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- Monte Carlo recap
- Markov Chain Monte Carlo (MCMC)
  - Gibbs sampling
  - Metropolis-Hastings
- Diagnostics
  - Warm-up
  - Convergence
  - S_{eff}, MCSE, and autocorrelation
- Difficult geometries

Bayesian Statistics and Data Analysis Lecture 5

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It's all about expectations

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

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

We can easily evaluate $p(y|\theta)p(\theta)$ for any θ, but the integral $\int p(y|\theta)p(\theta)d\theta$ is usually difficult.

We can use the unnormalized posterior $q(\theta|y) = p(y|\theta)p(\theta)$, for example, in

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

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

Monte Carlo

- Monte Carlo methods we have discussed so far
  - Inverse CDF works for 1D
  - Analytic transformations work for only certain distributions
  - Grid methods works in less than a few dimensions
  - Rejection sampling works mostly in 1D (truncation is a special case)
  - Importance sampling is reliable only in special cases
- What to do in high dimensions?
  - Markov chain Monte Carlo (Ch 11-12)
  - Laplace, Variational*, EP* (Ch 4, 13*, next course)

Markov chains

- Andrey Markov proved weak law of large numbers and central limit theorem for certain dependent-random sequences, which were later named Markov chains
- The probability of each event depends only on the state attained in the previous event (or finite number of previous events)

$$p(\theta_t|\theta_{t-1}, \theta_{t-2}, \dots) = p(\theta_t|\theta_{t-1})$$

- $T_t(\theta_t \mid \theta_{t-1}) \equiv p(\theta_t|\theta_{t-1})$ is usually refered to as the transition distribution
- Under some assumptions $p(\theta_t|\theta_{t-1})$ will converge (in total variation) to *one* stationary distribution $p(\theta)$
- Goal in MCMC: Construct a transition distribution with $p(\theta|y)$ as the stationary distribution

Markov chain Monte Carlo (MCMC)

- Produce draws $\theta_{(t)}$ given $\theta_{(t-1)}$ from a Markov chain, with stationary distribution $p(\theta|y)$
  - \+ generic
  - \+ combine sequence of easier Monte Carlo draws to form a Markov chain
  - \+ chain goes where most of the posterior mass is
  - \+ asymptotically chain spends the $\alpha\%$ of time where $\alpha\%$ posterior mass is
  - \+ central limit theorem holds for expectations
  - \- draws are dependent
  - \- construction of efficient Markov chains is not always easy

Markov chain Monte Carlo (MCMC)

- Random variables $\theta_1, \theta_2, \ldots$ where θ_t depends only on the previous $\theta_{(t-1)}$

$$p(\theta_t | \theta_1, \ldots, \theta_{(t-1)}) = p(\theta_t | \theta_{(t-1)})$$

- 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 $p(\theta | y)$

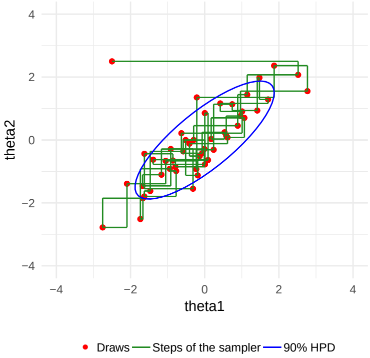
Gibbs sampling

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

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

- Will converge (in total variation) to $p(\theta|y)$ as $N \to \infty$
- j can be multiple (blocked) parameters
- 1D sampling ($|j| = 1$) is generally easy
- Related to the (stochastic) EM algorithm

Gibbs sampling



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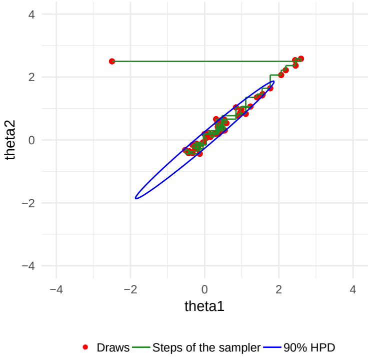
Gibbs sampling

- With *conditionally* conjugate priors, the sampling from the conditional distributions is easy for wide range of models
- BUGS / WinBUGS / OpenBUGS / JAGS
- No algorithm parameters to tune
- 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...

Gibbs sampling



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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?

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
     (b) calculate acceptance ratio
     $$r = \frac{p(\theta^*|y)}{p(\theta_{t-1}|y)}$$
     (c) set
     $$\theta_t = \begin{cases} \theta^* & \text{with probability } \min(r, 1) \\ \theta_{t-1} & \text{otherwise} \end{cases}$$
     ie, if $p(\theta^*|y) > p(\theta_{t-1}|y)$ accept the proposal always and otherwise accept the proposal with probability r
- 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!

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

- 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 $p(\theta|y)$

Why Metropolis algorithm works

1. Prove that simulated series is a Markov chain which has unique stationary distribution
   a) irreducible
      = positive probability of eventually reaching any state from any other state
   b) aperiodic
      = aperiodic (return times are not periodic)
      - holds for a random walk on any proper distribution (except for trivial exceptions)
   c) recurrent / not transient
      = probability to return to a state i is 1 as $T \to \infty$
      - holds for a random walk on any proper distribution (except for trivial exceptions)

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Why Metropolis algorithm works

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

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Metropolis-Hastings algorithm

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

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

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
- Good proposal distribution resembles the target distribution
  - if the shape of the target distribution is unknown, usually normal or t distribution is used
- After the proposal distribution 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

demo

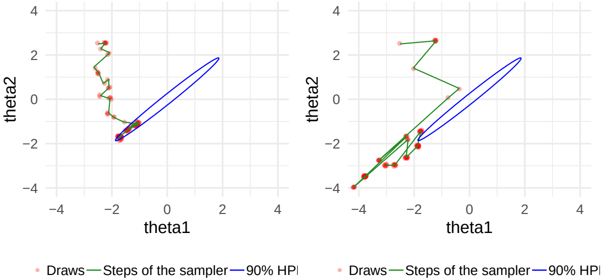
- Generic rule for rejection rate is 60-90%

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

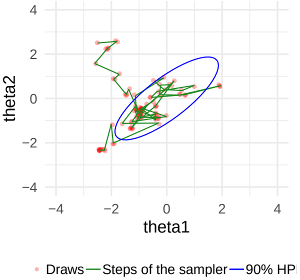
Metropolis

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



Warm-up

- Asymptotically chain spends the α% of time where α% posterior mass is
  - but in finite time the initial part of the Markov chain may be non-representative



- Warm-up period = (non-representative) draws from the beginning of the Markov chain
  - remove warm-up before using samples for inference
  - warm-up may include also phase for adapting algorithm parameters
- Also called burn-in

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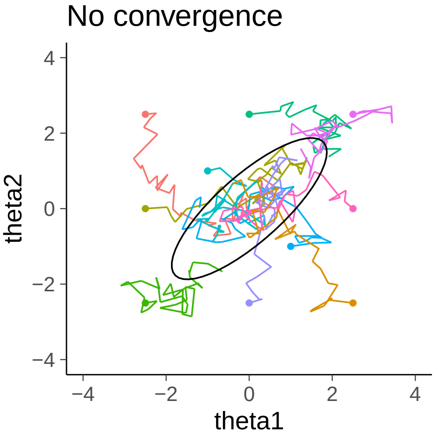
Assesing convergence

- Several Markov chains make convergence diagnostics easier
- Start chains from different starting points – preferably overdispersed



- Remove warm-up draws and run chains long enough

Several chains

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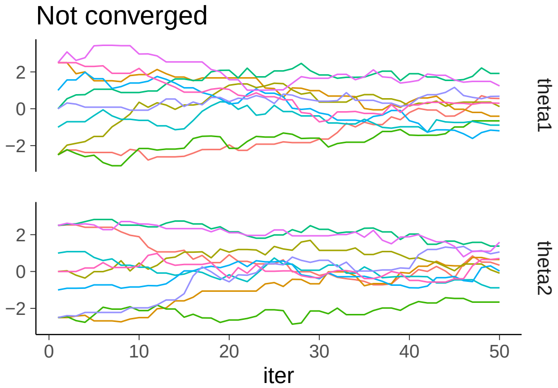

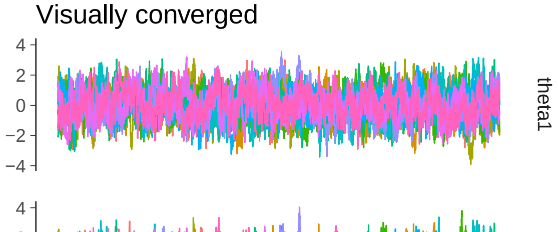

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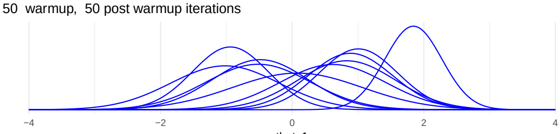
$\widehat{R}$: comparison of within and between variances of the chains

- $\widehat{R}$ or potential scale reduction factor (PSRF)
- Compare means and variances of the chains
  W = within chain variance estimate
  var_hat_plus = total variance estimate



$\widehat{R}$

- M chains, each having N draws
- Within chains variance W

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

- Between chains variance B

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

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

  - B/N is variance of the means of the chains

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

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

$\widehat{R}$

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

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

  - this *overestimates* marginal posterior variance if the starting points are overdispersed

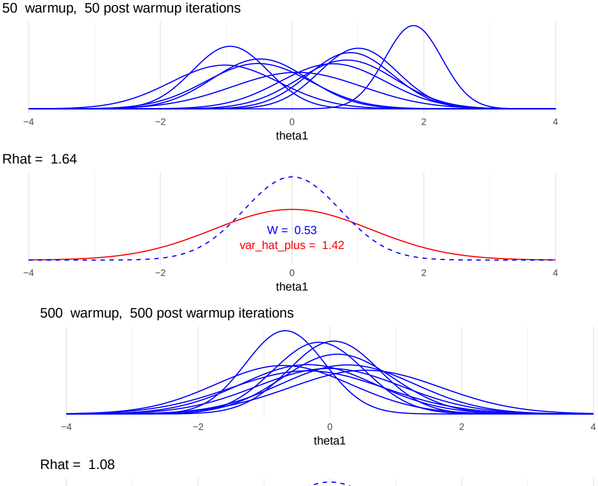
- Given finite N, W *underestimates* marginal posterior variance
  - single chains have not yet visited all points in the distribution
  - when $N \to \infty, \quad \mathrm{E}(W) \to \mathrm{var}(\theta|y)$

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

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

$\widehat{R}$

- BDA3: $\widehat{R}$ aka *potential scale reduction factor* (PSRF)
- Compare means and variances of the chains
  W = within chain variance estimate
  var_hat_plus = total variance estimate



$\widehat{R}$

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

- Estimates how much the scale 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
- 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

$\widehat{R}$

- Additional $\widehat{R}$ methods to assess convergence
- Split-$\widehat{R}$
  - Examines *mixing* and *stationarity* of chains
  - To examine stationarity chains are split to two parts: compare means and variances of the split chains
- Rank normalized $\widehat{R}$
  - Does not requires that the target distribution has finite mean and variance

MCMC draws are dependent

- Monte Carlo estimates still valid (central limit theorem)

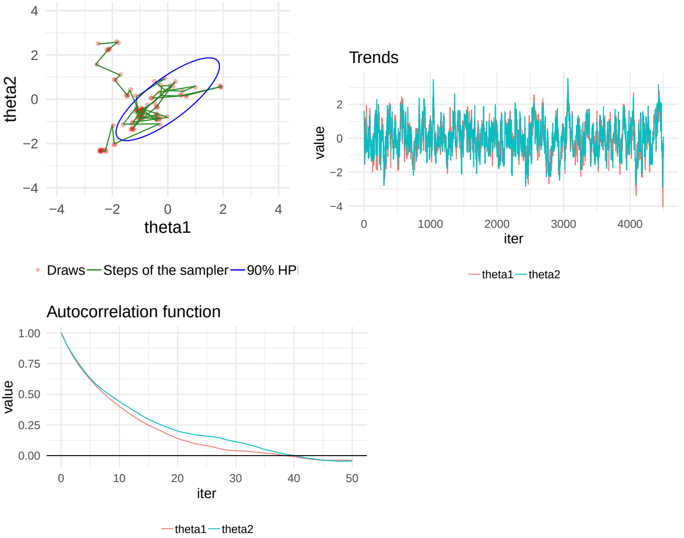
$$E_{p(\theta|y)}[f(\theta)] \approx \frac{1}{S}\sum_{s=1}^{S} f(\theta^{(s)})$$

- Estimation of Monte Carlo error is more difficult
  - evaluation of *effective* sample size, S_{eff}.

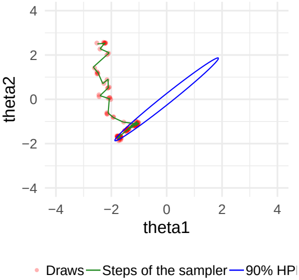
MCMC Autocorrelation

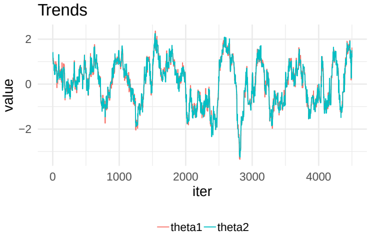
- Auto correlation function
  - describes the correlation given a certain lag
  - can be used to compare efficiency of MCMC methods

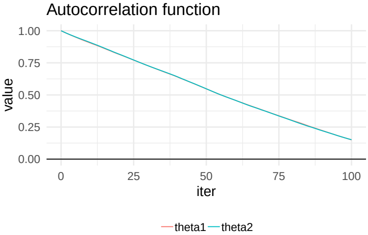
Autocorrelation



Autocorrelation







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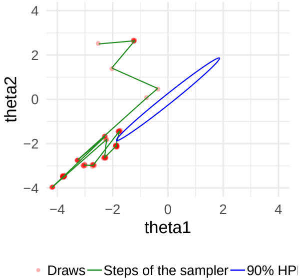
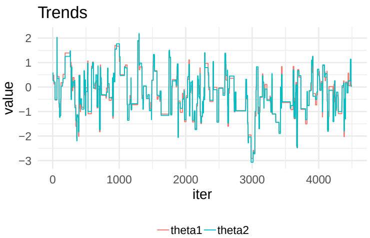
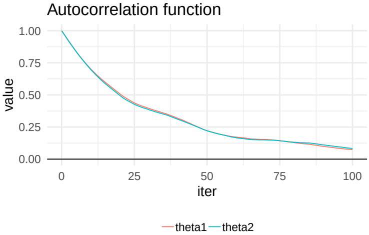






Autocorrelation

- The autocorrleation 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 $S_{\text{eff}} = S/\tau$, and τ is sum of autocorrelations

  - τ describes how many dependent draws correspond to one independent draw
  - Here $S = NM$ (in BDA3 $N = nm$ and $n_{\text{eff}} = N/\tau$)
  - BDA3 focuses on S_{eff} and not the Monte Carlo error directly

Autocorrelation

- 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
- 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

Estimating τ

- Estimation of τ

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

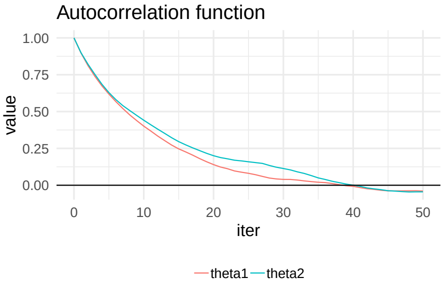
where $\hat{\rho}_t$ is empirical autocorrelation

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

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

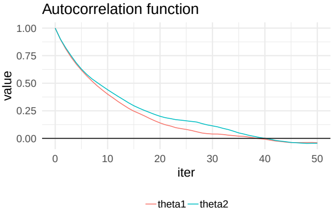
Geyer's adaptive window estimator of τ

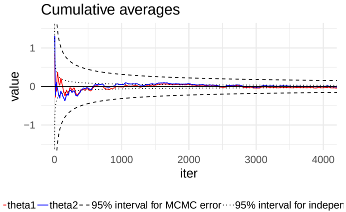
- Truncation T can be decided adaptively
  - for stationary, irreducible, recurrent Markov chain
  - let $\Gamma_m = \rho_{2m} + \rho_{2m+1}$, which is sum of two consequent autocorrelations
  - Γ_m is positive, decreasing and convex function of m
- Initial positive sequence estimator (Geyer's IPSE)
  - Choose the largest m so, that all values of the sequence $\hat{\Gamma}_1, \ldots, \hat{\Gamma}_m$ are positive



Effective sample size, S_{eff}

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





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

$$\approx 24$$

Effective sample size, S_{eff}

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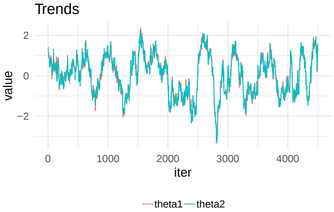

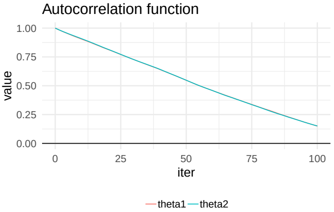

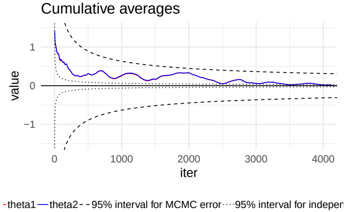

$$\hat{\tau} = 1 + 2\sum_{t=1}^{T} \hat{\rho}_t$$

$$\approx 104$$

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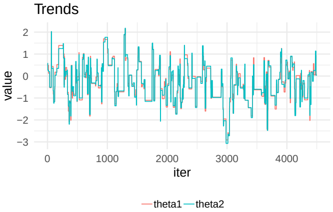

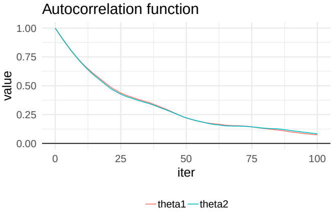

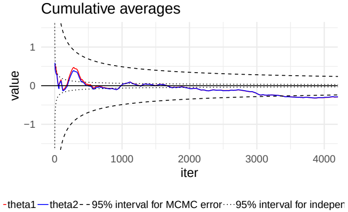

$$\hat{\tau} = 1 + 2\sum_{t=1}^{T} \hat{\rho}_t$$

$$\approx 63$$

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Problematic distributions

- Nonlinear dependencies
  - optimal proposal depends on location
- 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

demo