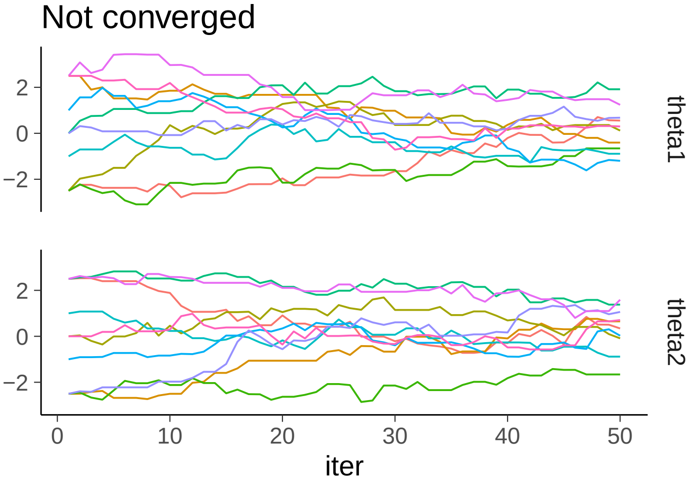

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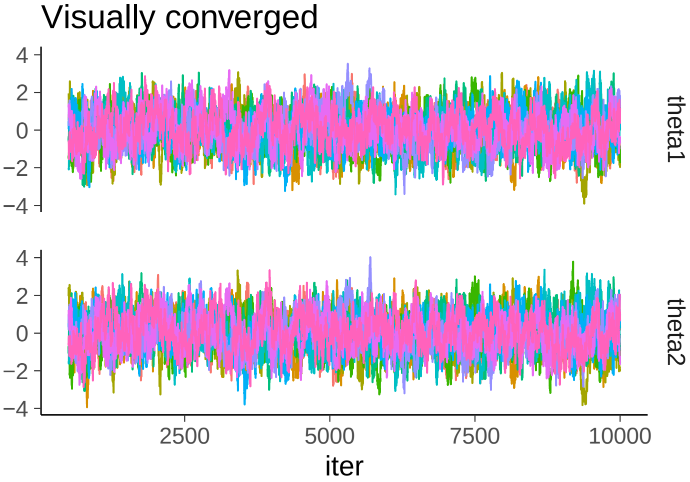

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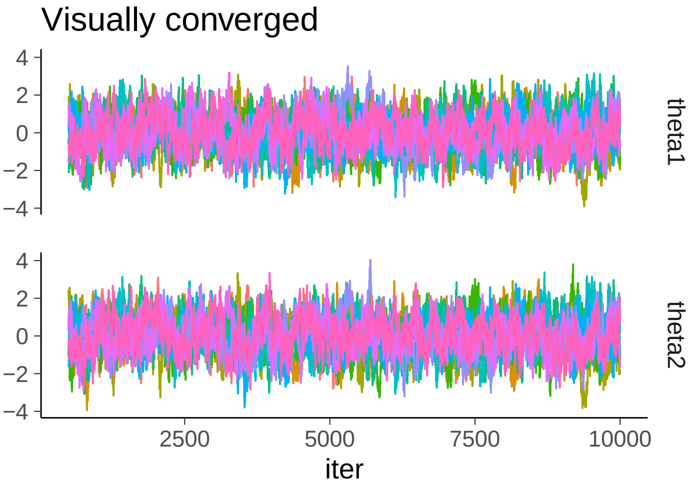

Visual convergence check is not sufficient

$\widehat{R}$: 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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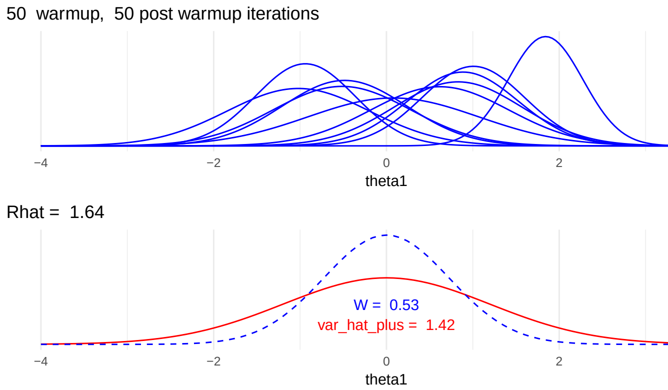

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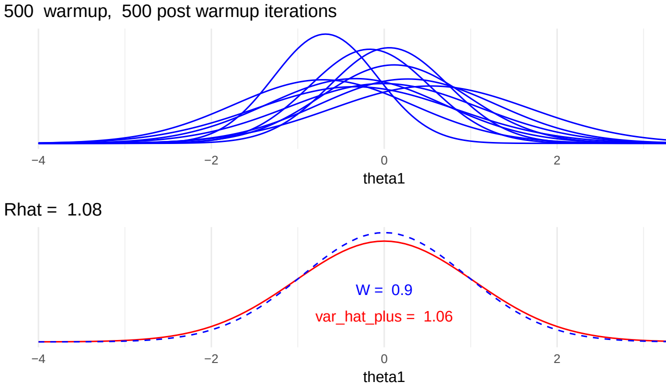

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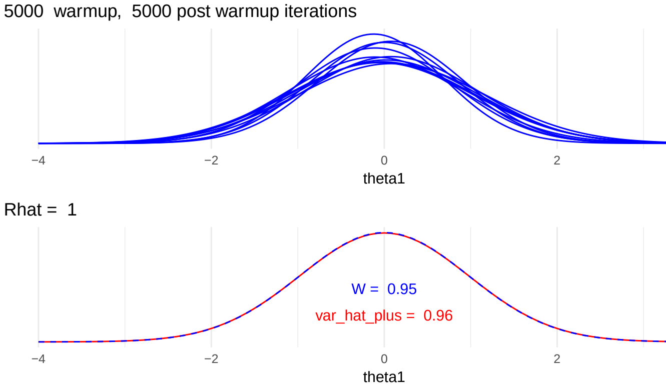

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- M chains, each having N draws (with new R-hat notation)

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

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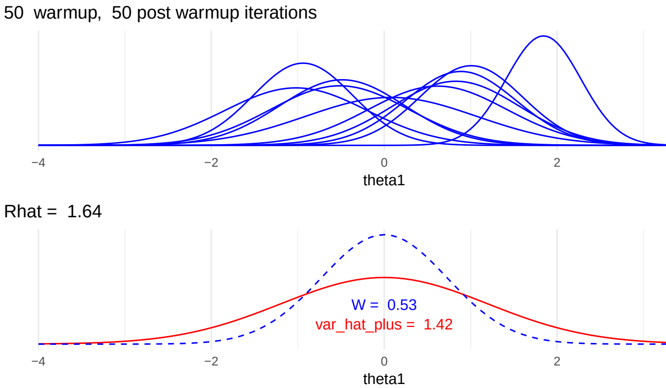

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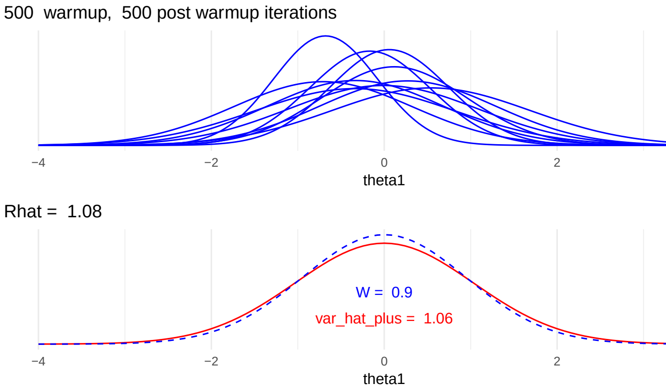

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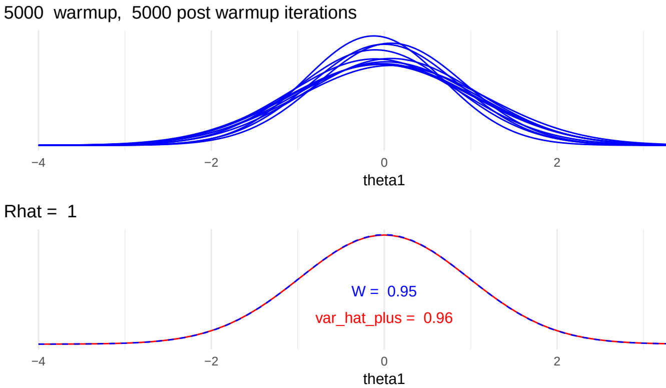

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- If $\widehat{R}$ close to 1, it is still possible that chains have not converged
  - if starting points were not overdispersed
  - distribution far from normal (especially if infinite variance)
  - just by chance when N is finite

Split-$\widehat{R}$

- BDA3: split-$\widehat{R}$
- Examines *mixing* and *stationarity* of chains
- To examine stationarity chains are split to two parts
  - after splitting, we have M chains, each having N draws
  - scalar draws $\theta_{nm} \quad (n = 1, \dots, N; m = 1, \dots, M)$
  - 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 R-hat for assessing convergence of MCMC. Bayesian Analysis, doi:10.1214/20-BA1221. https://projecteuclid.org/euclid.ba/1593828229.

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Time series analysis

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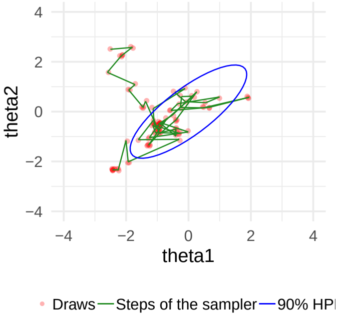
- Auto correlation function
  - describes the correlation given a certain lag
  - can be used to compare efficiency of MCMC algorithms and parameterizations

Auto correlation



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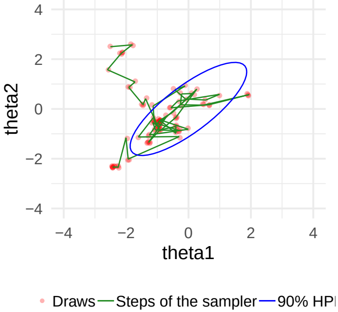

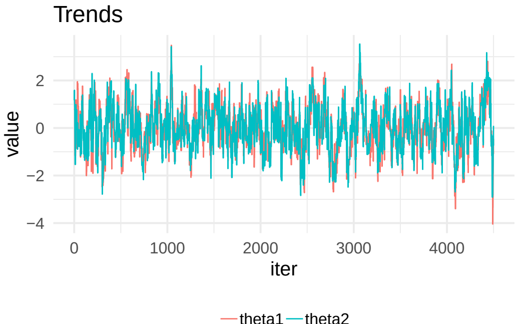

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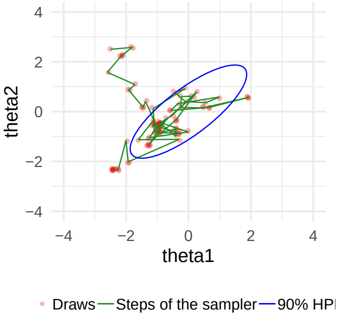

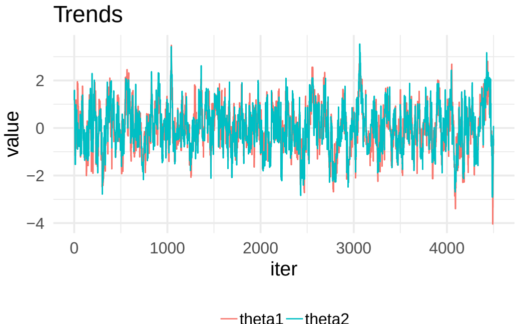

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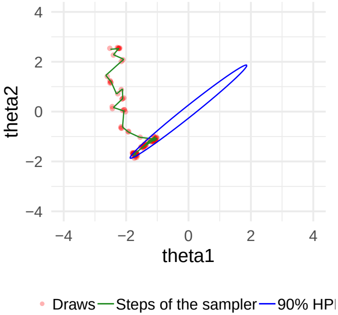

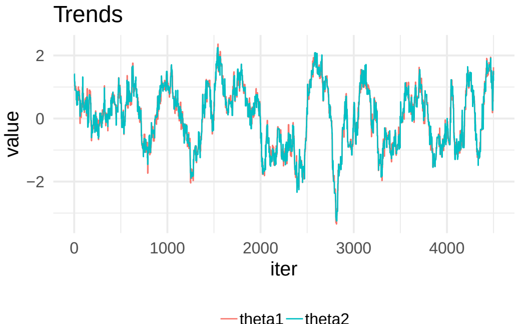

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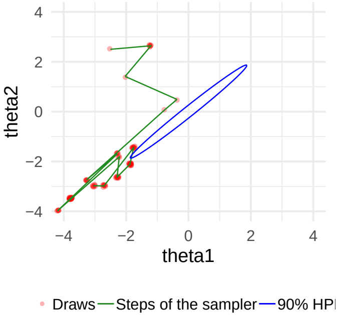

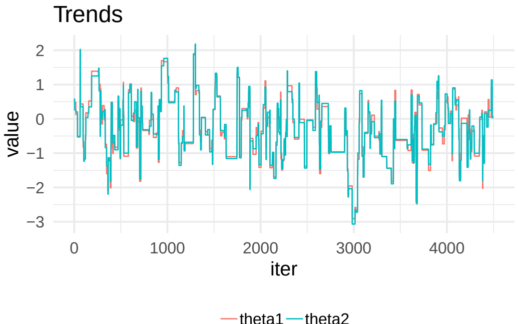

Time series analysis

- 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

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

where $\hat{\rho}_{n,m}$ is autocorrelation at lag n for chain m

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
- This combines $\widehat{R}$ and autocorrelation estimates
  - takes into account if the chains are not mixing (the chains have not converged)

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  - takes into account if the chains are not mixing (the chains have not converged)
- BDA3 has slightly different and less accurate equation. The above equation is used in Stan 2.18+
- Compared to a method which computes the autocorrelation from a single chain, the multi-chain estimate has smaller variance

Time series analysis

- Estimation of τ

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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

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

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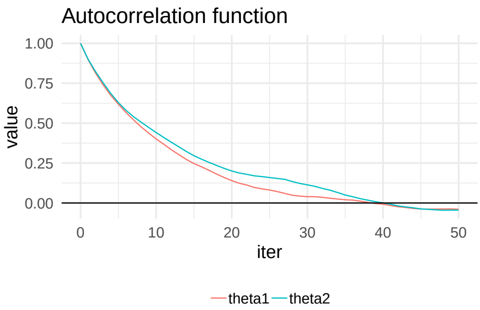
  - let $\Gamma_m = \rho_{2m} + \rho_{2m+1}$, which is sum of two consequent autocorrelations
  - Γ_m is positive, decreasing and convex function of m
- Initial positive sequence estimator (Geyer's IPSE)
  - Choose the largest m so, that all values of the sequence $\hat{\Gamma}_1, \ldots, \hat{\Gamma}_m$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



Effective sample size

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

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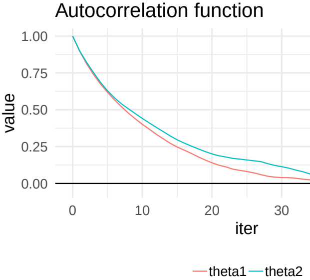

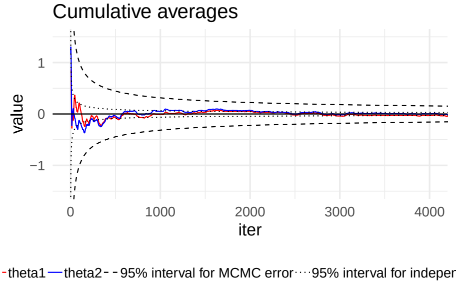

$$\hat{\tau} = 1 + 2\sum_{t=1}^{T} \hat{\rho}_t$$

$$\approx 24$$

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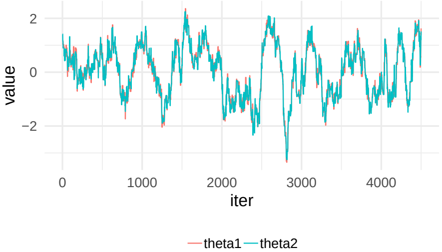
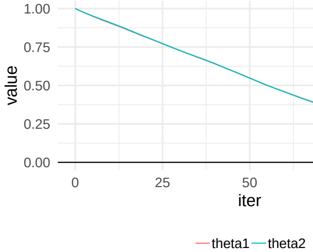
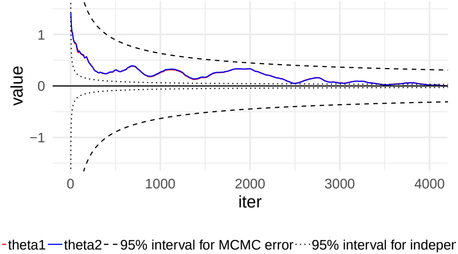
Trends



Autocorrelation function



Cumulative averages



$$\hat{\tau} = 1 + 2\sum_{t=1}^{T} \hat{\rho}_t$$
$$\approx 104$$

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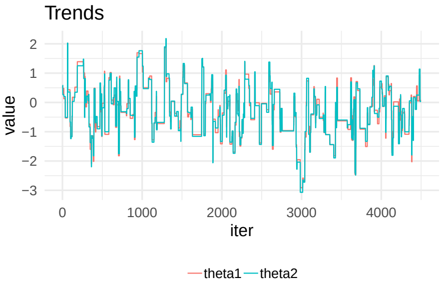

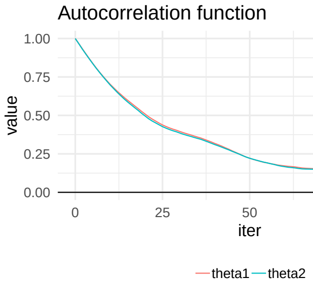

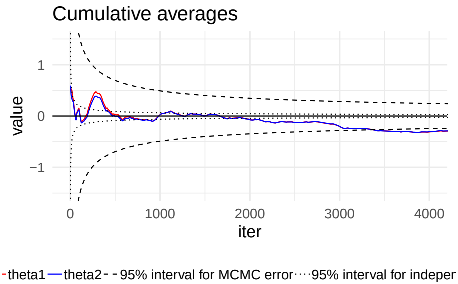

$$\hat{\tau} = 1 + 2\sum_{t=1}^{T} \hat{\rho}_t$$

$$\approx 63$$

Problematic distributions

- Nonlinear dependencies
  - optimal proposal depends on location

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