Chapter 11

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

It's all about expectations

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

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- Monte Carlo methods which can sample from $p(\theta^{(s)}|y)$ 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
  - Factorization works only for certain joint distributions
  - Grid evaluation and sampling works in less than a few dimensions
  - Rejection sampling works mostly in 1D (truncation is a special case)
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- What to do in high dimensions?
    - Markov chain Monte Carlo (Ch 11-12)
    - Laplace approximation, Variational Bayes*, Expectation Propagation* (Ch 4,13*)

Markov chain

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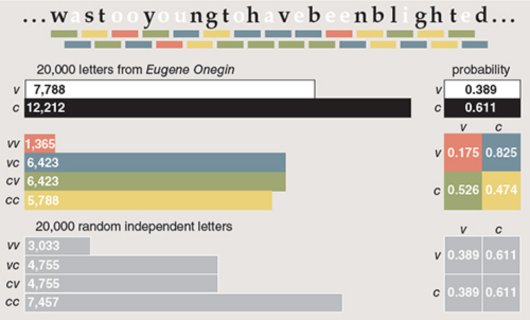
- The probability of each event depends only on the state attained in the previous event (or finite number of previous events)
- Markov's one example was the sequence of letters in Pushkin's novel "Yevgeniy Onegin" https://www.americanscientist.org/article/first-links-in-the-markov-chain

Markov chain

He was too young to have been blighted
by the cold world's corrupt finesse;
his soul still blossomed out, and lighted
at a friend's word, a girl's caress.
In heart's affairs, a sweet beginner,
he fed on hope's deceptive dinner;
the world's éclat, its thunder-roll,
still captivated his young soul.
He sweetened up with fancy's icing
the uncertainties within his heart;
for him, the objective on life's chart
was still mysterious and enticing—
something to rack his brains about,
suspecting wonders would come out.



- Example of a simple Markov chain: weather example

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

Markov chain

- Set of random variables $\theta^1, \theta^2, \ldots$, so that with all values of t, θ^t depends only on the previous $\theta^{(t-1)}$

$$p(\theta^t|\theta^1, \ldots, \theta^{(t-1)}) = p(\theta^t|\theta^{(t-1)})$$

- Chain has to be initialized with some starting point θ^0
- Transition distribution $T_t(\theta^t|\theta^{t-1})$ (may depend on t)
- By choosing a suitable transition distribution, the stationary distribution of Markov chain is $p(\theta|y)$

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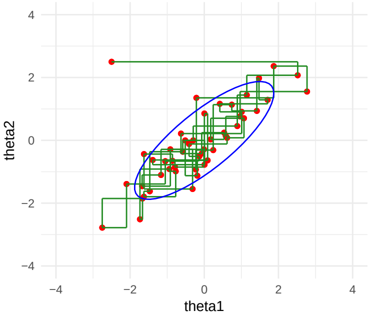
- demo



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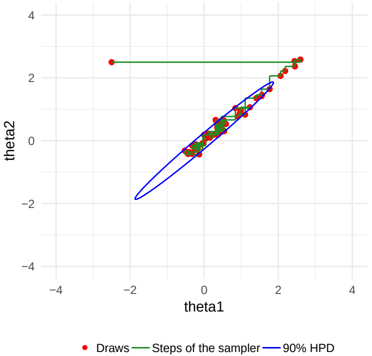
- Slow if parameters are highly dependent in the posterior
  - demo continues



Conditional vs joint

- How about sampling θ jointly?
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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?
  http://elevanth.org/blog/2017/11/28/build-a-better-markov-chain/

Metropolis algorithm

- Algorithm
  1. starting point θ^0
  2. $t = 1, 2, \ldots$
     (a) pick a proposal θ^* from the proposal distribution $J_t(\theta^*|\theta^{t-1})$. 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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     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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  - $p(\theta^*|y)$ 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

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

  - proposal distribution $J_t(\theta^*|\theta^{t-1}) = \mathrm{N}(\theta^*|\theta^{t-1}, \sigma_p^2)$
- Demo
  http://elevanth.org/blog/2017/11/28/build-a-better-markov-chain/,
  source: https://chi-feng.github.io/mcmc-demo/app.html?
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Why Metropolis algorithm works

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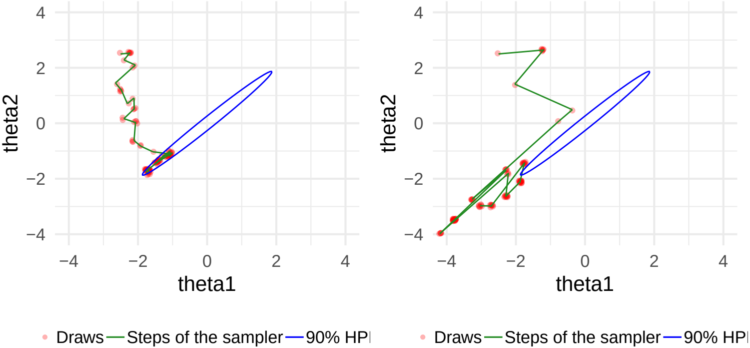
- Generic rule for rejection rate is 60-90% (but depends on dimensionality and a specific algorithm variation)

Gibbs sampling

- Specific case of Metropolis-Hastings algorithm
  - single updated (or blocked)
  - proposal distribution is the conditional distribution
    $\rightarrow$ 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
  - demo



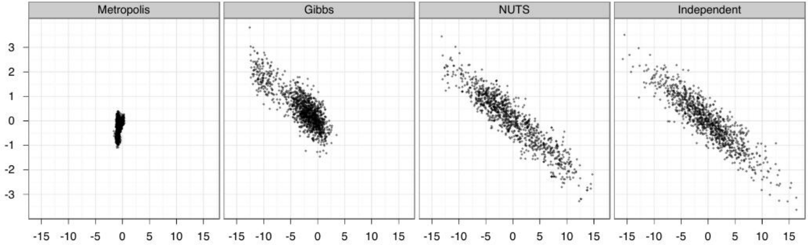
Dynamic Hamiltonian Monte Carlo and NUTS

- 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/, source: https://chi-feng.github.io/mcmc-demo/app.html?algorithm=HamiltonianMC&target=donut

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

Iterative simulation

Difficulties of inference from iterative simulation

1. if the iterations have not proceeded long enough, the simulations may be grossly unrepresentative of the target distribution.
2. within-sequence correlation

    aside from any convergence issues, simulation inference from correlated draws is generally less precise than from the same number of independent draws $\Rightarrow$ effective sample size

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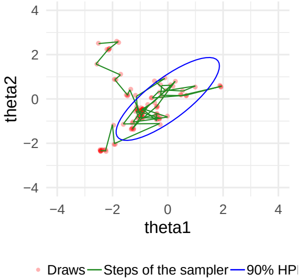

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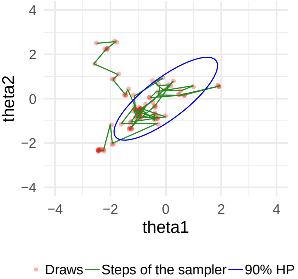

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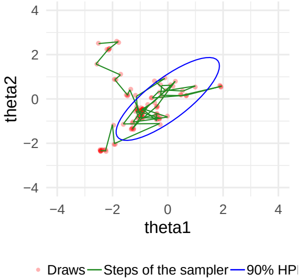


- Warm-up = remove draws from the beginning of the chain
  - warm-up may include also phase for adapting algorithm parameters
- Convergence diagnostics
  - Do we get samples from the target distribution?

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

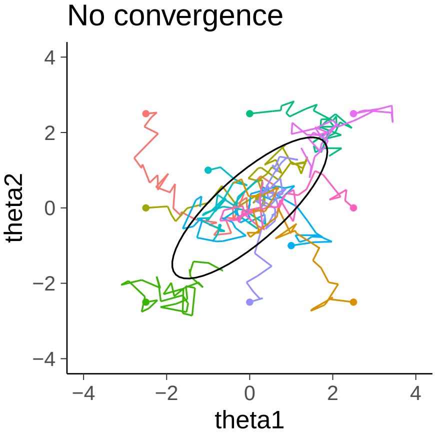
Remedies

We handle the special problems of iterative simulation in three ways

1. multiple sequences with starting points dispersed throughout parameter space
2. we monitor the convergence of all quantities of interest by comparing variation between and within simulated sequences
3. if the simulation efficiency is unacceptably low (in the sense of requiring too much real time), the algorithm can be altered

Several chains

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



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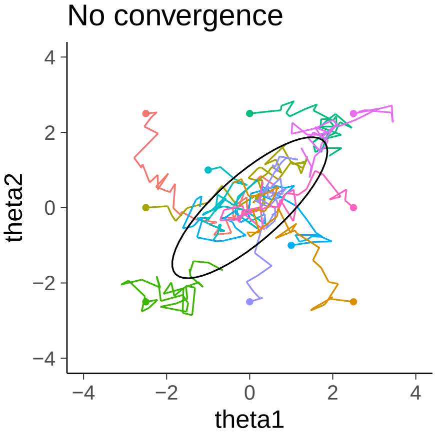

- Remove draws from the beginning of the chains and run chains long enough so that it is not possible to distinguish where each chain started and the chains are well mixed

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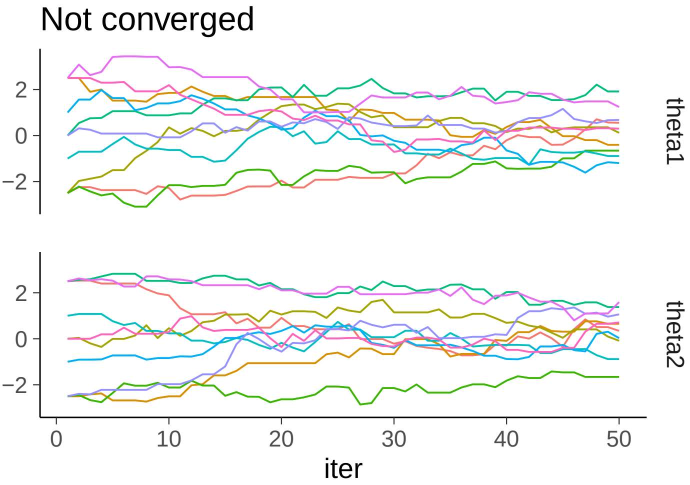

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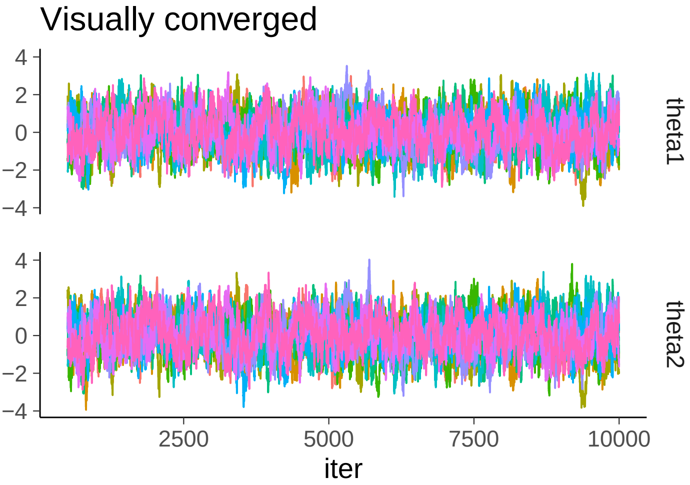

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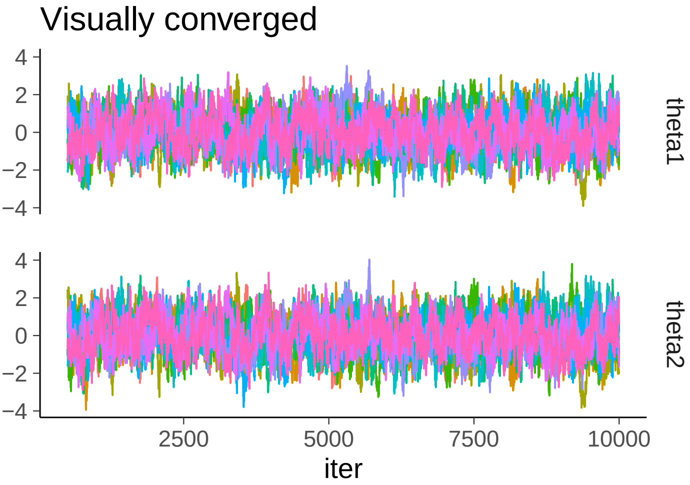

Visual convergence check is not sufficient

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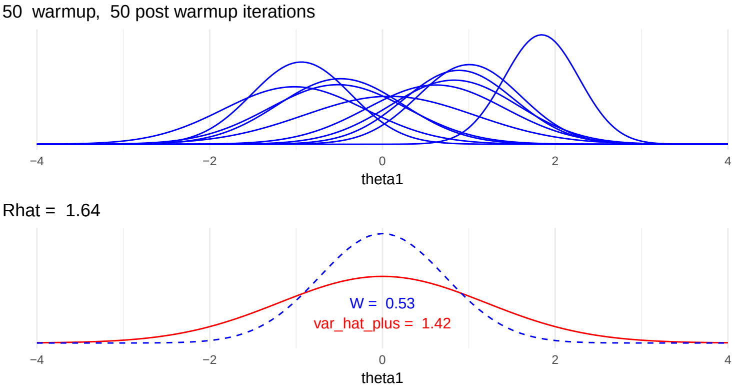

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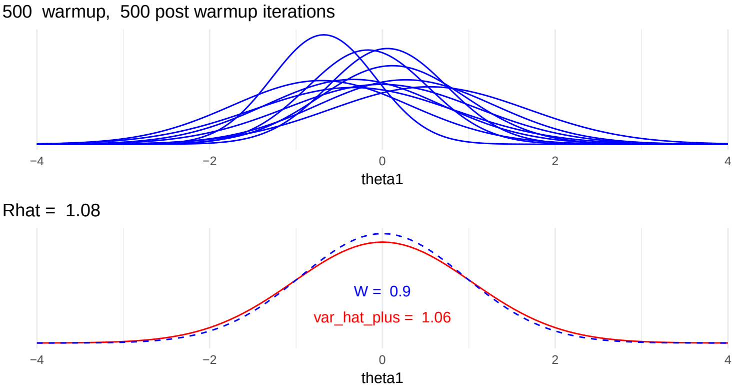

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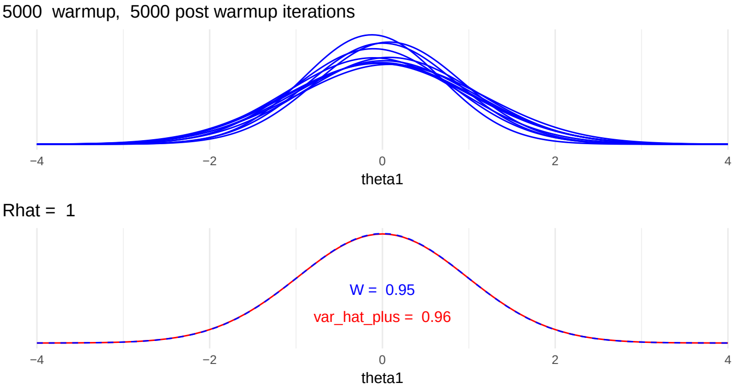

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- As $\widehat{\mathrm{var}}^{+}(\theta|y)$ overestimates and W underestimates, compute

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

$\widehat{R}$

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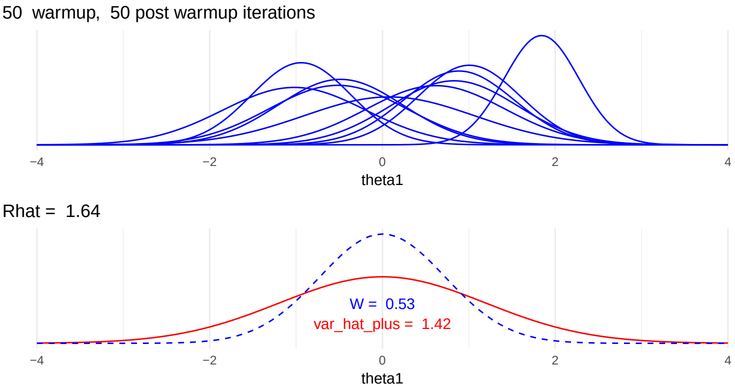

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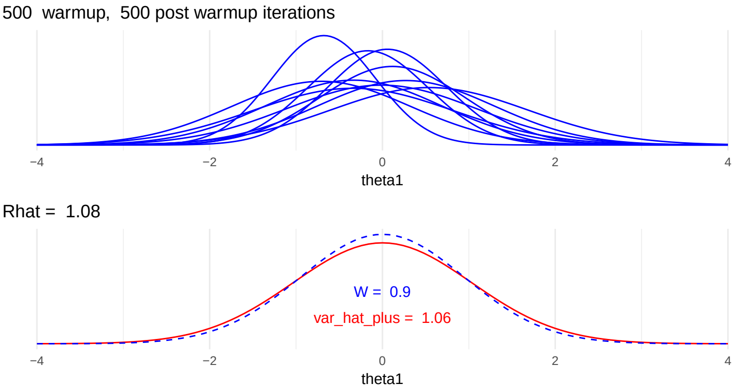

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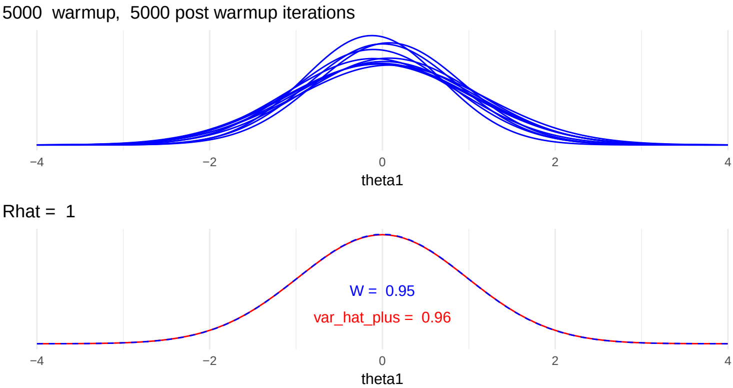

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- If $\widehat{R}$ close to 1, it is still possible that chains have not converged
  - if starting points were not overdispersed
  - distribution far from normal (especially if infinite variance)
  - just by chance when n is finite

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 $\widehat{R}$

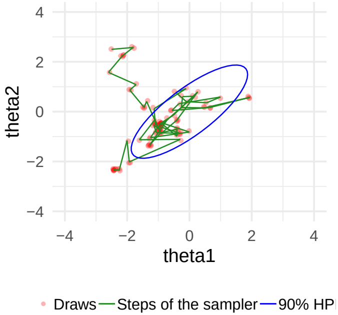
- Original $\widehat{R}$ requires that the target distribution has finite mean and variance
- Rank normalization fixes this and is also more robust given finite but high variance
- Folding improves detecting scale differences between chains
- Paper proposes also local convergence diagnostics and practical MCSE estimates for quantiles
- Notation updated compared to BDA3

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.

Time series analysis

- 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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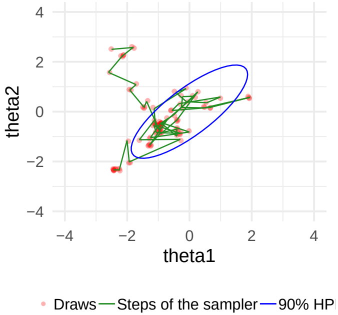

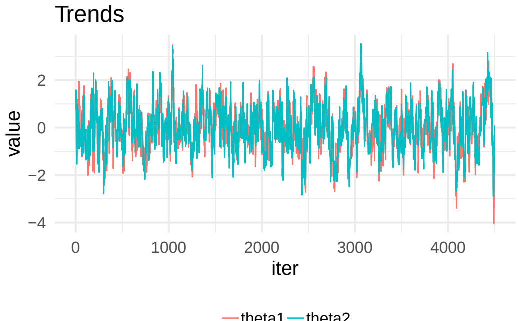

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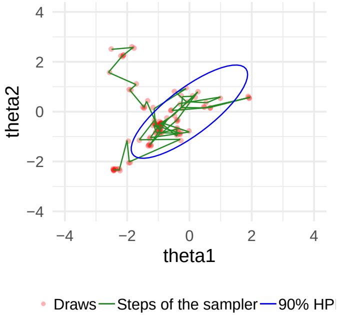

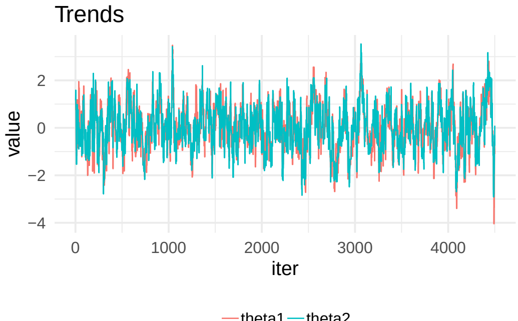

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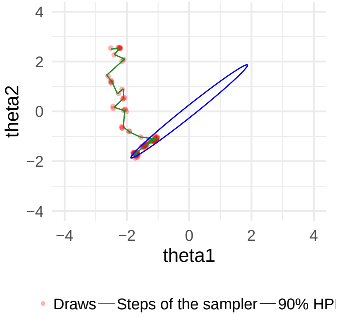

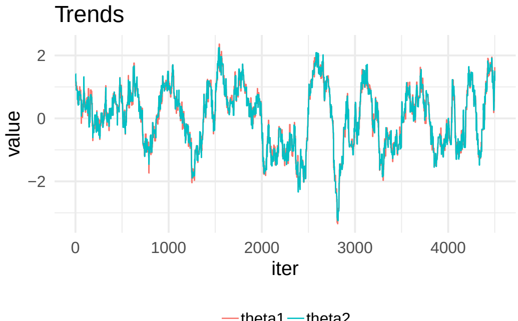

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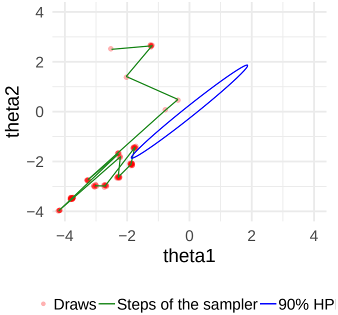

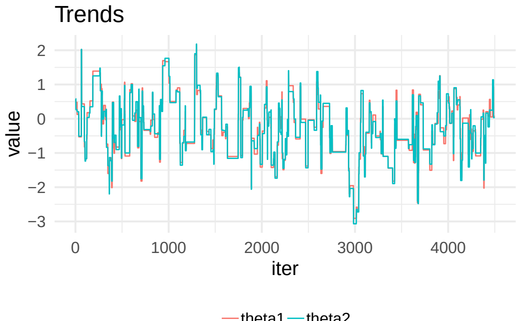

Time series analysis

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- For expectation $\bar{\theta}$

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  - BDA3 focuses on S_{eff} and not the Monte Carlo error directly new R-hat paper discusses more about MCSEs for different quantities

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- Compared to a method which computes the autocorrelation from a single chain, the multi-chain estimate has smaller variance

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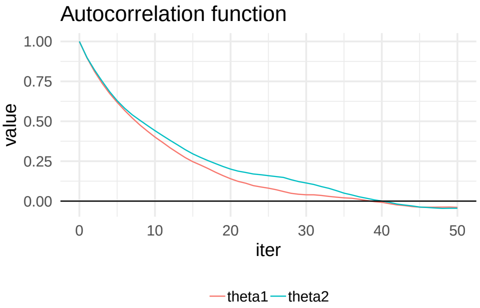
- Initial positive sequence estimator (Geyer's IPSE)
  - Choose the largest m so, that all values of the sequence $\hat{\Gamma}_1, \ldots, \hat{\Gamma}_m$ are positive



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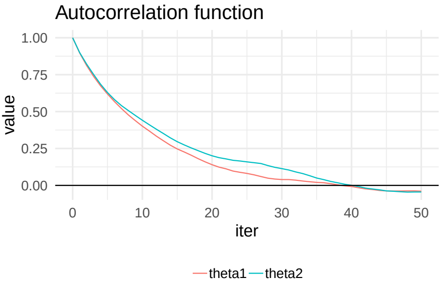

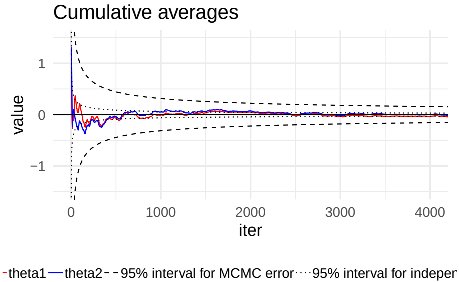

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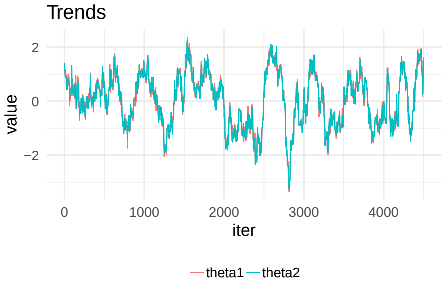

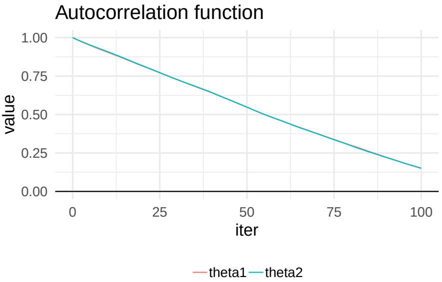

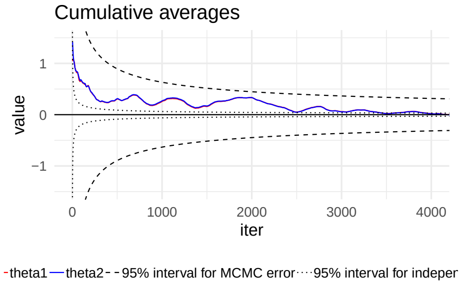

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Effective sample size

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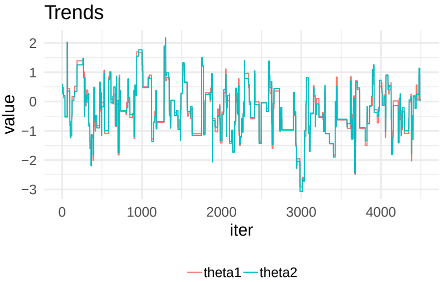

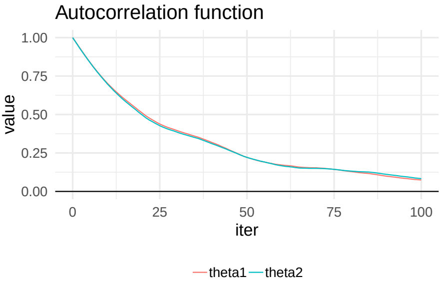

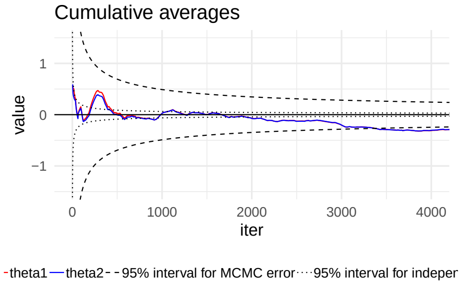

$$\hat{\tau} = 1 + 2\sum_{t=1}^{T} \hat{\rho}_t$$

$$\approx 63$$

Problematic distributions

- Nonlinear dependencies
    - optimal proposal depends on location

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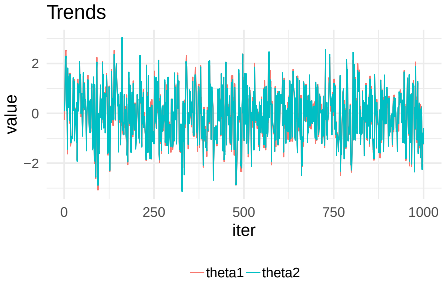
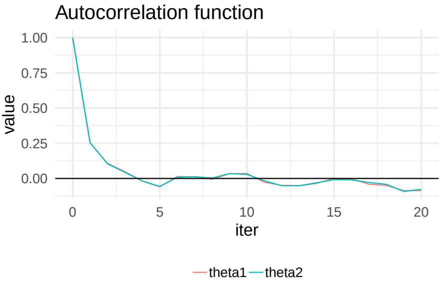
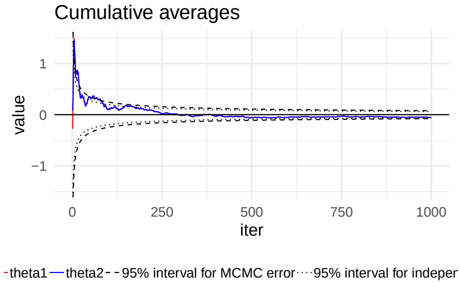
- Multimodal
  - difficult to move from one mode to another
- Long-tailed with non-finite variance and mean
  - central limit theorem for expectations does not hold

Ch. 12: HMC, NUTS, and dynamic HMC

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







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

$$\approx 1.6$$

Further diagnostics

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

Note

- Basics of Markov chains: http://www.netlab.tkk.fi/opetus/s38143/luennot/english.shtml, see Lecture 4.
  To prove that Metropolis algorithm works, it is sufficient to show that chain is irreducible, aperiodic and not transient.
- Nice animations with discussion http://elevanth.org/blog/2017/11/28/build-a-better-markov-chain/
  And just the animations with more options to experiment https://chi-feng.github.io/mcmc-demo/

- Metropolis algorithm
  Don't confuse rejection in the rejection sampling and in Metropolis algorithm.
  In the rejection sampling, the rejected samples are thrown away.
  In Metropolis algorithm the rejected proposals are thrown away, but time moves on and the previous sample $x(t)$ is also the sample $x(t+1)$.
    - When rejecting a proposal, the previous sample is repeated in the chain, they have to be included and they are valid samples from the distribution.
    - For basic Metropolis, it can be shown that optimal rejection rate is 55–77%, so that on even the optimal case quite many of the samples are repeated samples.
      However, high number of rejections is acceptable as then the accepted proposals are on average further away from the previous point. It is better to jump further away 23–45% of time than more often to jump really close.

- Transition distribution vs. proposal distribution Transition distribution is a property of Markov chain. In Metropolis algorithm the transition distribution is a mixture of a proposal distribution and a point mass in the current point. BDA uses also term jumping distribution to refer to proposal distribution.
- Convergence
  Theoretical convergence in an infinite time is different than practical convergence in a finite time. There is no exact moment when chain has converged and thus it is not possible to detect when the chain has converged (except for rare perfect sampling methods not discussed in BDA3).

  The convergence diagnostics can help to find out if the chain is unlikely to be representative of the target distribution. Furthermore, even if would be able to start from a independent sample from the posterior so that chain starts from the convergence, the mixing can be so slow that we may require very large number of samples before the samples are representative of the target distribution.

If starting point is selected at or near the mode, less time is needed to reach the area of essential mass, but still the samples in the beginning of the chain are not presentative of the true distribution unless the starting point was somehow samples directly from the target distribution.

Laplace, VB, EP: motivation

- MCMC methods could be expensive to compute, especially for large sample sizes n.
- Moreover, many MCMC algorithms require a rough estimate of some key posterior quantities, such as the posterior variance.
- These issues motivates the development of **deterministic approximations** of the posterior distribution
- Compared to MCMC methods, the accuracy of this class of approximations can not be reduced by running the algorithm longer.
- On the other hand, deterministic approximations are typically very fast to compute and sufficiently reliable in several applied contexts.

Laplace approximation

- Let $\pi(\theta|\mathbf{X})$ be a continuous and differentiable posterior density in $\Theta \subseteq \Re^p$
- The Laplace approximation is one of the first approximation methods that has been proposed. It was known even before the advent of MCMC.
- The key idea is approximating the log-posterior density $\log \pi(\theta|\mathbf{X})$ using a **Taylor expansion** around the mode $\hat{\theta}_{MAP}$ yielding

$$\log \pi(\theta|\mathbf{X}) \approx \log \pi(\hat{\theta}_{MAP}|\mathbf{X}) - \frac{1}{2}(\theta - \hat{\theta}_{MAP})^T \hat{M}(\theta - \hat{\theta}_{MAP}) + \text{const}$$

where M is the negative Hessian of $\log \pi(\theta|\mathbf{X})$ evaluated at $\hat{\theta}_{MAP}$, ie,

$$\hat{M} = -\left.\frac{\partial^2}{\partial\theta\partial\theta^T} \log \pi(\theta|\mathbf{X})\right|_{\theta=\hat{\theta}_{MAP}}$$

- This expansion leads to the following multivariate Gaussian approximate posterior

$$\pi(\theta|\mathbf{X}) \approx N_p(\hat{\theta}_{MAP}, \hat{M}^{-1})$$

- A fairly strong asymptotic justification of the Laplace approximation is based on the Bernstein–von Mises theorem.
- Here we are also assuming that $\hat{\theta}_{MAP}$ and $n\hat{M}^{-1}$ are consistent estimators for the "true" parameter value θ_0 and for the inverse Fisher information matrix, respectively.
- Hence, in several cases and for n large enough, the law $\pi(\theta|\mathbf{X})$ is roughly a Gaussian centered at the mode and with variance depending on the Fisher information.

+ The Laplace approximation is an old and simple method that has appealing asymptotic guarantees. Moreover, it only requires the computation of the Hessian and the MAP.

- Refined higher order improvements of expected posterior functionals can be obtained.
  - On the other hand, especially when the sample size n is relatively small, the quadratic approximation of $\log \pi(\theta|\mathbf{X})$ may perform poorly.
  - For example, if the posterior is not symmetric and unimodal, the MAP is not a good estimate for the posterior mean, thus leading to inaccurate Gaussian approximations.
  - Furthermore, if the parameter space Θ is bounded, a Gaussian approximation could be quite problematic $\Rightarrow$ a reparametrization should be considered.
  - Finally, it is unclear how to handle discrete parameter spaces.

Approximation methods

- Let $\pi(\theta|\mathbf{X})$ be the intractable posterior distribution and let $q(\theta)$ be a density belonging to $\mathcal{Q}$, where $\mathcal{Q}$ is a general class of tractable densities.
- An optimal approximation $\hat{q}(\theta) \in \mathcal{Q}$ of the posterior distribution is defined as

$$\hat{q}(\theta) = \arg\min_{q \in \mathcal{Q}} \mathcal{D}\{q(\theta), \pi(\theta|\mathbf{X})\}$$

  where $\mathcal{D}$ is some divergence or metric over the space of probability distributions.
- An example is the Kullback-Leibler divergence $\mathcal{D}(\cdot, \cdot) = KL(\cdot||\cdot)$
  - $KL(q(\theta||\pi(\theta|\mathbf{X}))$ divergence leads to the variational Bayes method
  - $KL(\pi(\theta|\mathbf{X})||q(\theta)$ divergence leads to the expectation propagation method