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- This lecture introduces also necessary diagnostics to check whether MCMC results are useful

Chapter 11

- 11.1 Gibbs sampler
- 11.2 Metropolis and Metropolis-Hastings
- 11.3 Using Gibbs and Metropolis as building blocks
- 11.4 Inference and assessing convergence (important)
 - potential scale reduction \widehat{R} (R-hat)
- 11.5 Effective number of simulation draws (important)
 - effective sample size (ESS / S_{eff})
- 11.6 Example: hierarchical normal model (quick glance)

Chapter 11 demos

- demo11_1: Gibbs sampling
- demo11_2: Metropolis sampling
- demo11_3: Convergence of Markov chain
- demo11_4: split- \widehat{R} and effective sample size (ESS or $S_{\rm eff}$)
- demo11_5: Diagnostics with posterior and bayesplot packages

$$E_{p(\theta|y)}[f(\theta)] = \int f(\theta)p(\theta|y)d\theta,$$
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• Monte Carlo methods which can sample from $p(\theta^{(s)} \mid y)$ using only $q(\theta^{(s)} \mid y)$

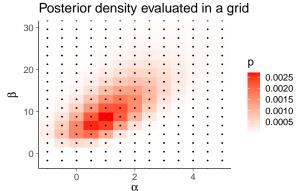
$$E_{p(\theta|y)}[f(\theta)] \approx \frac{1}{S} \sum_{s=1}^{S} f(\theta^{(s)})$$

Monte Carlo

- Monte Carlo methods we have discussed so far
 - Inverse CDF works for 1D
 - Analytic transformations work for only certain distributions
 - Factorization works only for certain joint distributions
 - Grid evaluation and sampling works in a few dimensions
 - Rejection sampling works mostly in 1D (truncation is a special case)
 - Importance sampling is reliable only in special cases

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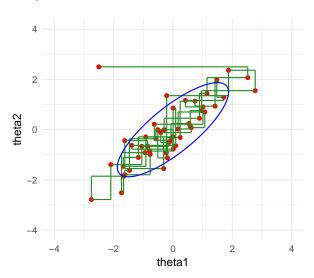
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- What to do in high dimensions?
 - Markov chain Monte Carlo (Ch 11-12)
 - Laplace, Variational*, EP* (Ch 4,13*)

Automatically focuses density evaluations where most of the posterior mass is



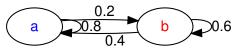
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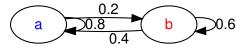
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 - Deep learning language models are super big Markov models

• Example of a simple Markov chain

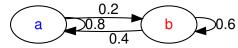


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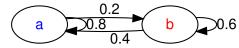
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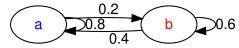
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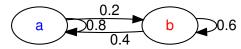
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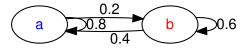
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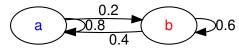


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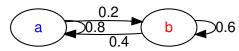
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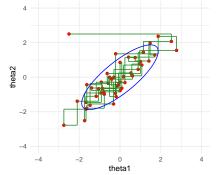
• From A^s we get p(a) = 0.75 and p(b) = 0.25

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

• 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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Markov chain

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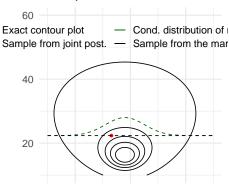
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- Transition distribution $T_t(\theta^t \mid \theta^{t-1})$ (may depend on t)
 - by choosing a suitable transition distribution, the stationary distribution of Markov chain is $p(\theta \mid y)$

- Alternate sampling from 1D conditional distributions
 - e.g. normal distribution, sample alternating from $p(\mu \mid \sigma^2, y)$ and $p(\sigma^2 \mid \mu, y)$

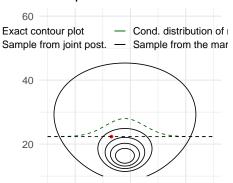
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Joint posterior



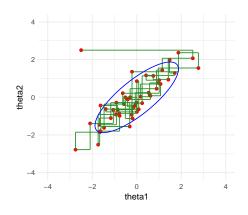
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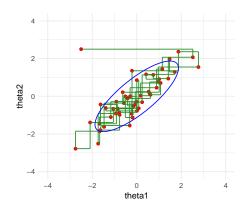
1D is easy even if no conjugate prior and analytic posterior

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- demo11 1



Draws — Steps of the sampler — 90% HPD

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Basic algorithm

sample
$$\theta_j^t$$
 from $p(\theta_j \mid \theta_{-j}^{t-1}, y)$, where $\theta_{-j}^{t-1} = (\theta_1^t, \dots, \theta_{j-1}^t, \ \theta_{j+1}^{t-1}, \dots, \theta_d^{t-1})$

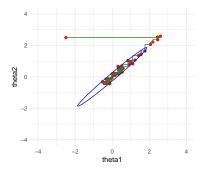
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- Slow if parameters are highly dependent in the posterior
 - demo11_1 continues



Conditional vs joint

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

Conditional vs joint

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

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

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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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- $p(\theta^* \mid y)$ 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!

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

$$\begin{pmatrix} \theta_1 \\ \theta_2 \end{pmatrix} \middle| y \sim N \begin{pmatrix} \begin{pmatrix} y_1 \\ y_2 \end{pmatrix}, \begin{pmatrix} 1 & \rho \\ \rho & 1 \end{pmatrix} \end{pmatrix}$$

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

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Theoretically

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- Prove that this stationary distribution is the desired target distribution

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 - = probability to return to a state i is 1
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- 2. Prove that this stationary distribution is the desired target distribution $p(\theta \mid y)$
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which is the same as the probability of transition from θ_a to θ_b , since we have required that $J_t(\cdot \mid \cdot)$ is symmetric

- since their joint distribution is symmetric, θ^{t-1} and θ^t have the same marginal distributions, and so $p(\theta \mid y)$ is the stationary distribution of the Markov chain of θ

Metropolis-Hastings algorithm

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

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

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 - ightarrow many steps accepted, but the chain moves slowly due to small steps
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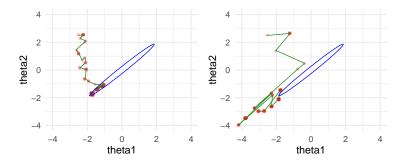
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- Generic rule for rejection rate is 60-90% (but depends on dimensionality and a specific algorithm variation)

Gibbs sampling

- Specific case of Metropolis-Hastings algorithm
 - single updated (or blocked)
 - proposal distribution is the conditional distribution
 - → proposal and target distributions are same
 - ightarrow 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



Draws—Steps of the sampler—90% HPI

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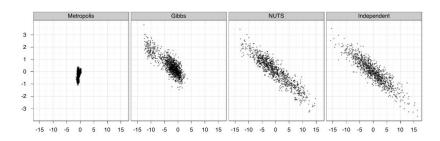
Dynamic Hamiltonian Monte Carlo and NUTS

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

HMC / NUTS

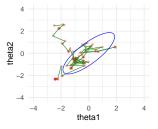
Comparison of algorithms on **highly correlated** 250-dimensional Gaussian distribution

- •Do **1,000,000** draws with both Random Walk Metropolis and Gibbs, thinning by 1000
- •Do 1,000 draws using Stan's NUTS algorithm (no thinning)
- •Do 1,000 independent draws (we can do this for multivariate normal)



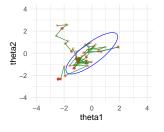
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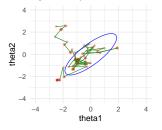
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- Draws—Steps of the sampler—90% HP
- Warm-up = remove draws from the beginning of the chain
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- Convergence diagnostics
 - Is the sample representative of the target distribution?

MCMC draws are dependent

 Monte Carlo estimates still valid (central limit theorem holds as proved by Andrey Markov)

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

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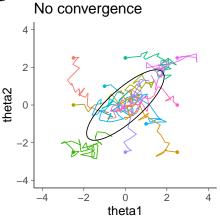
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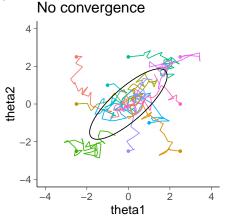
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- Estimation of Monte Carlo error is more difficult
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 - given finite variance, the distribution of the expectation approaches normal distribution with variance $\sigma_{\theta}^2/\text{ESS}$

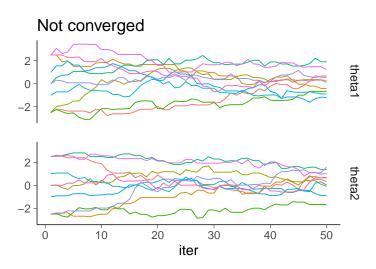
- Use of several chains make convergence diagnostics easier
- Start chains from different starting points preferably overdispersed

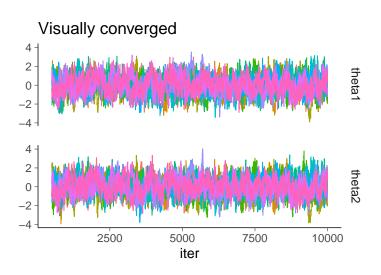


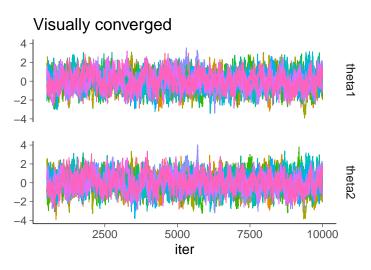
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 Remove draws from the beginning of the chains and run chains long enough so that it is not possible to distinguish where each chain started and the chains are well mixed



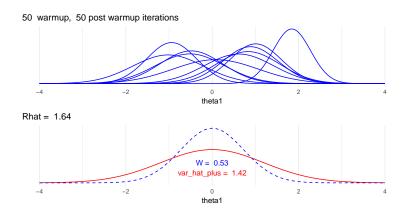




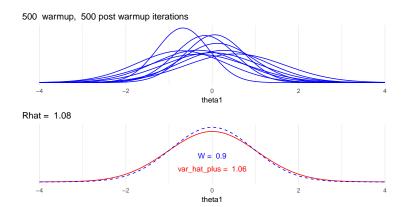
Visual convergence check is not sufficient

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

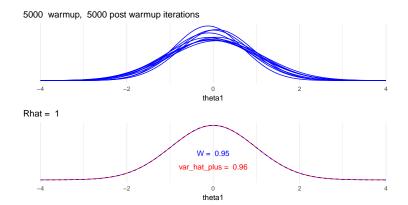
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Between chains variance B

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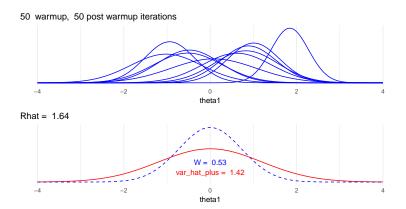
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- As $\widehat{\text{var}}^+(\theta \mid y)$ overestimates and W underestimates, compute

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

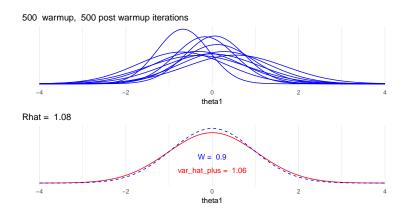
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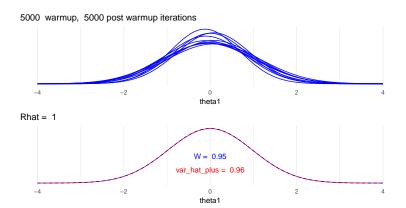
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- If \widehat{R} close to 1, it is still possible that chains have not converged
 - if starting points were not overdispersed
 - distribution far from normal (especially if infinite variance)
 - just by chance when N is finite

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

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 - inverse normal-cdf of ranks

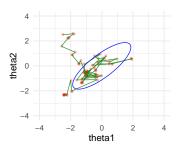
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- Notation updated compared to BDA3

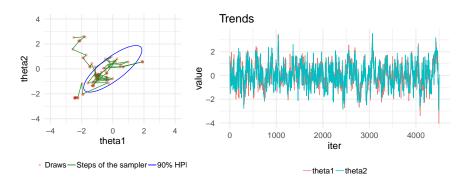
- Autocorrelation function
 - describes the correlation given a certain lag
 - can be used to compare efficiency of MCMC algorithms and parameterizations

Autocorrelation

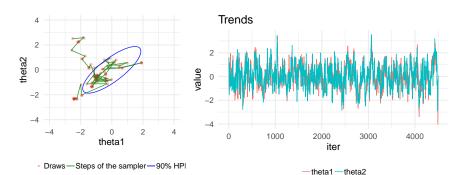


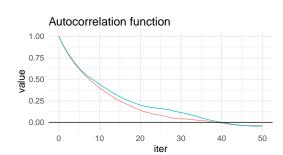
Draws—Steps of the sampler—90% HPI

Autocorrelation

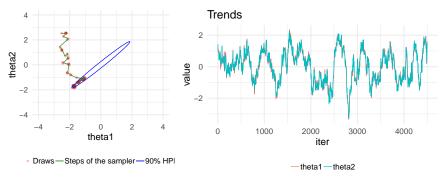


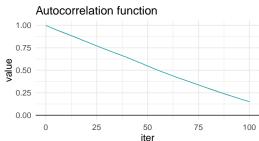
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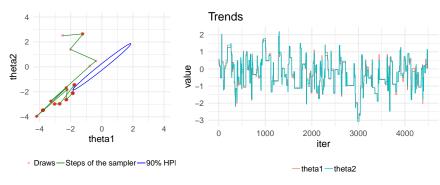


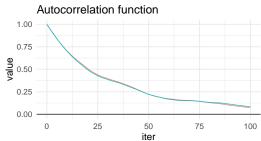
Autocorrelation (slow mixing due to small step size)





Autocorrelation (slow mixing due to many rejections)

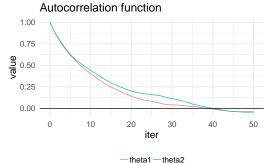




- Time series analysis can be used to estimate Monte Carlo error in case of MCMC
- For expectation $\bar{\theta}$

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

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



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

Estimation of the autocorrelation using several chains

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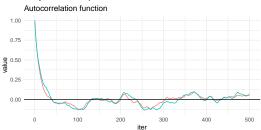
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 - takes into account if the chains are not mixing (the chains have not converged)
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- Compared to a method which computes the autocorrelation from a single chain, the multi-chain estimate has smaller variance

• Estimation of τ

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

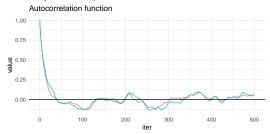
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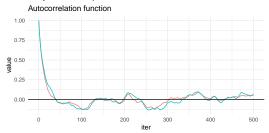
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- noise is larger for longer lags (less observations)
- · less noisy estimate is obtained by truncating

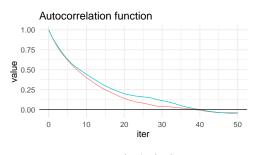
$$\hat{\tau} = 1 + 2\sum_{t=1}^{T} \hat{\rho}_t$$

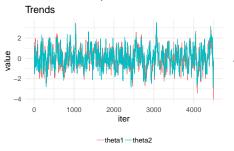
Geyer's adaptive window estimator

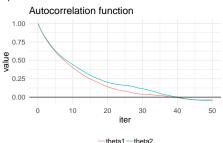
- Truncation can be decided adaptively
 - for stationary, irreducible, recurrent Markov chain
 - let $\Gamma_m = \rho_{2m} + \rho_{2m+1}$, which is sum of two consequent autocorrelations
 - Γ_m is positive, decreasing and convex function of m

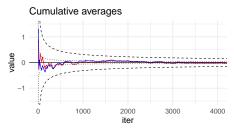
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 - Γ_m is positive, decreasing and convex function of m
- Initial positive sequence estimator (Geyer's IPSE)
 - Choose the largest m so, that all values of the sequence $\hat{\Gamma}_1, \dots, \hat{\Gamma}_m$ are positive



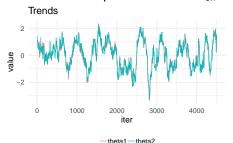


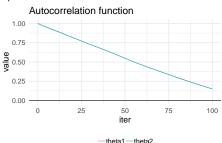


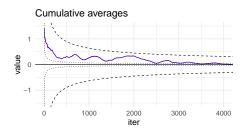


$$\hat{\tau} = 1 + 2 \sum_{t=1}^{T} \hat{\rho}_{t}$$

$$\approx 24$$

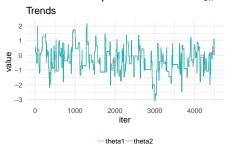


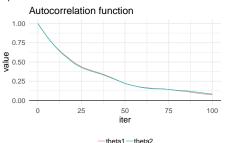


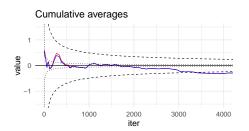


$$\hat{\tau} = 1 + 2 \sum_{t=1}^{T} \hat{\rho}_t$$

$$\approx 104$$







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

$$\approx 63$$

Monte Carlo standard error (MCSE)

- MCSE is obtained as discussed in lecture 4, but replacing the sample size S with the effective sample size ESS.
- See Digits case study for how many iterations to run and how many digits to report https://avehtari.github.io/casestudies/Digits/digits.html

ESS and MCSE in posterior package

Simulated 4 chains with AR(0.3) process

ESS and MCSE in posterior package

Simulated 4 chains with AR(0.3) process

variable	mean	sd	pareto_khat	ess_mean	<pre>mcse_mean</pre>
xn	0.01	0.99	-0.07	2280	. 0.02
xt3	0.02	1.6	0.33	2452	. 0.03
xt2	0.05	2.9	0.52	2903 .	. 0.05
xt1	0.33	93.	1.0	3976 .	. 1.5

ESS and MCSE in posterior package

Simulated 4 chains with AR(0.3) process

```
/variable mean pareto_khat ess_mean mcse_mean ess_q95 mcse_q95
       0.01
                 -0.07
                          2280.
                                  0.02
                                        3251.
                                                 0.04
хn
                 0.33
xt3
       0.02
                          2452. 0.03
                                        3251.
                                                0.09
xt2 0.05
                 0.52
                         <del>2903.</del> 0.05
                                        3251.
                                                0.13
                1.0 <del>3976.</del> <del>1.5</del>
xt1
    0.33
                                        3251.
                                                 0.49
```

Bulk-ESS and Tail-ESS in posterior package

- ESS depends on the quantity
- For quick diagnostic purposes the default summary shows
 - median and median absolute deviation (mad), which are valid in case of infinite mean and variance, too
 - if mad is much smaller than sd, suspect infinite variance
 - Rank-normalized \widehat{R} rhat
 - Bulk-ESS (ess_bulk) is generic ESS for sampling efficiency in bulk using rank normalized values (works for infinite variance)
 - Tail-ESS (ess_tail) is the minimum ESS for 5%- and 95%-quantiles

drt |> summarise_draws()

variable	mean	median	sd	mad	q5	q95	rhat	ess_bulk	ess_tail	
xn	0.01	0.00	0.99	0.99	-1.6	1.6	1.00	2284.	3189.	
xt3	0.02	0.00	1.6	1.1	-2.3	2.3	1.00	2284.	3189.	
xt2	0.05	0.00	2.9	1.2	-2.8	2.9	1.00	2284.	3189.	
xt1	0.33	0.00	93.	1.5	-5.8	6.1	1.00	2284.	3189.	

ESS and MCSE

- ESS and MCSE depend on the quantity
 - Bulk-ESS and Tail-ESS are useful diagnostic summaries, but eventually need to look at the ESS / MCSE for the quantity of interest

Diagnostic tools

For this week's assignment:

- \widehat{R} , ESS, MCSE
 - library(posterior)
 - th |> summarise_draws(Rhat=basic_rhat, ESS=mean_ess)
 - th |> summarise_draws(mean, mean_mcse)
 - th |> summarize_draws(~quantile(.x, probs = c(0.05, 0.95)))
 - see demo11_5 and Digits case study for the examples how to use these

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- Python
 - see ArviZ package

- Nonlinear dependencies
 - optimal proposal depends on location

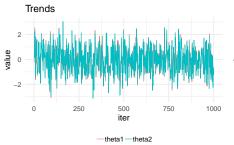
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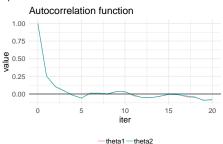
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- Long-tailed with non-finite variance and mean
 - central limit theorem for expectations does not hold

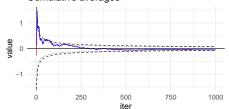
Next week: HMC, NUTS, and dynamic HMC

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





Cumulative averages



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

$$\approx 1.6$$

Further diagnostics

- Pareto- \hat{k} diagnostic for checking whether variance is finite
- Dynamic HMC/NUTS has additional diagnostics
 - divergences
 - tree depth exceedences

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