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})

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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- Grid (equal spacing) evaluation with self-normalization

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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)
  - Importance sampling is reliable only in special cases

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

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  - Deep learning language models are super big Markov models

Markov chain

- Example of a simple Markov chain

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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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- 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 $p(\theta \mid y)$

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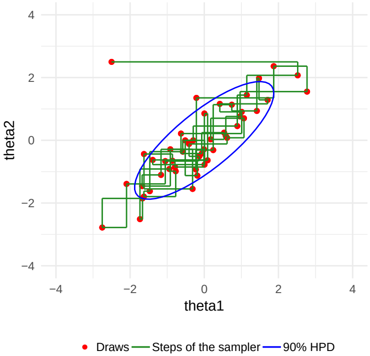

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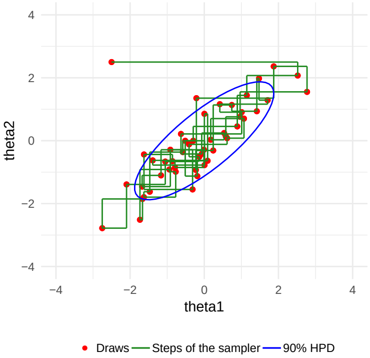

- Basic algorithm

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

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

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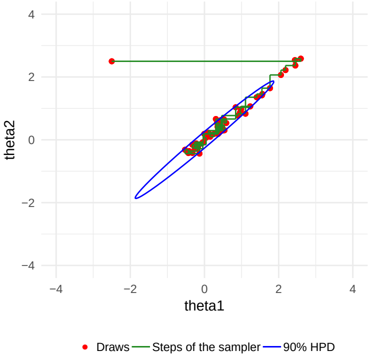
- Slow if parameters are highly dependent in the posterior
  - demo11_1 continues



Conditional vs joint

- How about sampling θ jointly?
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Conditional vs joint

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

Metropolis algorithm

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

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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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- step c is executed by generating a random number from $\mathrm{U}(0, 1)$
- $p(\theta^* \mid y)$ and $p(\theta^{t-1} \mid y)$ have the same normalization terms, and thus instead of $p(\cdot \mid y)$, unnormalized $q(\cdot \mid y)$ 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

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

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

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- Theoretically
  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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   c) recurrent / not transient
      = probability to return to a state *i* is 1
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   which is the same as the probability of transition from 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 and θ^{t-1} 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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- After the shape has been selected, it is important to select the scale
  - small scale
    $\rightarrow$ many steps accepted, but the chain moves slowly due to small steps
  - big scale
    $\rightarrow$ long steps proposed, but many of those rejected and again chain moves slowly

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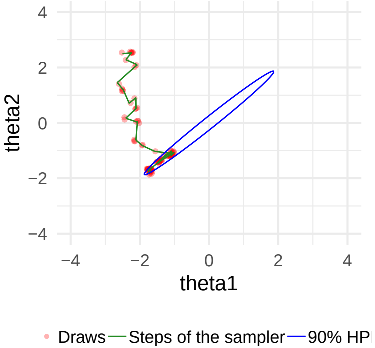
  - small scale
    $\rightarrow$ many steps accepted, but the chain moves slowly due to small steps
  - big scale
    $\rightarrow$ long steps proposed, but many of those rejected and again chain moves slowly
- Generic rule for rejection rate is 60-90% (but depends on dimensionality and a specific algorithm variation)

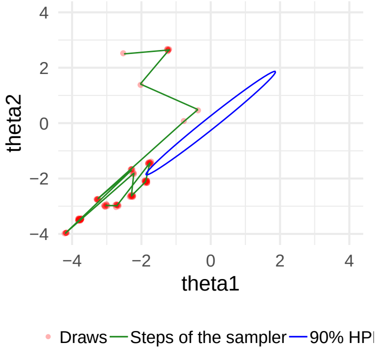
Gibbs sampling

- 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

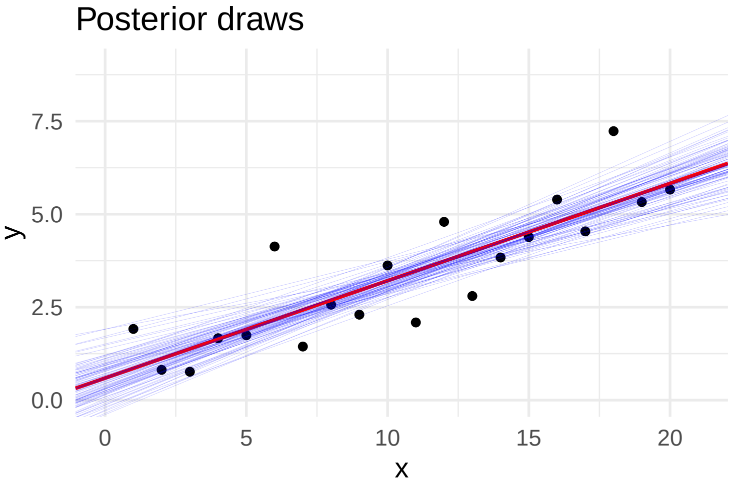




Dynamic Hamiltonian Monte Carlo and NUTS

- 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
    - state-of-the-art MCMC used by most modern probabilistic programming frameworks
- More next week

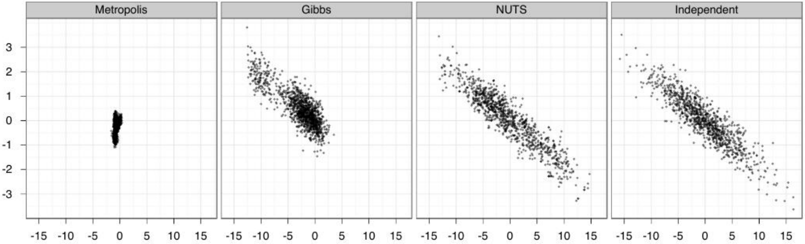
Example of uncertainty in modeling



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

Warm-up and convergence diagnostics

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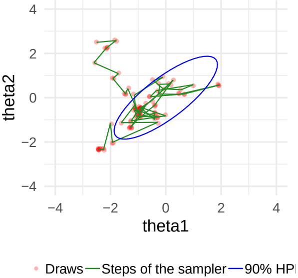

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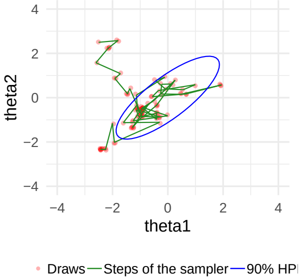

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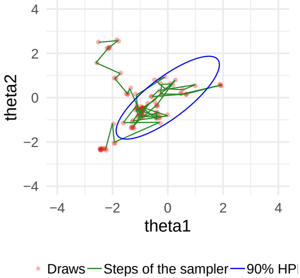


- Warm-up = remove draws from the beginning of the chain
  - warm-up may include also phase for adapting algorithm parameters
- Convergence diagnostics
  - Is the sample representative of the target distribution?

MCMC draws are dependent

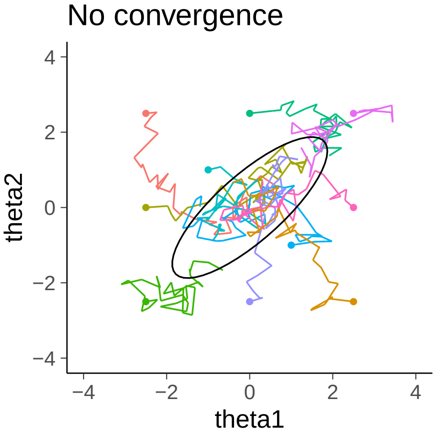
- Monte Carlo estimates still valid (central limit theorem holds)

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

- 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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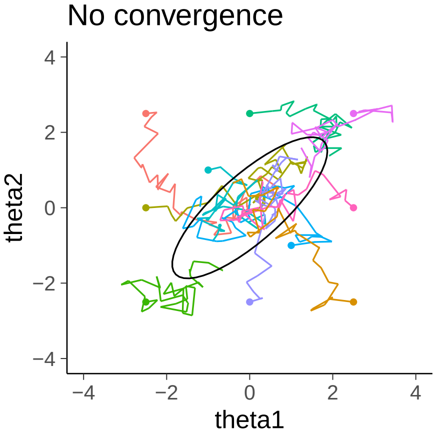
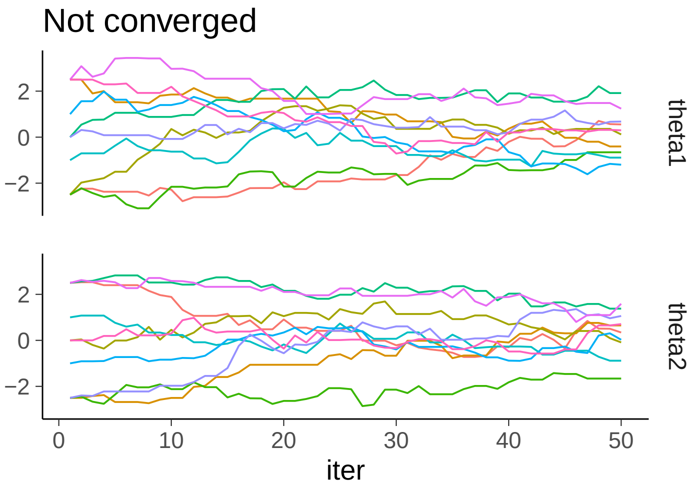


- Remove draws from the beginning of the chains and run chains long enough so that it is not possible to distinguish where each chain started and the chains are well mixed

Several chains



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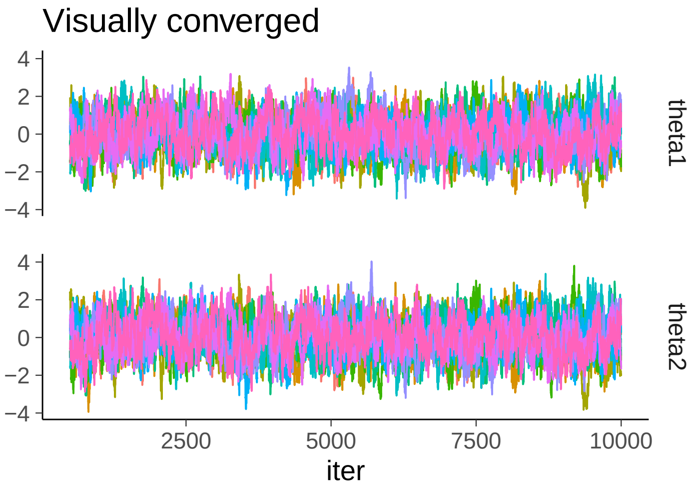

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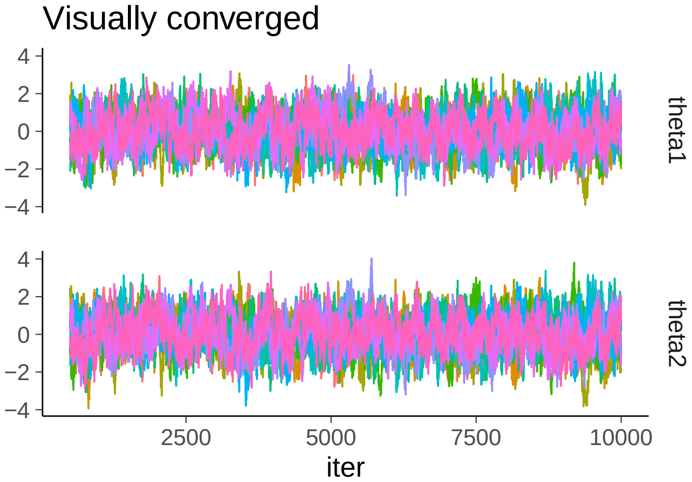

Visual convergence check is not sufficient

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

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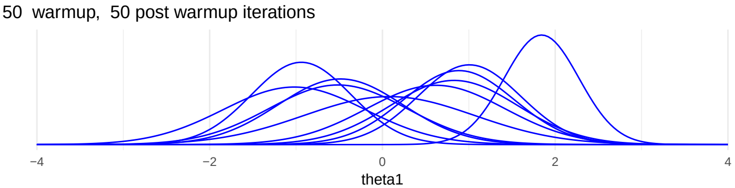

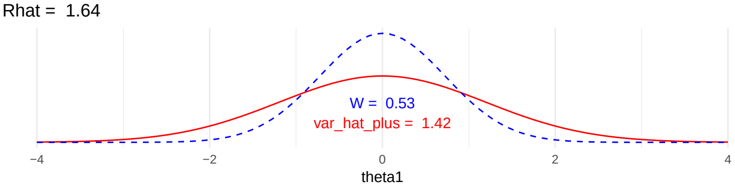

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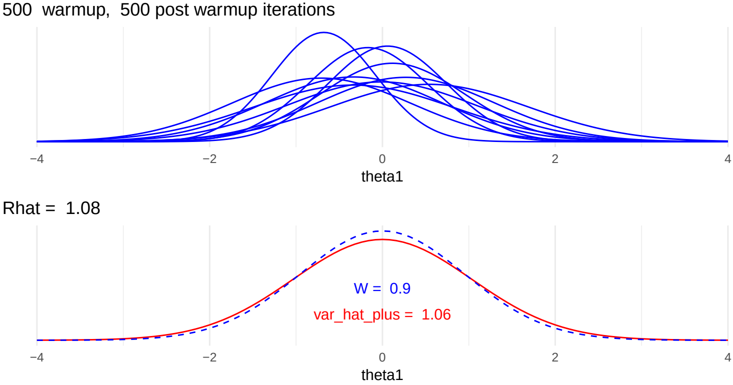

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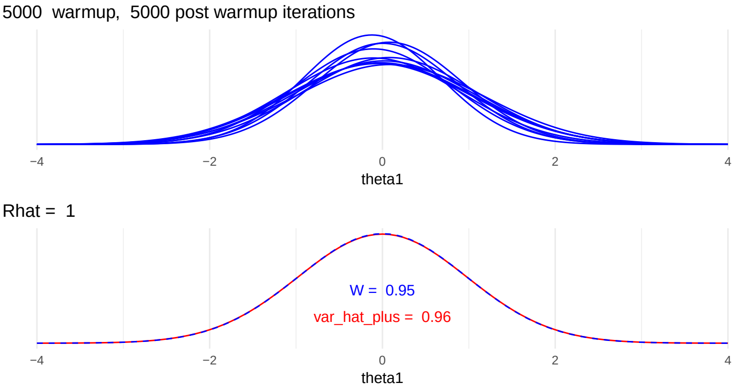

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$$\widehat{\mathrm{var}}^{+}(\theta \mid y) = \frac{N-1}{N}W + \frac{1}{N}B$$

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

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

$\widehat{R}$

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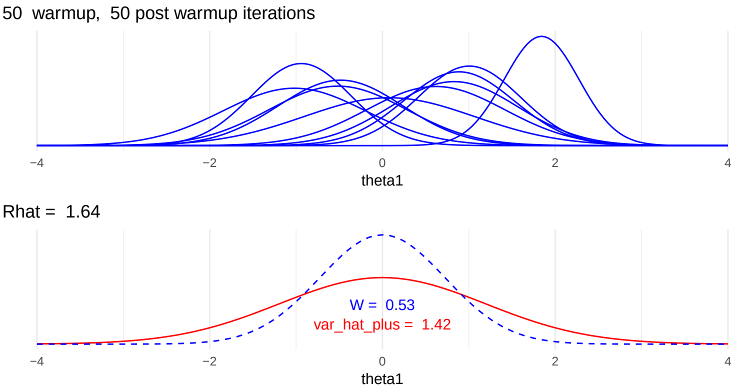

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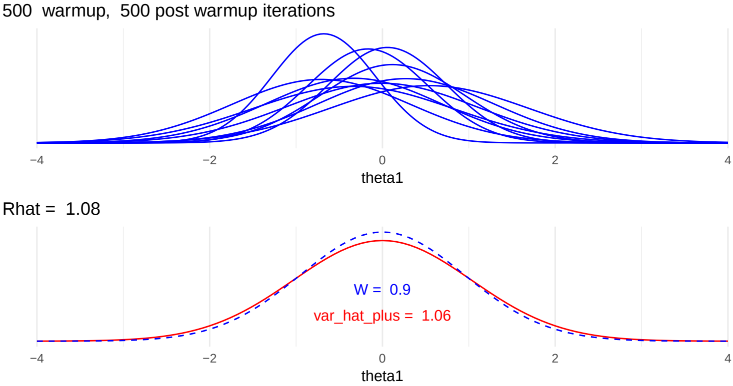

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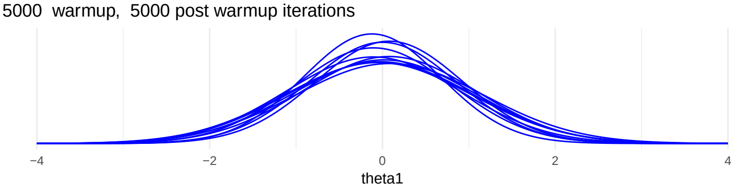

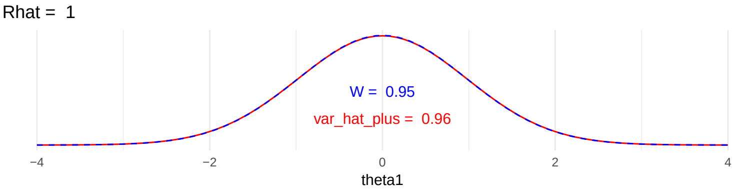

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- Estimates how much the scale of ψ could reduce if $N \to \infty$
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- If $\widehat{R}$ close to 1, it is still possible that chains have not converged
  - if starting points were not overdispersed
  - 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 $\theta_{nm} \quad (n = 1, \ldots, N; m = 1, \ldots, M)$
  - 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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- Notation updated compared to BDA3

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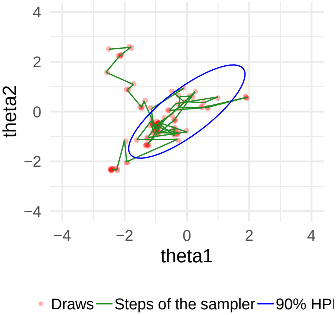
Time series analysis

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

Autocorrelation



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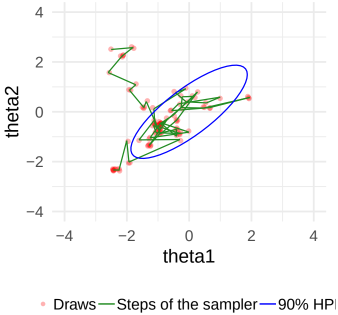

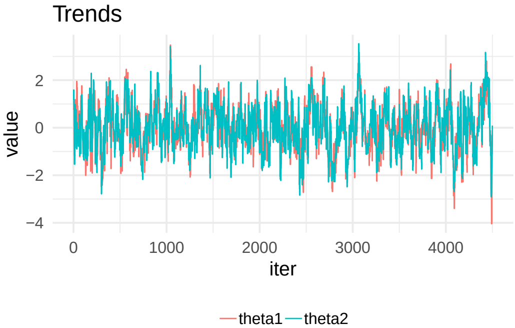

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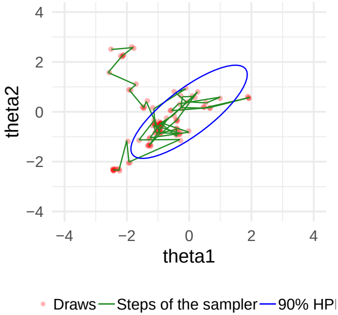
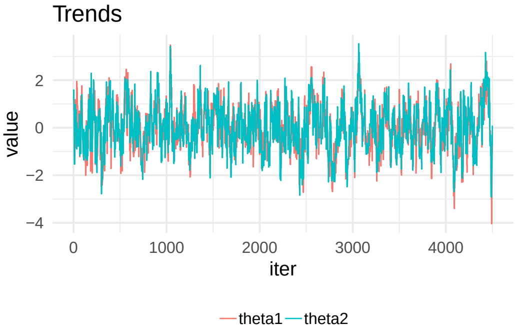
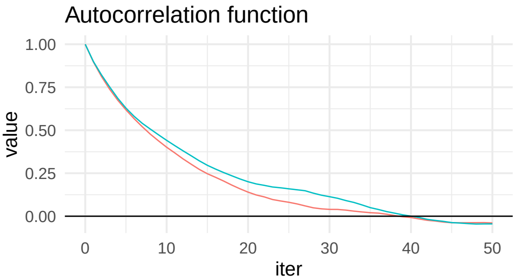
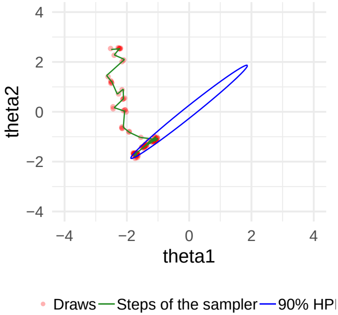
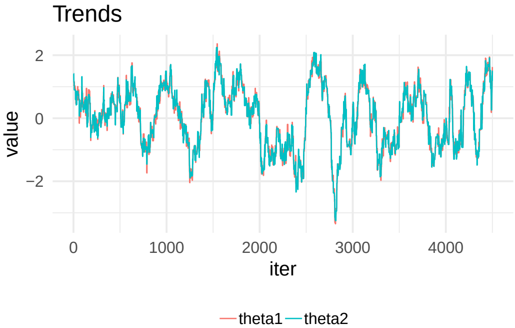


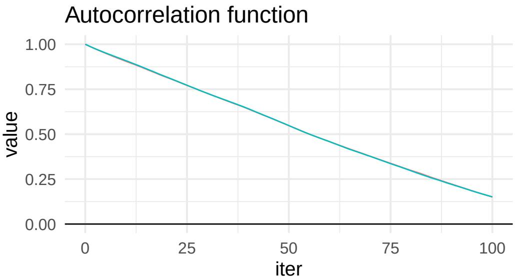




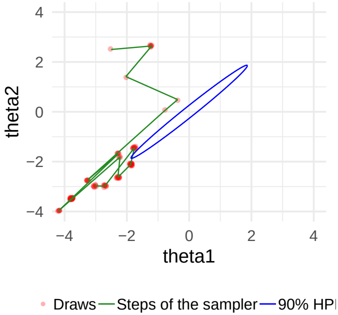
Autocorrelation (slow mixing due to small step size)

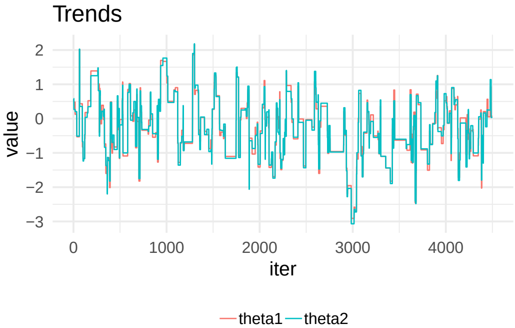


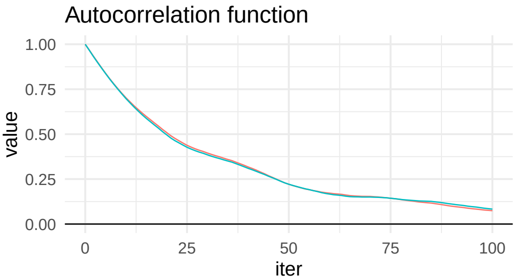




Autocorrelation (slow mixing due to many rejections)





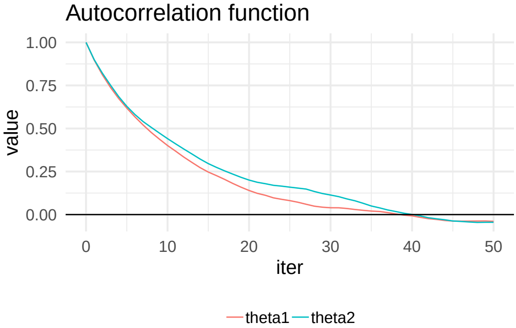


Time series analysis

- 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 $n_{\mathrm{eff}} = N/\tau$)
  - 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

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

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

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- BDA3 has slightly different and less accurate equation. The above equation is used in Stan 2.18+

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

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

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

Time series analysis

- Estimation of τ

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

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

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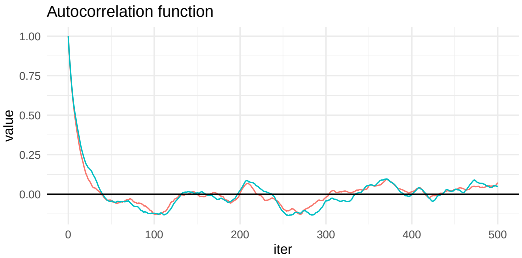

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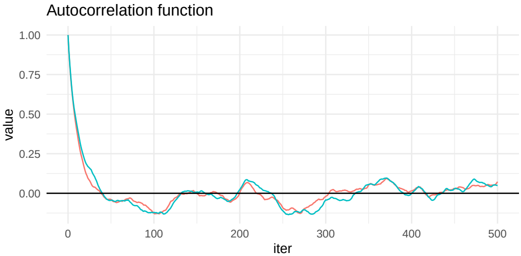

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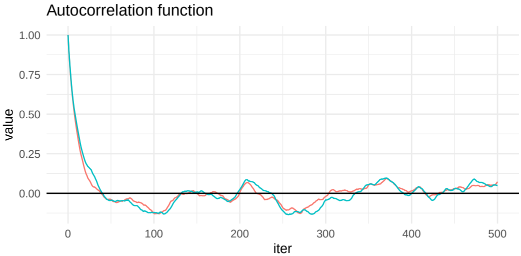

- empirical autocorrelation function is noisy and thus estimate of τ is noisy
- noise is larger for longer lags (less observations)
- less noisy estimate is obtained by truncating

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

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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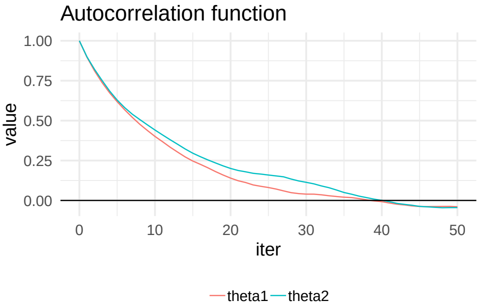
  - Γ_m is positive, decreasing and convex function of m
- Initial positive sequence estimator (Geyer's IPSE)
  - Choose the largest m so, that all values of the sequence $\hat{\Gamma}_1, \ldots, \hat{\Gamma}_m$ are positive



Effective sample size

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

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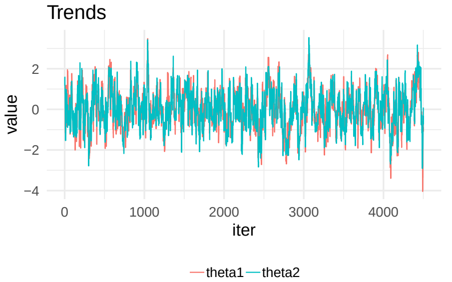
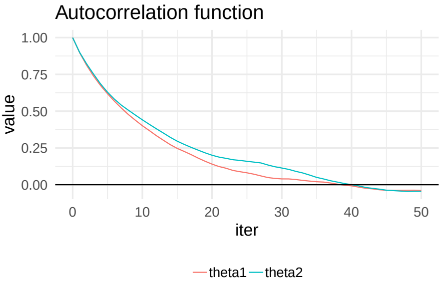
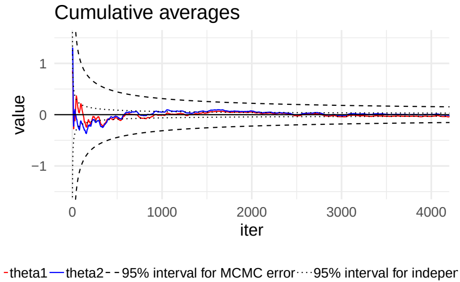






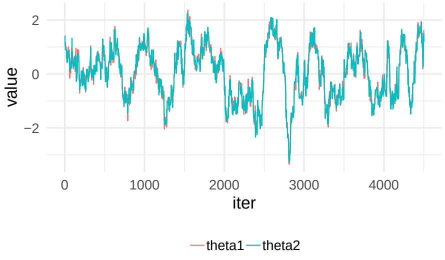
$$\hat{\tau} = 1 + 2\sum_{t=1}^{T} \hat{\rho}_t$$

$$\approx 24$$

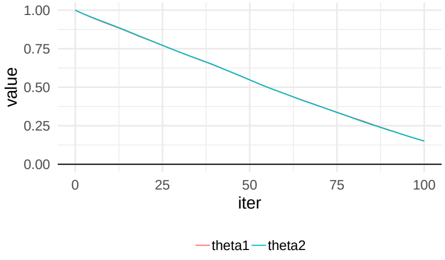
Effective sample size

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

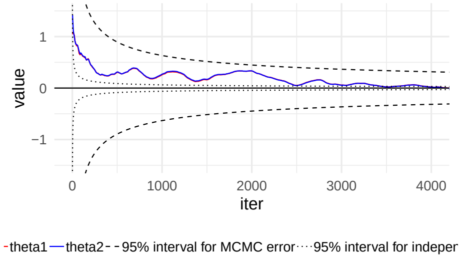
Trends



Autocorrelation function



Cumulative averages



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

$$\approx 104$$

Effective sample size

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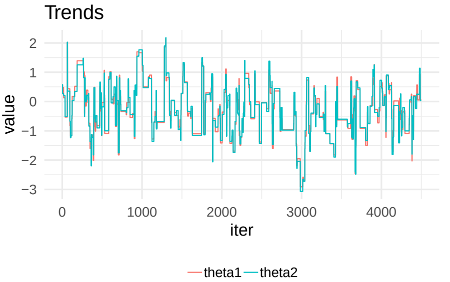

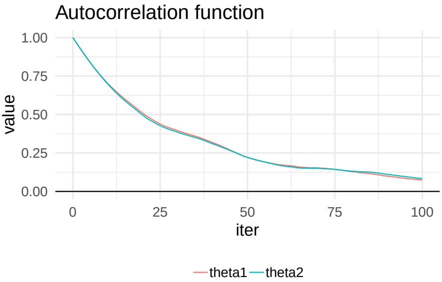

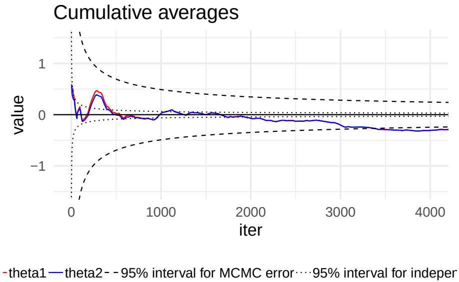

$$\hat{\tau} = 1 + 2\sum_{t=1}^{T} \hat{\rho}_t$$

$$\approx 63$$

Problematic distributions

- Nonlinear dependencies
  - optimal proposal depends on location

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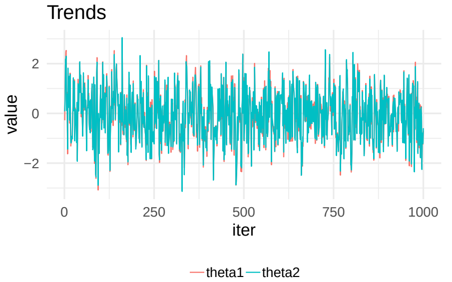
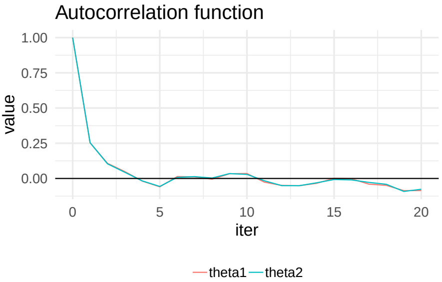
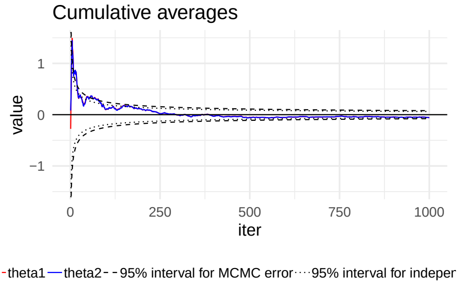
  - optimal proposal depends on location
- Funnels
  - optimal proposal depends on location
- Multimodal
  - difficult to move from one mode to another
- Long-tailed with non-finite variance and mean
  - central limit theorem for expectations does not hold

Next week: HMC, NUTS, and dynamic HMC

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







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

$$\approx 1.6$$

Further diagnostics

- Dynamic HMC/NUTS has additional diagnostics
  - divergences
  - tree depth exceedences
  - fraction of missing information