

Hamiltonian Monte Carlo and Stan

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 - the performance scales well with the number of dimensions
 - this lecture introduces the basic HMC and No-U-Turn-Sampler based dynamic HMC
 - other useful variants have been developed recently

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 - this lecture introduces the basic HMC and No-U-Turn-Sampler based dynamic HMC
 - other useful variants have been developed recently
- Stan is the most popular probabilistic programming framework
 - many recent probprog frameworks use dynamic HMC samplers
 - this lecture introduces Stan language and main features
 - later you can also use higher level packages built on top of Stan

BDA Chapter 12

- 12.1 Efficient Gibbs samplers (not part of the course)
- 12.2 Efficient Metropolis jump rules (not part of the course)
- 12.3 Further extensions to Gibbs and Metropolis (not part of the course)
- 12.4 Hamiltonian Monte Carlo (important)
- 12.5 Hamiltonian dynamics for a simple hierarchical model (useful example)
- 12.6 Stan: developing a computing environment (useful intro)

Extra material for HMC / NUTS

- An introduction for applied users with good visualizations:
Monnahan, Thorson, and Branch (2016) Faster estimation of Bayesian models in ecology using Hamiltonian Monte Carlo.
<https://dx.doi.org/10.1111/2041-210X.12681>
- A technical review of why HMC works:
Neal (2012). MCMC using Hamiltonian dynamics.
<https://arxiv.org/abs/1206.1901>
- The No-U-Turn Sampler:
Hoffman and Gelman (2014). The No-U-Turn Sampler: Adaptively Setting Path Lengths in Hamiltonian Monte Carlo.
<https://jmlr.csail.mit.edu/papers/v15/hoffman14a.html>
- Multinomial variant of NUTS:
Betancourt (2018). A Conceptual Introduction to Hamiltonian Monte Carlo. <https://arxiv.org/abs/1701.02434>

Extra material for Stan

- Gelman, Lee, and Guo (2015) Stan: A probabilistic programming language for Bayesian inference and optimization.
http://www.stat.columbia.edu/~gelman/research/published/stan_jebbs_2.pdf
- Carpenter et al (2017). Stan: A probabilistic programming language. Journal of Statistical Software 76(1).
<https://doi.org/10.18637/jss.v076.i01>
- Stan User's Guide, Language Reference Manual, and Language Function Reference (in html and pdf)
<https://mc-stan.org/users/documentation/>
 - easiest to start from Example Models in User's guide
- Basics of Bayesian inference and Stan, part 1 Jonah Gabry & Lauren Kennedy (StanCon 2019 Helsinki tutorial)
 - <https://www.youtube.com/watch?v=ZRpo41l02KQ&index=6&list=PLuwyh42iHquU4hUBQs20hkBsKSMrp6H0J>
 - <https://www.youtube.com/watch?v=6cc4N1vT8pk&index=7&list=PLuwyh42iHquU4hUBQs20hkBsKSMrp6H0J>

Chapter 12 demos

- demo12_1: HMC
- <https://chi-feng.github.io/mcmc-demo/>
- <http://elevanth.org/blog/2017/11/28/build-a-better-markov-chain/>
- cmdstanr_demo, rstan_demo
- <http://sumsar.net/blog/2017/01/bayesian-computation-with-stan-and-farmer-jons/>
- <http://mc-stan.org/documentation/case-studies.html>
- <https://mc-stan.org/cmdstanr/>
- <https://mc-stan.org/rstan/>

Hamiltonian Monte Carlo

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Hamiltonian Monte Carlo

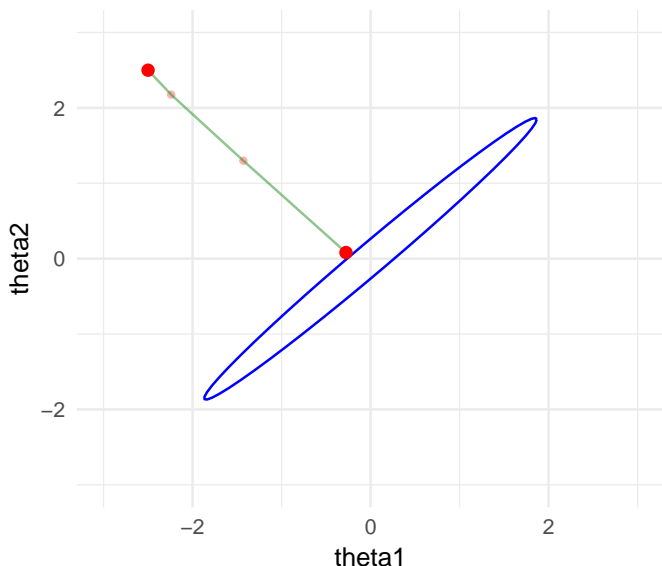
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- Now most popular probabilistic programming frameworks use it (Stan, PyMC, TFP, Pyro, Turing.jl, etc.)
- Also used as the a high-fidelity reference in Approximate Inference in Bayesian Deep Learning competition
https://izmailovpavel.github.io/neurips_bdl_competition/

Hamiltonian Monte Carlo

- Uses log density (negative log density is called energy)
- Uses gradient of log density for more efficient sampling

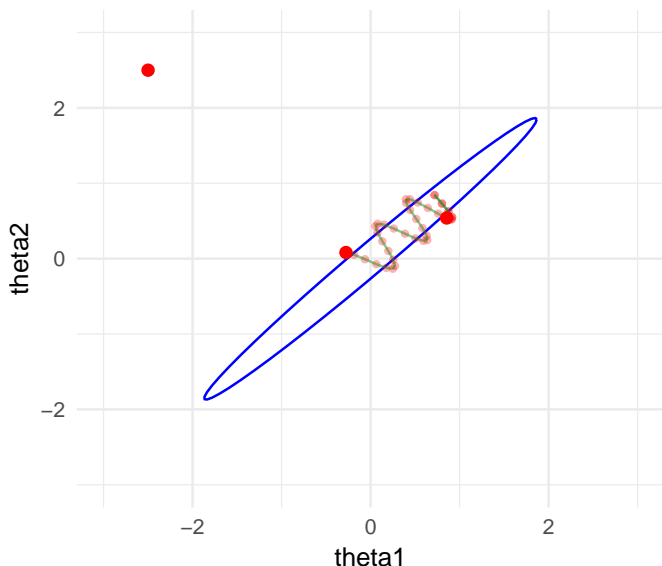
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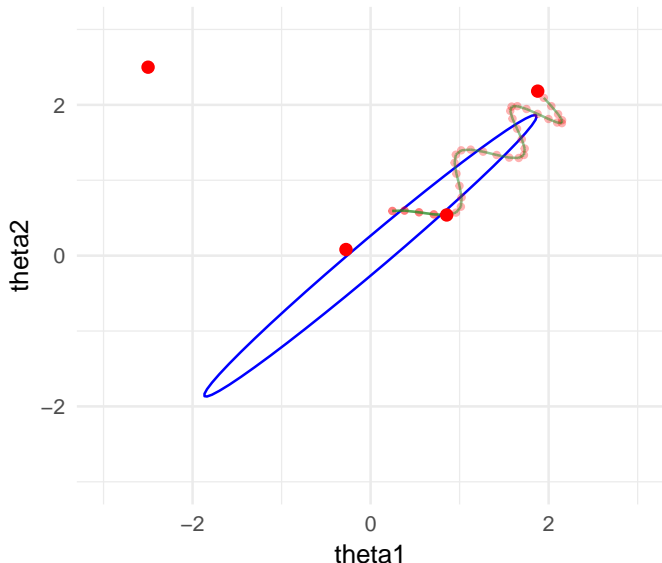
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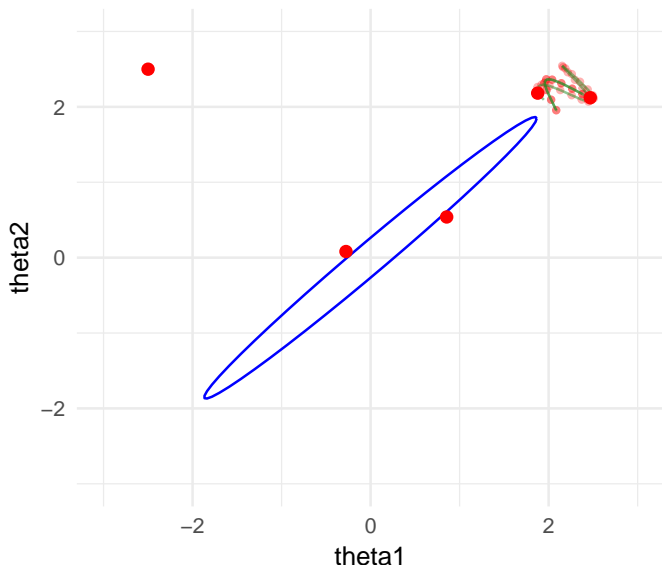
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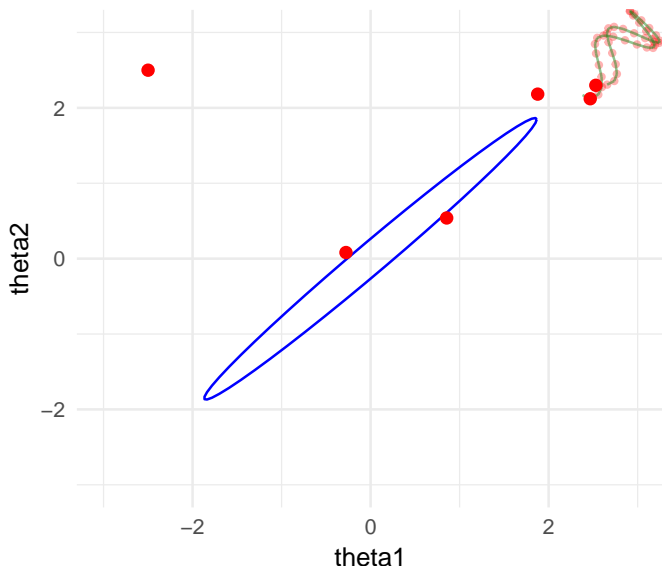
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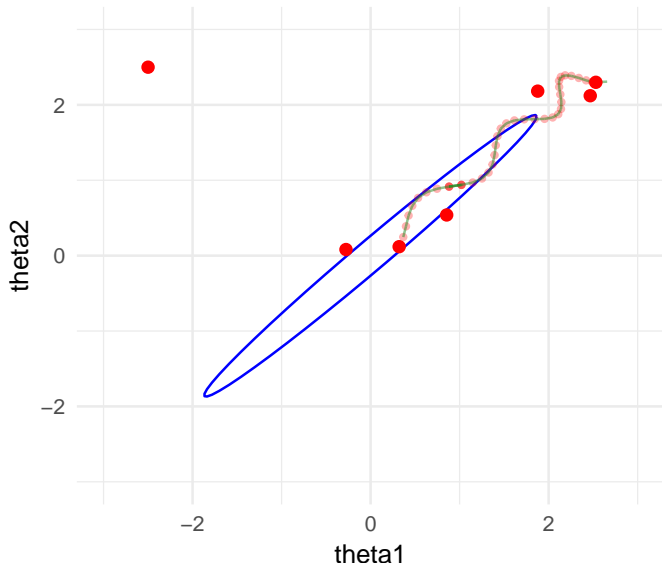
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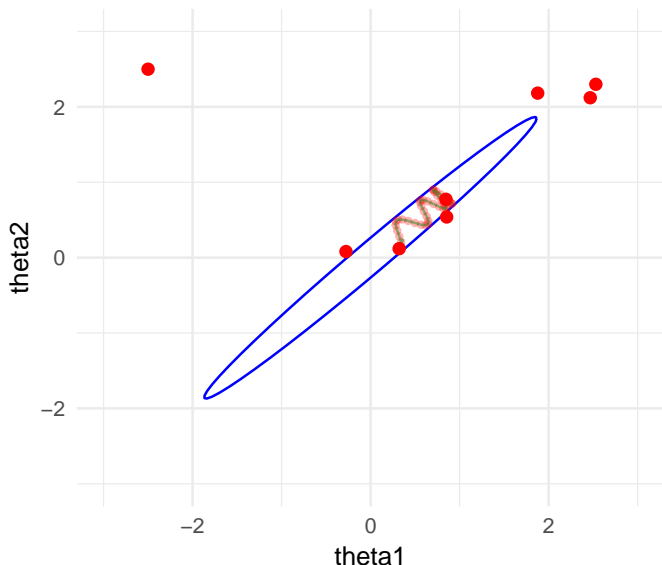
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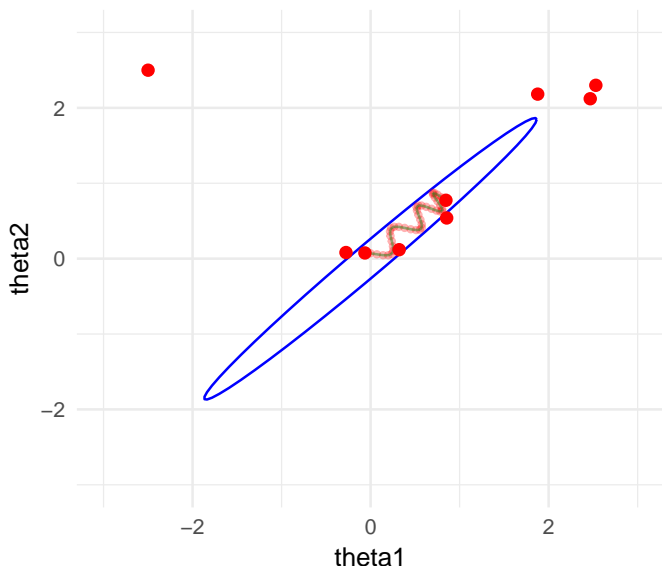
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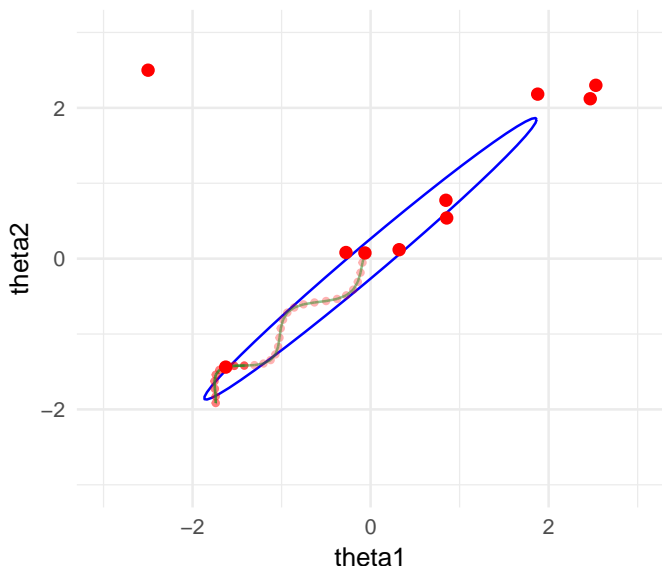
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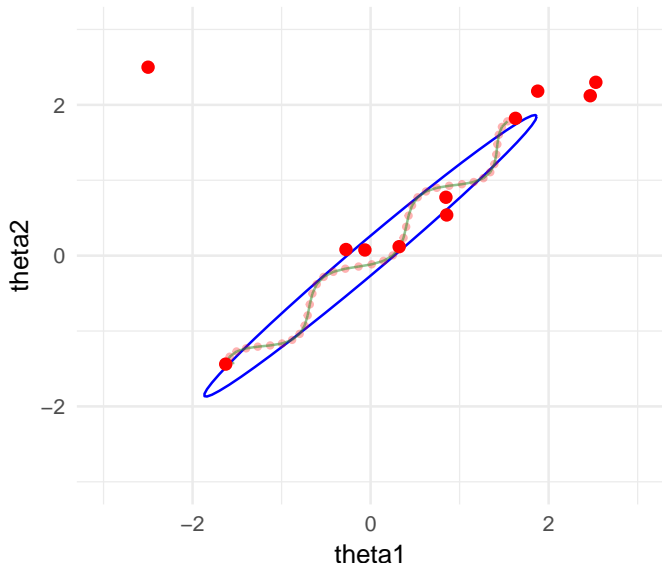
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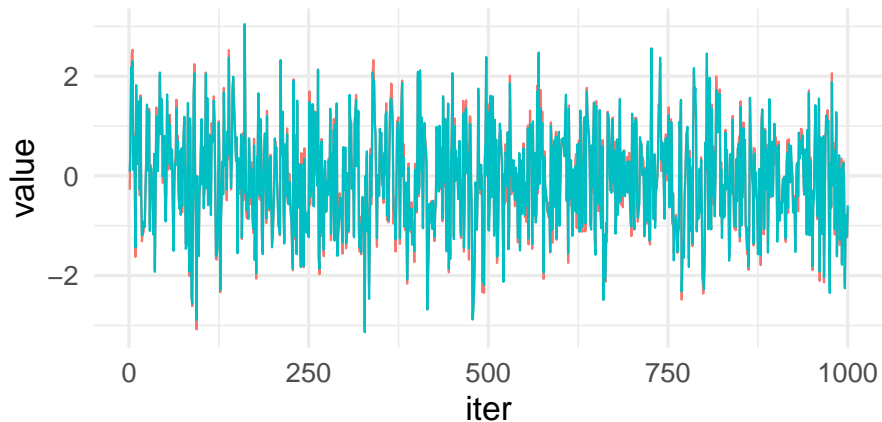
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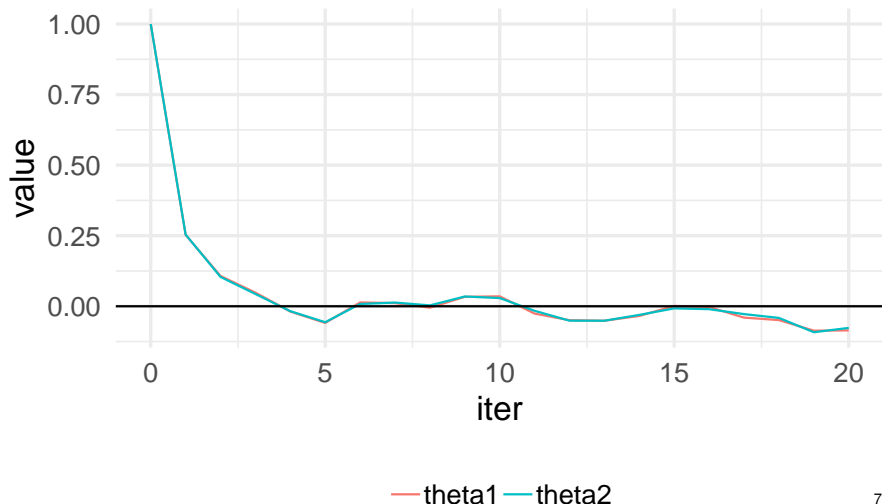
Trends



Hamiltonian Monte Carlo

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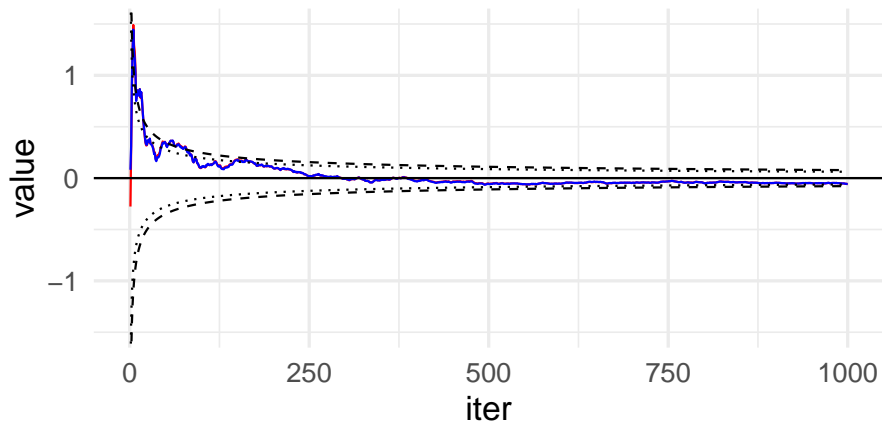
Autocorrelation function



Hamiltonian Monte Carlo

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- Uses gradient of log density for more efficient sampling

Cumulative averages



- θ_1 — θ_2 - - 95% interval for MCMC error ··· 95% interval for independent samples

Hamiltonian Monte Carlo / No-U-Turn sampling

1. HMC basics (static HMC)

Hamiltonian Monte Carlo / No-U-Turn sampling

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2. HMC + leapfrog discretization + Metropolis (static HMC)
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4. NUTS + multinomial (dynamic HMC)
 - Betancourt (2018)

Hamiltonian Monte Carlo

- Related methods
 - Factorizing $p(\theta_1, \theta_2) = p(\theta_1 | \theta_2)p(\theta_2)$: sample from
 - 1) $p(\theta_2)$,
 - 2) $p(\theta_1 | \theta_2)$

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jump distribution is a combination of proposal distribution and point mass at the previous value
- HMC
 - Augment with ϕ (the same dimensionality as θ)
 - - 1) sample directly from $p(\phi)$,
 - 2) make a special joint Metropolis step for $p(\theta, \phi) = p(\theta)p(\phi)$

Hamiltonian Monte Carlo

- 1) Sample from $p(\phi)$
 - define $p(\phi) = \text{normal}(0, 1)$
- 2) Metropolis update for $p(\theta, \phi) = p(\theta)p(\phi)$
 - proposal from Hamiltonian dynamic simulation

Hamiltonian dynamic simulation

- Statistical mechanics and canonical distribution

$$\begin{aligned} p(\theta, \phi) &= p(\theta)p(\phi) \\ &= \frac{1}{Z} \exp(-(U(\theta) + K(\phi))) \\ &= \frac{1}{Z} \exp(-H(\theta, \phi)) \end{aligned}$$

where

- U is potential energy function
- K is kinetic energy function
- H is Hamiltonian energy function
- ϕ is called a momentum variable

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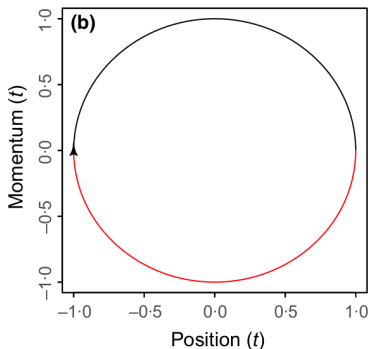
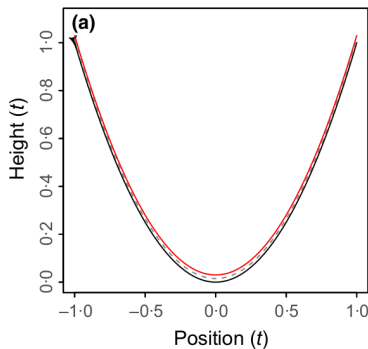
where

- U is potential energy function
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- The potential energy is the negative log density
 $U(\theta) = -\log(p(\theta)) + C$

Hamiltonian dynamic simulation

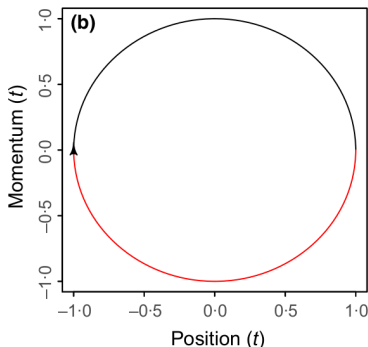
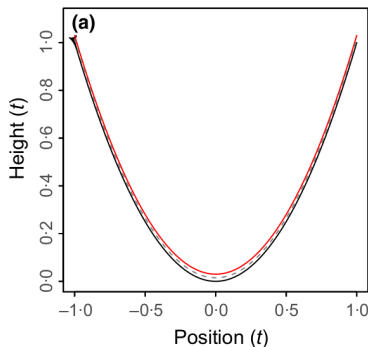
Equations of motion, use also the gradient

$$\frac{d\theta_i}{dt} = \frac{\partial H}{\partial \phi_i}$$
$$\frac{d\phi_i}{dt} = -\frac{\partial H}{\partial \theta_i}$$



Hamiltonian Monte Carlo

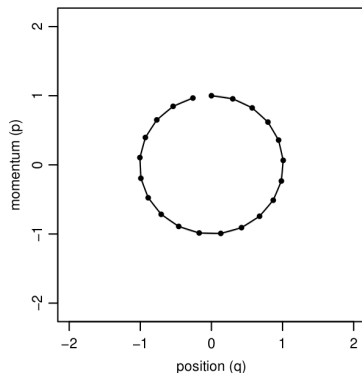
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 - proposal from Hamiltonian dynamic simulation
 $p(\theta, \phi) \propto \exp(-H(\theta, \phi))$



Leapfrog discretization

- Leapfrog discretization
 - preserves volume
 - reversible
 - discretization error does not usually grow in time

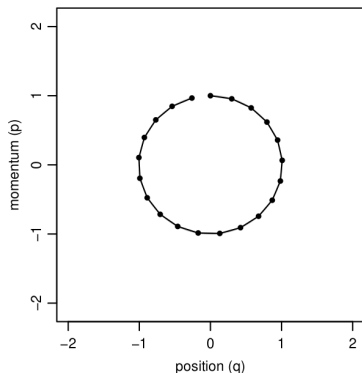
(c) Leapfrog Method, stepsize 0.3



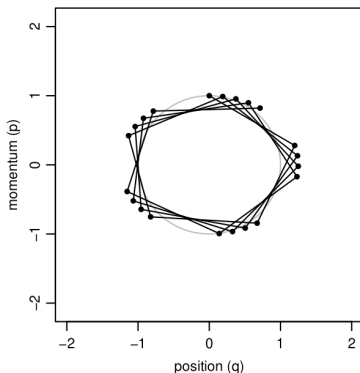
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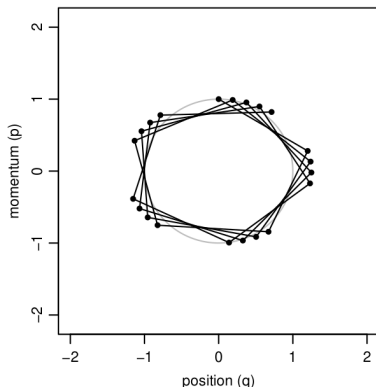


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Leapfrog discretization + Metropolis

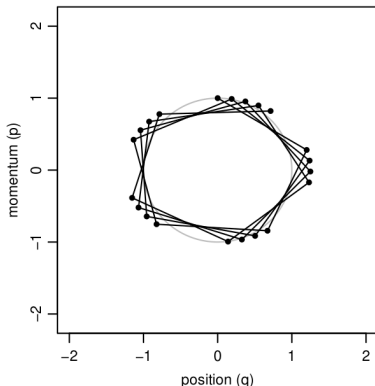
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 - due to the discretization error the simulation steps away from the constant contour



From Neal (2012)

Leapfrog discretization + Metropolis

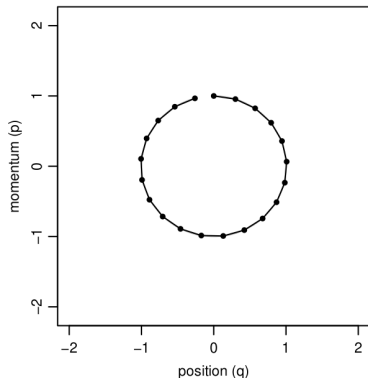
- Leapfrog discretization
 - due to the discretization error the simulation steps away from the constant contour
- Metropolis step with $r = \exp(-H(\theta^*, \phi^*) + H(\theta^{(t-1)}, \phi^{(t-1)}))$
 - accept if the Hamiltonian energy in the end is higher
 - accept with some probability if the Hamiltonian energy in the end is lower



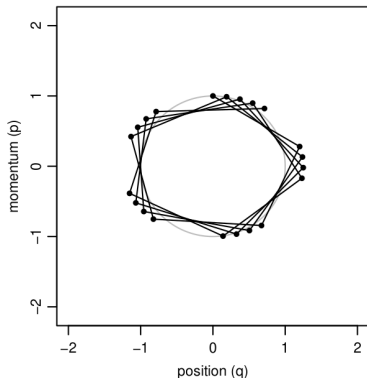
Two steps of Hamiltonian Monte Carlo

- Perfect simulation keeps $p(\theta, \phi)$ constant

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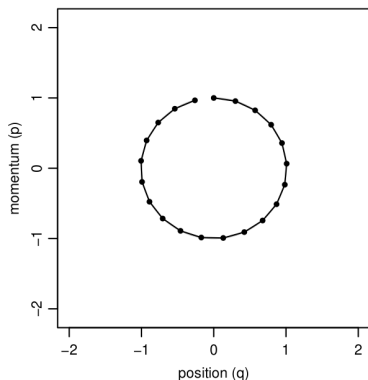
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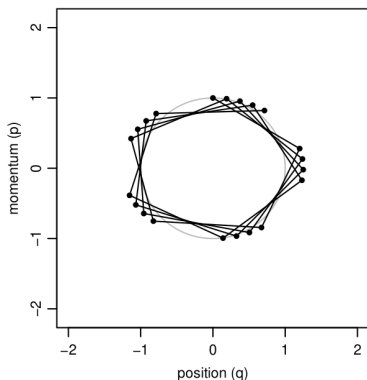
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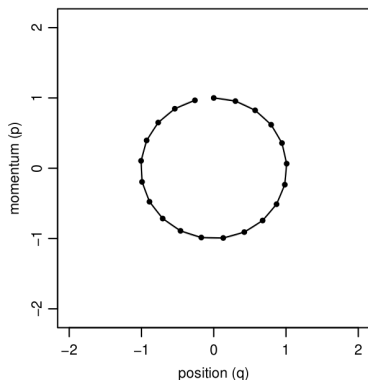
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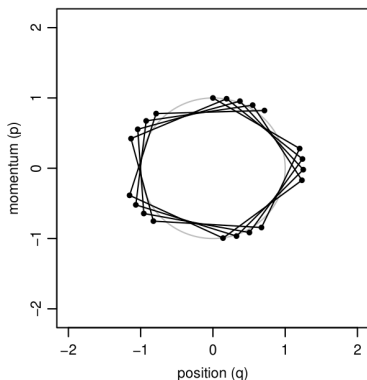
Two steps of Hamiltonian Monte Carlo

- Perfect simulation keeps $p(\theta, \phi)$ constant
- Discretized simulation keeps changes in $p(\theta, \phi)$ small
- Alternating sampling from $p(\phi)$ is crucial for moving to (θ, ϕ) points with different joint density

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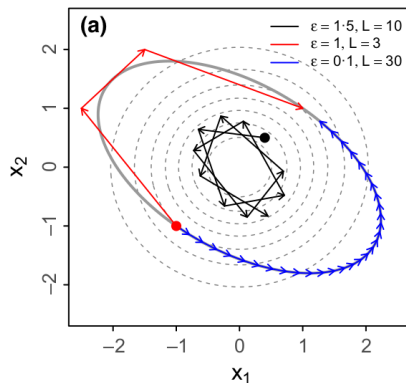


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Leapfrog discretization, step size

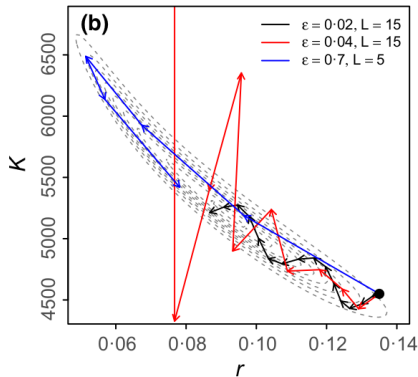
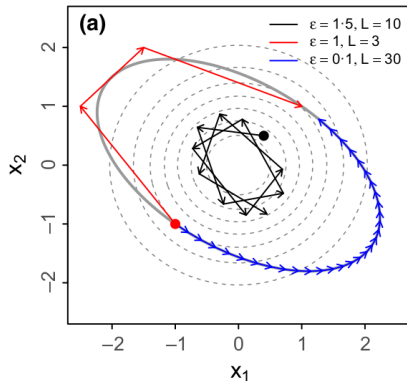
- Small step size \rightarrow high acceptance rate, but many log density and gradient evaluations
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From Monnahan et al (2017)

Leapfrog discretization, step size

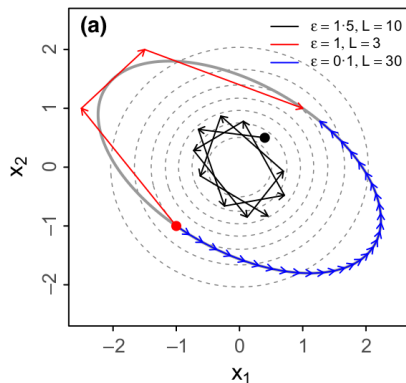
- Small step size \rightarrow high acceptance rate, but many log density and gradient evaluations
- Big step size \rightarrow less log density and gradient evaluations, but lower acceptance rate and the simulation may diverge



From Monnahan et al (2017)

Leapfrog discretization, the number of steps

- Many steps can reduce random walk
- Many steps require many log density and gradient evaluations



From Monnahan et al (2017)

Static Hamiltonian Monte Carlo

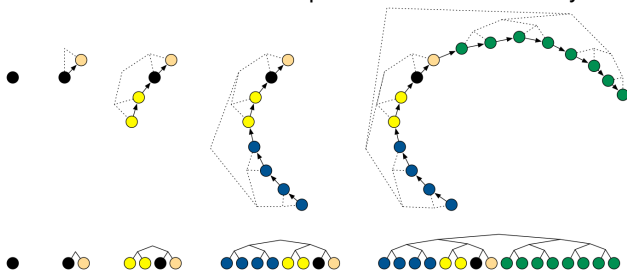
- Fixed number of steps
- Demo <https://chi-feng.github.io/mcmc-demo/>

No-U-Turn sampler

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 - NUTS is a dynamic HMC algorithm, where dynamic refers to the dynamic trajectory length

No-U-Turn sampler

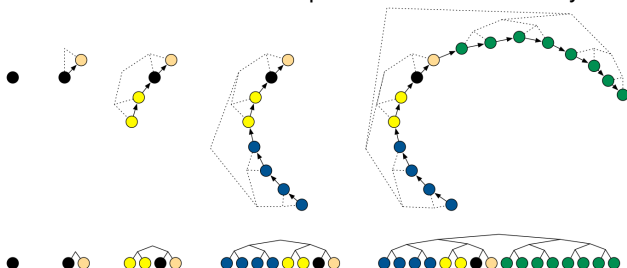
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 - simulate until a U-turn is detected
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from Hoffman & Gelman (2014)

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from Hoffman & Gelman (2014)

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 - need to simulate in two directions
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No-U-Turn sampler with multinomial sampling

- Original NUTS
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Mass matrix and the step size adaptation

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Mass matrix and the step size adaptation

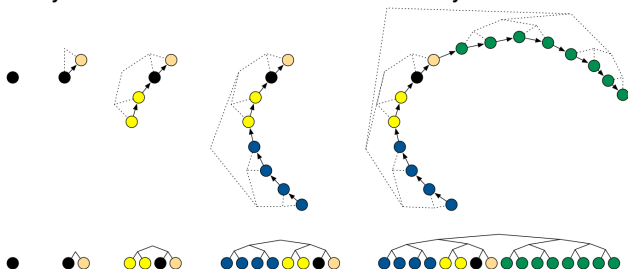
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- After adaptation the algorithm parameters are fixed and some more iterations run to finish the warmup

Max tree depth diagnostic

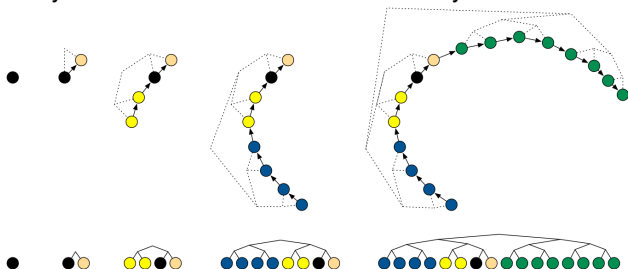
- NUTS specific diagnostic
 - the dynamic simulation is build as a binary tree



from Hoffman & Gelman (2014)

Max tree depth diagnostic

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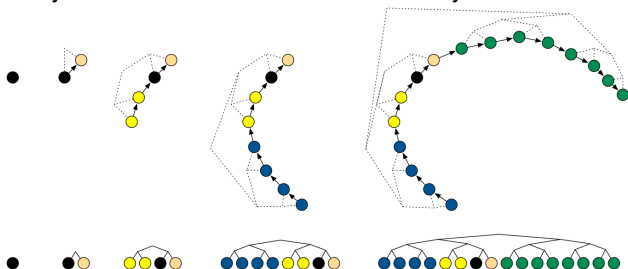


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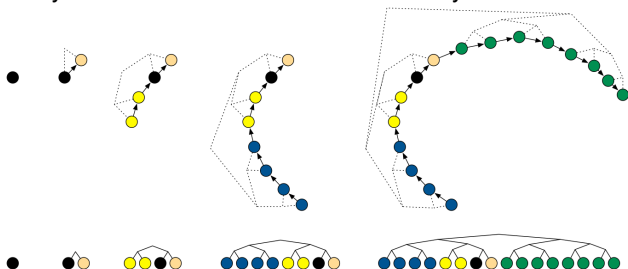


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- maximum simulation length, i.e. maximum number of steps, is capped to avoid very long waiting times in case of bad behavior
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 - very low inefficiency can indicate problems that need to be inverse-distance
 - moderate inefficiency doesn't invalidate the result

Max tree depth diagnostic

- NUTS specific diagnostic
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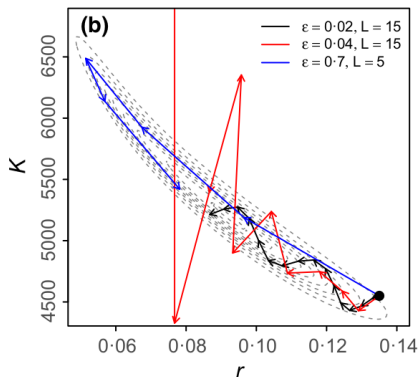


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 - very low inefficiency can indicate problems that need to be inverse-distance
 - moderate inefficiency doesn't invalidate the result
- Different parameterizations matter

Divergences

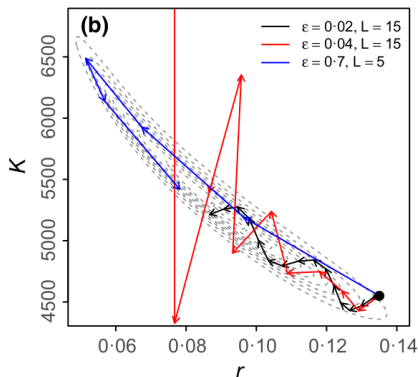
- HMC specific: indicates that Hamiltonian dynamic simulation has problems with unexpected fast changes in log-density (compared to the used step size)
 - indicates possibility of biased estimates



From Monnahan et al (2017)

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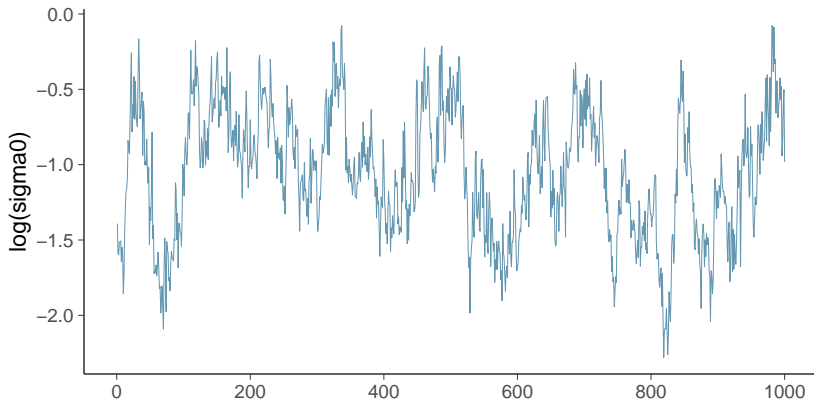
- Demo <https://chi-feng.github.io/mcmc-demo/>

Divergences

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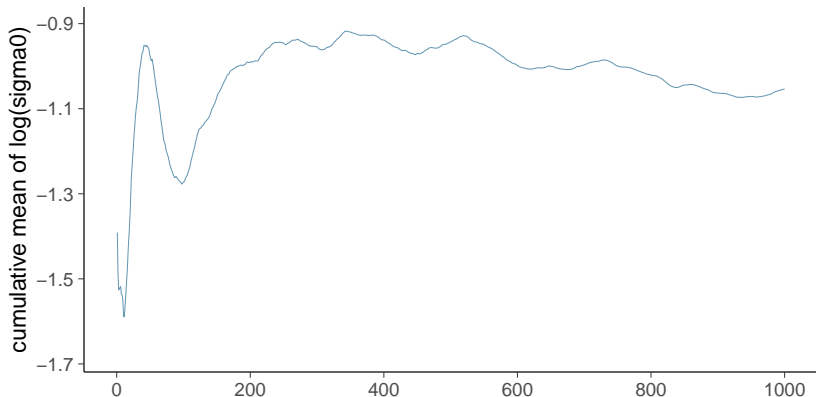
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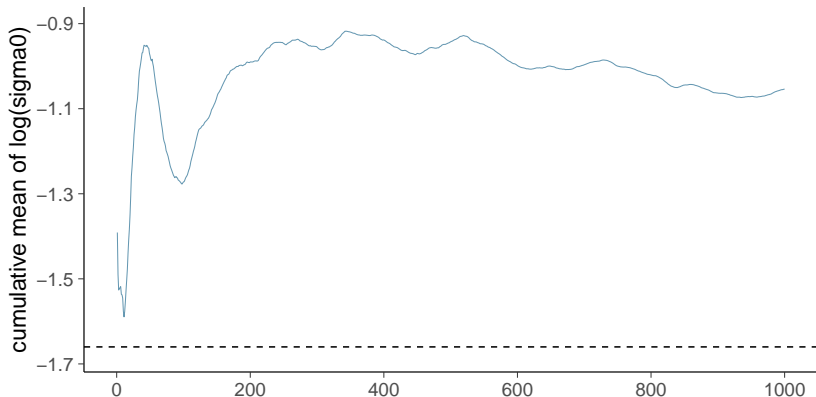
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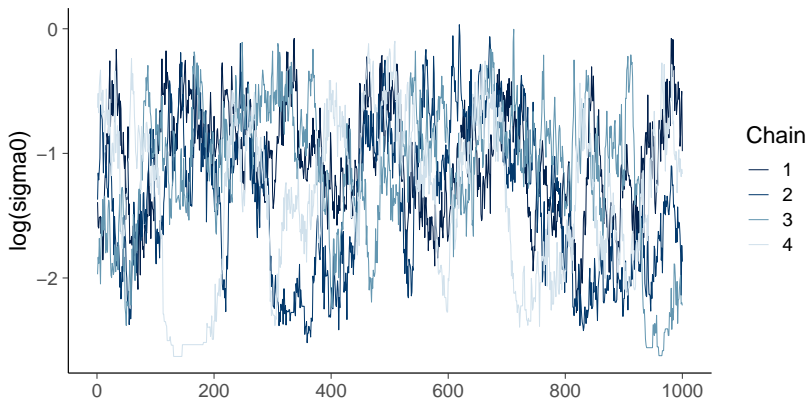
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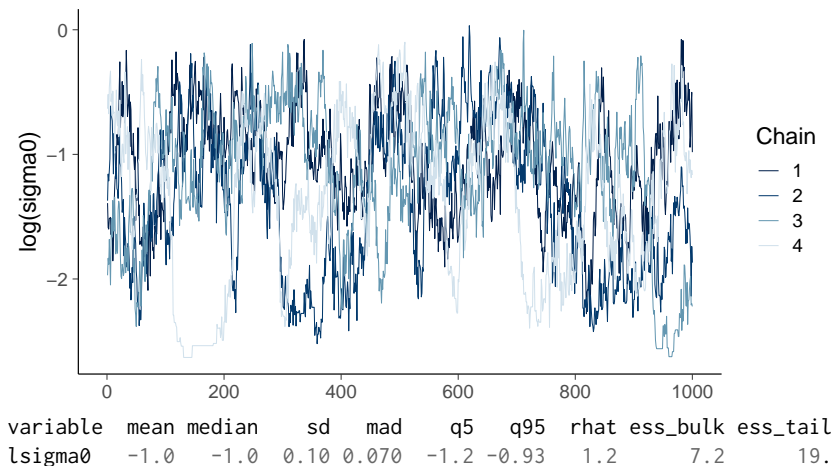
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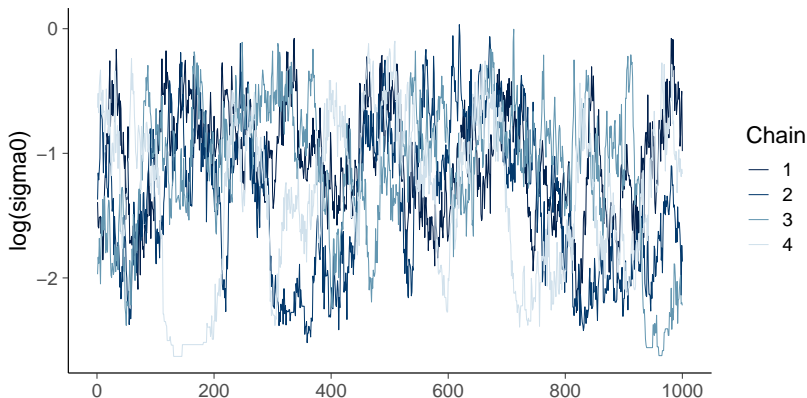
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Divergences

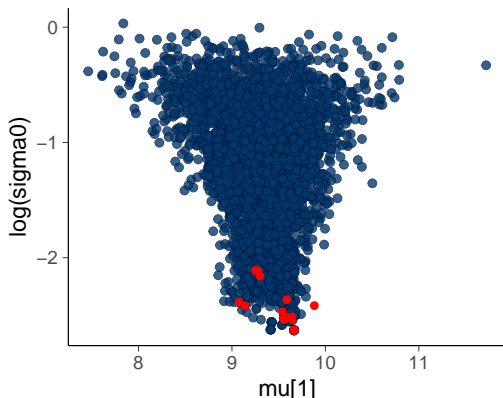
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See <https://mc-stan.org/misc/warnings> for details.

Divergences

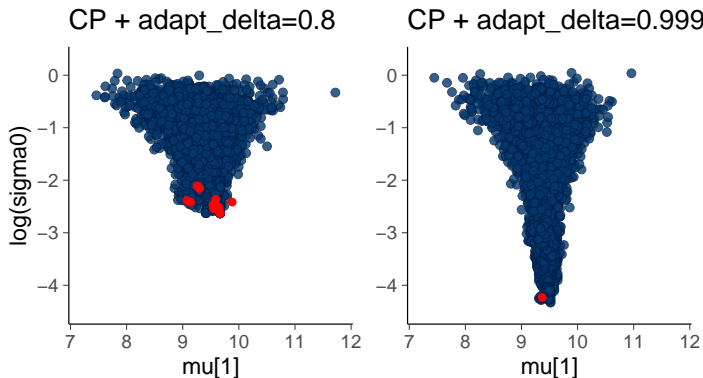
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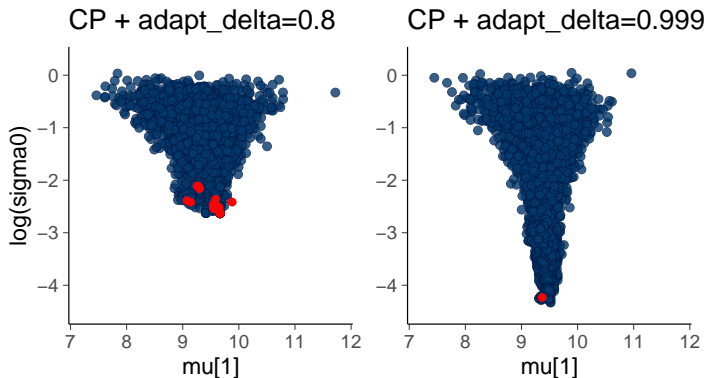
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Divergences

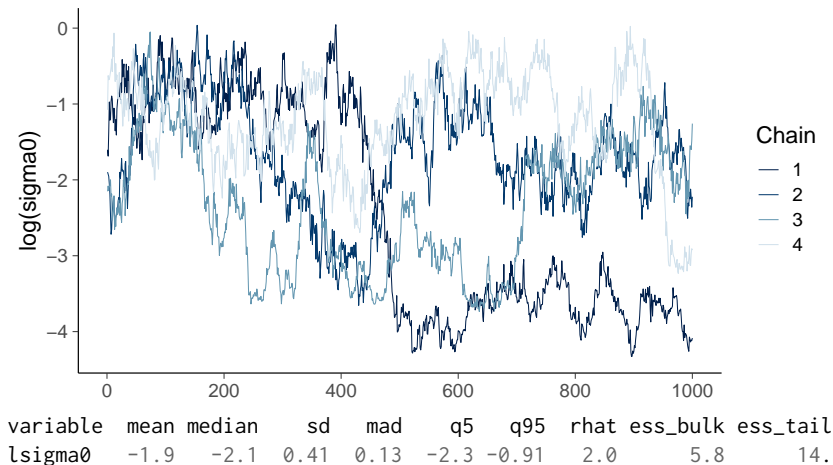
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variable	mean	median	sd	mad	q5	q95	rhat	ess_bulk	ess_tail
lsigma0	-1.9	-2.1	0.41	0.13	-2.3	-0.91	2.0	5.8	14.

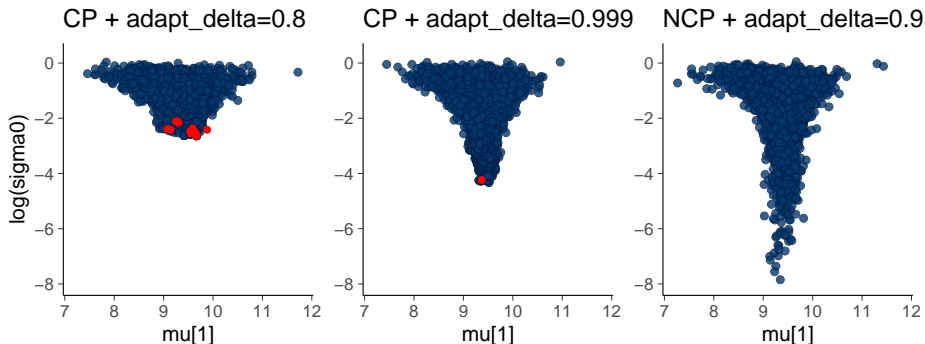
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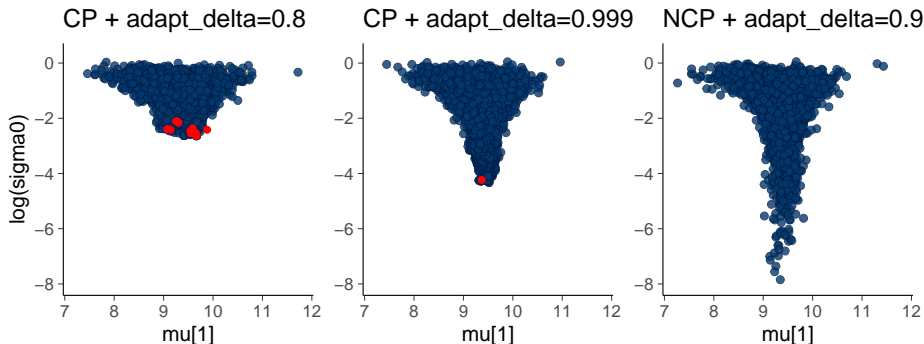
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With NCP parameterization

variable	mean	median	sd	mad	q5	q95	rhat	ess_bulk	ess_tail
sigma0	0.27	0.24	0.19	0.20	0.023	0.64	1.0	1571.	1737.
lsigma0	-1.7	-1.4	1.1	0.87	-3.8	-0.45	1.0	1571.	1737.

Problematic distributions

- Nonlinear dependencies
 - simple mass matrix scaling doesn't help
- Funnels
 - optimal step size depends on location
- Multimodal
 - difficult to move from one mode to another
- Long-tailed with non-finite variance and mean
 - efficiency of exploration is reduced
 - central limit theorem doesn't hold for mean and variance

Some other recent HMC and gradient based variants

- ChEES-HMC (Hoffman et al., 2021)
 - a GPU friendly adapted but fixed simulation length
 - static after adaptation
- MEADS (Hoffman & Sountsov, 2022)
 - a GPU friendly multi-chain adaptation for generalized HMC (Horowitz, 1991) in which the momentum is partially updated frequently
 - instead of simulation length, need to choose the partial update rate
- MALT (Riou-Durand and Vogrinc, 2022; Riou-Durand et al., 2022)
 - a GPU friendly method related to GHMC
 - but avoids momentum flips after rejection

Probabilistic programming language

- Wikipedia “A probabilistic programming language (PPL) is a programming language designed to describe probabilistic models and then perform inference in those models”

Probabilistic programming language

- Wikipedia “A probabilistic programming language (PPL) is a programming language designed to describe probabilistic models and then perform inference in those models”
- To make probabilistic programming useful
 - inference has to be as automatic as possible
 - diagnostics for telling if the automatic inference doesn't work
 - easy workflow (to reduce manual work)
 - fast enough (manual work replaced with automation)

Probabilistic programming

- Enables agile workflow for developing probabilistic models
 - language
 - automated inference
 - diagnostics
- Many frameworks Stan, PyMC, Pyro (Uber), TFP (Google), Turing.jl, JAGS, ELFI, ...
 - Short review of the landscape:
Štrumbelj et al. (2023). Past, Present, and Future of Software for Bayesian Inference. *Statistical Science*, accepted for publication. Preprint http://www.stat.columbia.edu/~gelman/research/published/Bayesian_software_review-8.pdf.

Stan - probabilistic programming framework

- Language, inference engine, user interfaces, documentation, case studies, diagnostics, packages, ...
 - autodiff to compute gradients of the log density



mc-stan.org

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- Language, inference engine, user interfaces, documentation, case studies, diagnostics, packages, ...
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mc-stan.org

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- Several full time developers, 40+ developers, more than 100 contributors
- R, Python, Julia, Scala, Stata, command line interfaces
- More than 200 R packages using Stan



mc-stan.org

Stan

- Stanislaw Ulam (1909-1984)
 - Monte Carlo method
 - H-Bomb

Binomial model - Stan code

Domain-specific language for constructing models
with common *distributed as* \sim notation

```
data {  
  int<lower=0> N;           // number of experiments  
  int<lower=0,upper=N> y;  // number of successes  
}  
  
parameters {  
  real<lower=0,upper=1> theta; // parameter of the binomial  
}  
  
model {  
  theta ~ beta(1, 1);      // prior  
  y ~ binomial(N, theta);  // observation / data model  
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- Stan checks that given data matches type and constraints

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- Data type and size are declared
- Stan checks that given data matches type and constraints
 - If you are not used to strong typing, this may feel annoying, but it will reduce the probability of coding errors, which will reduce probability of data analysis errors

Binomial model - Stan code

```
parameters {  
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```

- Only continuous parameters allowed (discrete parameters can often be integrated out in the model block)
- Parameters may have constraints
- Stan makes transformation to unconstrained space and samples in unconstrained space
 - e.g. log transformation for `<lower=a>`
 - e.g. logit transformation for `<lower=a, upper=b>`

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- Parameters may have constraints
- Stan makes transformation to unconstrained space and samples in unconstrained space
 - e.g. log transformation for `<lower=a>`
 - e.g. logit transformation for `<lower=a, upper=b>`
- For these declared transformation Stan automatically takes into account the Jacobian of the transformation (see BDA3 p. 21)

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e.g. y is distributed as $\text{binomial}(N, \theta)$

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- these can be written also as *log density increment statements*
left side of $|$ denotes what is distributed as, e.g., binomial

```
model {  
  target += beta_lpdf(theta | 1, 1);  
  target += binomial_lpmf(y | N, theta);  
}
```

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- `target` is the log posterior density (Lecture 4 discussed `log`)
- `_lpdf` for continuous, `_lpmf` for discrete distributions (left of $|$)
- if y are data, and θ is a parameter, then that term defines log likelihood
- for Stan sampler there is no difference between prior and likelihood, all that matters is the final `target`

Stan

- You can write in Stan language any program to compute the log density (Stan language is Turing complete)

Stan

- You can write in Stan language any program to compute the log density (Stan language is Turing complete)
- Stan compiles (transpiles) the model written in Stan language to C++
 - this makes the sampling for complex models and bigger data faster
 - also makes Stan models easily portable, you can use your own favorite interface and scripting language for manipulating data and inference results (e.g. R, Python, Julia, Stata, ...)

CmdStanR

RStan

```
library(cmdstanr)  
options(mc.cores = 1)
```

```
d_bin <- list(N = 10, y = 7)  
mod_bin <- cmdstan_model(stan_file = 'binom.stan')  
fit_bin <- mod_bin$sample(data = d_bin)
```

CmdStanR

RStan

```
library(cmdstanr)
options(mc.cores = 1)

d_bin <- list(N = 10, y = 7)
mod_bin <- cmdstan_model(stan_file = 'binom.stan')
fit_bin <- mod_bin$sample(data = d_bin)
```

PyStan

PyStan

```
import pystan  
import stan_utility
```

```
data = dict(N=10, y=8)  
model = stan_utility.compile_model('binom.stan')  
fit = model.sampling(data=data)
```

PyStan

PyStan

```
import pystan
import stan_utility

data = dict(N=10, y=8)
model = stan_utility.compile_model('binom.stan')
fit = model.sampling(data=data)
```

Stan

- Compilation (unless previously compiled model available)
- Warm-up including adaptation
- Sampling
- Generated quantities
- Save posterior draws
- Report divergences, ESS, \hat{R}

Difference between proportions

- An experiment was performed to estimate the effect of beta-blockers on mortality of cardiac patients
- A group of patients were randomly assigned to treatment and control groups:
 - out of 674 patients receiving the control, 39 died
 - out of 680 receiving the treatment, 22 died

Difference between proportions

```
data {  
  int<lower=0> N1;  
  int<lower=0> y1;  
  int<lower=0> N2;  
  int<lower=0> y2;  
}  
parameters {  
  real<lower=0,upper=1> theta1;  
  real<lower=0,upper=1> theta2;  
}  
model {  
  theta1 ~ beta(1, 1);  
  theta2 ~ beta(1, 1);  
  y1 ~ binomial(N1, theta1);  
  y2 ~ binomial(N2, theta2);  
}  
generated quantities {  
  real oddsratio;  
  oddsratio = (theta2/(1-theta2))/(theta1/(1-theta1));  
}
```


Difference between proportions

```
data {  
  int<lower=0> N1;  
  int<lower=0> y1;  
  int<lower=0> N2;  
  int<lower=0> y2;  
}  
parameters {  
  real<lower=0,upper=1> theta1;  
  real<lower=0,upper=1> theta2;  
}  
model {  
  theta1 ~ beta(1, 1);  
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}  
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}
```

Difference between proportions

```
generated quantities {  
  real oddsratio;  
  oddsratio = (theta2/(1-theta2))/(theta1/(1-theta1));  
}
```

- generated quantities is run after the sampling

Difference between proportions

```
d_bin2 <- list(N1 = 674, y1 = 39, N2 = 680, y2 = 22)
mod_bin2 <- cmdstan_model(stan_file = 'binom2.stan')
fit_bin2 <- mod_bin2$sample(data = d_bin2, refresh=1000)
```

```
> Running MCMC with 4 parallel chains...
```

```
Chain 1 Iteration:    1 / 2000 [  0%]  (Warmup)
Chain 1 Iteration: 1000 / 2000 [ 50%]  (Warmup)
Chain 1 Iteration: 1001 / 2000 [ 50%]  (Sampling)
Chain 1 Iteration: 2000 / 2000 [100%]  (Sampling)
```

```
...
```

```
All 4 chains finished successfully.
```

```
Mean chain execution time: 0.0 seconds.
```

```
Total execution time: 0.2 seconds.
```

Difference between proportions

```
options(posterior.num_args=list(sigfig=2))  
fit_bin2$summary()
```

	variable	mean	median	sd	mad	q5	q95	rhat	ess_bulk	ess_tail
1	lp__	-2.5e+2	-2.5e+2	1.0	0.74	-2.6e+2	-2.5e+2	1.0	1751.	2231.
2	theta1	5.9e-2	5.9e-2	0.0093	0.0093	4.5e-2	7.5e-2	1.0	3189.	2657.
3	theta2	3.4e-2	3.3e-2	0.0069	0.0067	2.3e-2	4.6e-2	1.0	3229.	2163.
4	oddsratio	5.7e-1	5.5e-1	0.16	0.15	3.5e-1	8.7e-1	1.0	2998.	2685.

Difference between proportions

```
options(posterior.num_args=list(sigfig=2))  
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	variable	mean	median	sd	mad	q5	q95	rhat	ess_bulk	ess_tail
1	lp__	-2.5e+2	-2.5e+2	1.0	0.74	-2.6e+2	-2.5e+2	1.0	1751.	2231.
2	theta1	5.9e-2	5.9e-2	0.0093	0.0093	4.5e-2	7.5e-2	1.0	3189.	2657.
3	theta2	3.4e-2	3.3e-2	0.0069	0.0067	2.3e-2	4.6e-2	1.0	3229.	2163.
4	oddsratio	5.7e-1	5.5e-1	0.16	0.15	3.5e-1	8.7e-1	1.0	2998.	2685.

- lp__ is the log density, ie, same as target

HMC specific diagnostics

```
fit_bin2$diagnostic_summary(diagnostics = c("divergences",  
                                             "treedepth"))
```

```
$num_divergent
```

```
[1] 0 0 0 0
```

```
$num_max_treedepth
```

```
[1] 0 0 0 0
```


HMC specific diagnostics

```
fit_bin2$diagnostic_summary(diagnostics = c("divergences",  
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```

```
$num_divergent
```

```
[1] 0 0 0 0
```

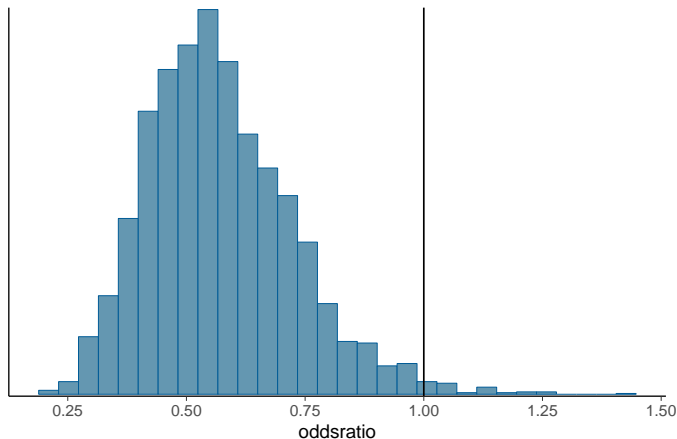
```
$num_max_treedepth
```

```
[1] 0 0 0 0
```

`rdiagnostic_summary()` includes E-BFMI diagnostic, which I'll skip in this course

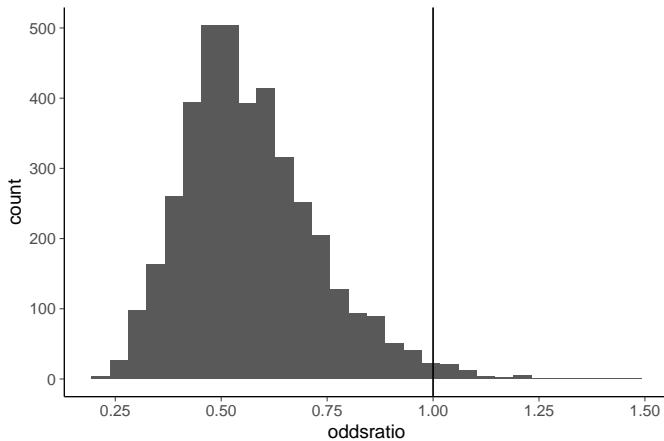
Difference between proportions (bayesplot)

```
draws <- fit_bin2$draws(format = "df")  
mcmc_hist(draws, pars = 'oddsratio') +  
  geom_vline(xintercept = 1) +  
  scale_x_continuous(breaks = c(seq(0.25, 1.5, by=0.25)))
```



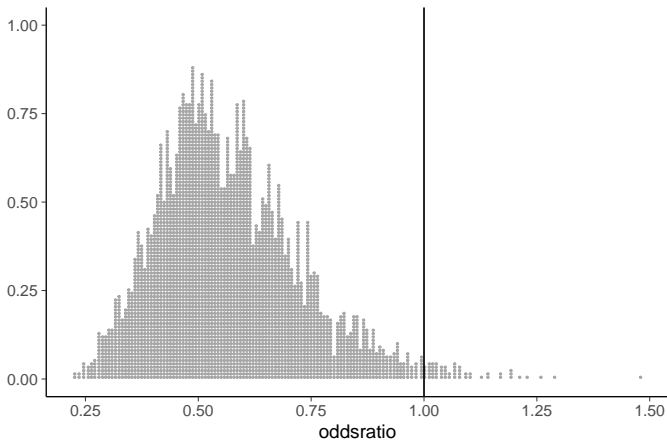
Difference between proportions (ggplot2)

```
draws <- fit_bin2$draws(format = "df")  
draws |> ggplot(aes(x=oddsratio)) +  
  geom_histogram() +  
  geom_vline(xintercept = 1) +  
  scale_x_continuous(breaks = c(seq(0.25, 1.5, by=0.25)))
```



Difference between proportions (ggdist dot plot)

```
draws <- fit_bin2$draws(format = "df")
draws |> ggplot(aes(x=oddsratio)) +
  geom_dotsinterval() +
  geom_vline(xintercept = 1) +
  scale_x_continuous(breaks = c(seq(0.25, 1.5, by=0.25)))
```



Difference between proportions (probability and MCSE)

Probability (and corresponding MCSE) that $\text{oddsratio} < 1$

```
> draws |>
  mutate_variables(p_oddsratio_lt_1 =
                    as.numeric(oddsratio<1)) |>
  subset_draws("p_oddsratio_lt_1") |>
  summarise_draws(prob=mean, MCSE=mcse_mean)
```

variable	prob	MCSE
p_oddsratio_lt_1	0.99	0.0023

posterior object formats

Default is draws_array

```
> fit_bin2$draws()
```

```
# A draws_array: 1000 iterations, 4 chains, and 4 variables  
, , variable = lp__
```

	chain			
iteration	1	2	3	4
1	-253	-253	-254	-253
2	-253	-253	-255	-252
3	-254	-252	-254	-253
4	-255	-253	-254	-254
5	-253	-253	-253	-253

```
, , variable = theta1
```

	chain			
iteration	1	2	3	4
1	0.054	0.052	0.045	0.049
2	0.062	0.060	0.070	0.058

```
...
```

posterior object formats

`draws_df` looks prettier and works with `ggplot()`

```
> fit_bin2$draws(format = "df")
```

```
# A draws_df: 1000 iterations, 4 chains, and 4 variables
```

	lp__	theta1	theta2	oddsratio
1	-253	0.054	0.033	0.59
2	-253	0.062	0.035	0.55
3	-254	0.047	0.026	0.54
4	-255	0.049	0.049	0.99
5	-253	0.068	0.035	0.50
6	-253	0.056	0.027	0.47
7	-253	0.071	0.031	0.43
8	-253	0.049	0.036	0.72
9	-253	0.049	0.036	0.72
10	-253	0.063	0.026	0.39

```
# ... with 3990 more draws
```

```
# ... hidden reserved variables {'.chain', '.iteration', '.draw'}
```

posterior object formats

draws_rvar makes it easy to compute derived quantities

```
> as_draws_rvars(fit_bin2$draws())
```

```
# A draws_rvars: 1000 iterations, 4 chains, and 4 variables
```

```
$lp__: rvar<1000,4>[1] mean ± sd:
```

```
[1] -253 ± 1
```

```
$theta1: rvar<1000,4>[1] mean ± sd:
```

```
[1] 0.059 ± 0.0093
```

```
$theta2: rvar<1000,4>[1] mean ± sd:
```

```
[1] 0.034 ± 0.0069
```

```
$oddsratio: rvar<1000,4>[1] mean ± sd:
```

```
[1] 0.57 ± 0.16
```


posterior object formats

`draws_rvar` makes it easy to compute derived quantities

```
> as_draws_rvars(fit_bin2$draws())
```

```
# A draws_rvars: 1000 iterations, 4 chains, and 4 variables
```

```
$lp__: rvar<1000,4>[1] mean ± sd:
```

```
[1] -253 ± 1
```

```
$theta1: rvar<1000,4>[1] mean ± sd:
```

```
[1] 0.059 ± 0.0093
```

```
$theta2: rvar<1000,4>[1] mean ± sd:
```

```
[1] 0.034 ± 0.0069
```

```
$oddsratio: rvar<1000,4>[1] mean ± sd:
```

```
[1] 0.57 ± 0.16
```

```
> with(draws, (theta2/(1-theta2))/(theta1/(1-theta1)))
```

```
rvar<1000,4>[1] mean ± sd:
```

```
[1] 0.5689 ± 0.1577
```

posterior object formats

draws_rvar makes it easy to compute derived quantities

```
> as_draws_rvars(fit_bin2$draws())
```

```
# A draws_rvars: 1000 iterations, 4 chains, and 4 variables
```

```
$lp__: rvar<1000,4>[1] mean ± sd:
```

```
[1] -253 ± 1
```

```
$theta1: rvar<1000,4>[1] mean ± sd:
```

```
[1] 0.059 ± 0.0093
```

```
$theta2: rvar<1000,4>[1] mean ± sd:
```

```
[1] 0.034 ± 0.0069
```

```
$oddsratio: rvar<1000,4>[1] mean ± sd:
```

```
[1] 0.57 ± 0.16
```

```
> with(draws, (theta2/(1-theta2))/(theta1/(1-theta1)))
```

```
rvar<1000,4>[1] mean ± sd:
```

```
[1] 0.5689 ± 0.1577
```

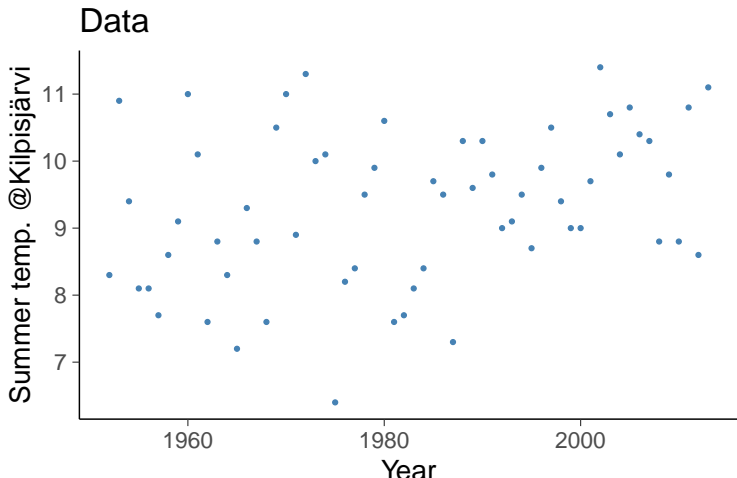
```
> draws$oddsratio<1
```

```
rvar<1000,4>[1] mean ± sd:
```

```
[1] 0.9865 ± 0.1154
```

Kilpisjärvi summer temperature

- Temperature at Kilpisjärvi in June, July and August from 1952 to 2013
- Is there change in the temperature?



Normal linear model

```
data {  
  int<lower=0> N;           // number of observations  
  vector[N] x;  
  vector[N] y;  
}  
  
parameters {  
  real alpha;              // intercept  
  real beta;               // slope  
  real<lower=0> sigma;     // observation model sd  
}  
  
transformed parameters {  
  vector[N] mu;  
  mu = alpha + beta*x;    // linear model  
}  
  
model {  
  y ~ normal(mu, sigma);  // observation model  
}
```

Normal linear model

```
data {  
  int<lower=0> N;           // number of observations  
  vector[N] x;  
  vector[N] y;  
}  
  
parameters {  
  real alpha;              // intercept  
  real beta;               // slope  
  real<lower=0> sigma;     // observation model sd  
}  
  
transformed parameters {  
  vector[N] mu;  
  mu = alpha + beta*x;    // linear model  
}  
  
model {  
  y ~ normal(mu, sigma);  // observation model  
}
```

Normal linear model

```
data {  
  int<lower=0> N;          // number of observations  
  vector[N] x;  
  vector[N] y;  
}  
  
parameters {  
  real alpha;             // intercept  
  real beta;              // slope  
  real<lower=0> sigma;    // observation model sd  
}  
  
transformed parameters {  
  vector[N] mu;  
  mu = alpha + beta*x;    // linear model  
}  
  
model {  
  y ~ normal(mu, sigma); // observation model  
}
```

Normal linear model

```
data {  
  int<lower=0> N;          // number of observations  
  vector[N] x;  
  vector[N] y;  
}  
  
parameters {  
  real alpha;             // intercept  
  real beta;              // slope  
  real<lower=0> sigma;    // observation model sd  
}  
  
transformed parameters {  
  vector[N] mu;  
  mu = alpha + beta*x;    // linear model  
}  
  
model {  
  y ~ normal(mu, sigma);  // observation model  
}
```

Normal linear model

```
data {  
  int<lower=0> N;           // number of observations  
  vector[N] x;  
  vector[N] y;  
}
```

- difference between `vector[N] x` and `array[N] real x`

Normal linear model

```
data {  
  int<lower=0> N;           // number of observations  
  vector[N] x;  
  vector[N] y;  
}
```

- difference between `vector[N] x` and `array[N] real x`
- only integer arrays: `array[N] int x`

Normal linear model

```
parameters {  
  real alpha;           // intercept  
  real beta;            // slope  
  real<lower=0> sigma;   // observation model sd  
}  
  
transformed parameters {  
  vector[N] mu;  
  mu = alpha + beta*x;  // linear model  
}
```

- transformed parameters are deterministic transformations of parameters and data

Student- t linear model

...

```
parameters {  
  real alpha;  
  real beta;  
  real<lower=0> sigma;  
  real<lower=1,upper=80> nu;  
}  
transformed parameters {  
  vector[N] mu;  
  mu = alpha + beta*x;  
}  
model {  
  nu ~ gamma(2, 0.1);           // prior for nu  
  y ~ student_t(nu, mu, sigma); // observation model  
}
```

Priors for normal linear model

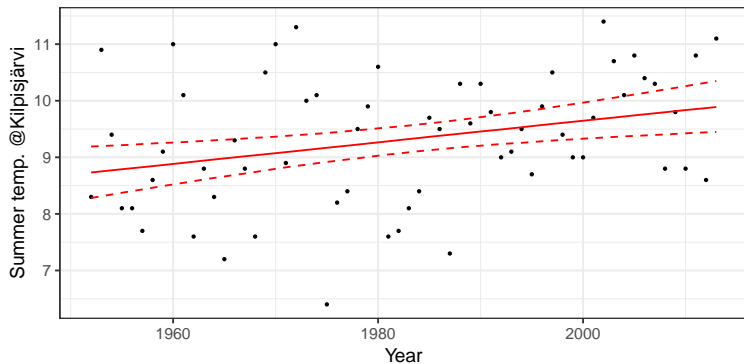
```
data {  
  int<lower=0> N; // number of observations  
  vector[N] x; //  
  vector[N] y; //  
  real pmualpha; // prior mean for alpha  
  real psalpha; // prior std for alpha  
  real pmubeta; // prior mean for beta  
  real psbeta; // prior std for beta  
}  
...  
transformed parameters {  
  vector[N] mu;  
  mu = alpha + beta*x;  
}  
model {  
  alpha ~ normal(pmualpha, psalpha); // prior for alpha  
  beta ~ normal(pmubeta, psbeta); // prior for beta  
  y ~ normal(mu, sigma); // observation model  
}
```

Priors

- Prior for temperature increase?

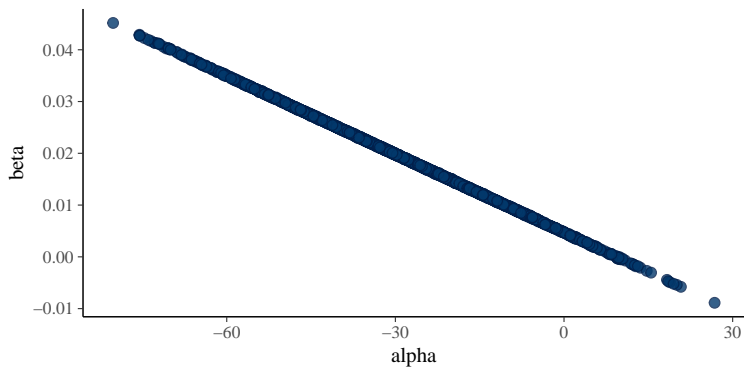
Kilpisjärvi summer temperature

Posterior fit



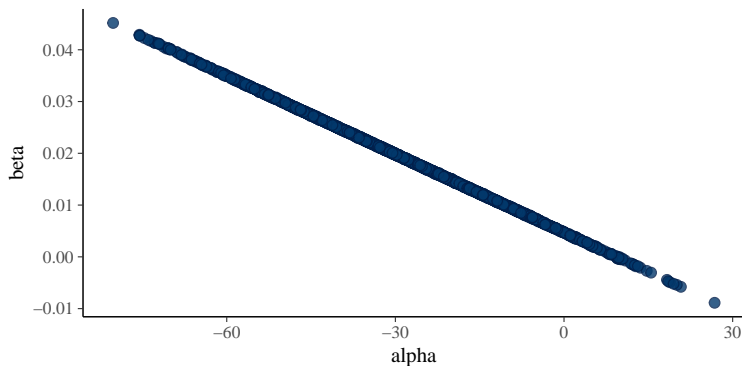
Kilpisjärvi summer temperature

Posterior draws of alpha and beta



Kilpisjärvi summer temperature

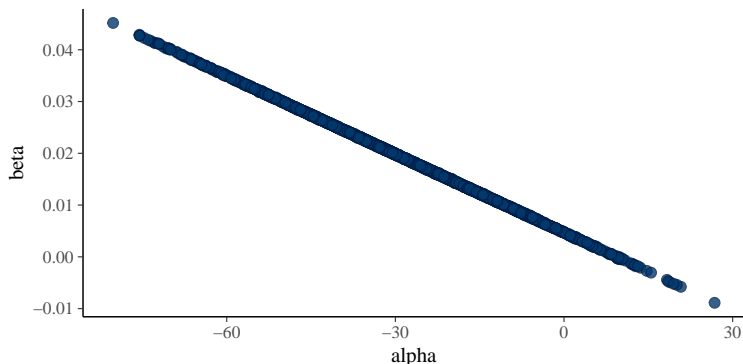
Posterior draws of alpha and beta



Warning: 1 of 4000 (0.0%) transitions hit the maximum treedepth limit of 10.
See <https://mc-stan.org/misc/warnings> for details.

Kilpisjärvi summer temperature

Posterior draws of alpha and beta



Warning: 1 of 4000 (0.0%) transitions hit the maximum treedepth limit of 10.
See <https://mc-stan.org/misc/warnings> for details.

Hitting maximum treedepth (maximum number of steps) does not invalidate results, but indicates inefficient sampling

Linear regression model in Stan

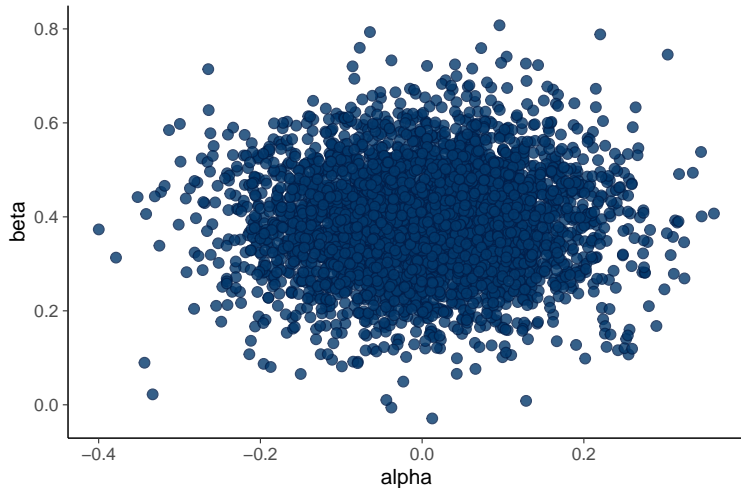
Center the data inside the model code

```
data {  
  int<lower=0> N; // number of observations  
  vector[N] x;  
  vector[N] y;  
  real xpred;      // covariate values for prediction  
}
```

```
transformed data {  
  vector[N] x_std;  
  vector[N] y_std;  
  real xpred_std;  
  x_std = (x - mean(x)) / sd(x);  
  y_std = (y - mean(y)) / sd(y);  
  xpred_std = (xpred - mean(x)) / sd(x);  
}
```

Kilpisjärvi summer temperature

Posterior draws of alpha and beta when data is centered



Kilpisjärvi summer temperature

Without centering

```
> fit_lin$summary(variables=c("alpha", "beta"),  
                    default_convergence_measures())
```

variable	rhat	ess_bulk	ess_tail
alpha	1.0	919.	897.
beta	1.0	919.	895.

With centering

```
> fit_lin_std$summary(variables=c("alpha", "beta"),  
                      default_convergence_measures())
```

variable	rhat	ess_bulk	ess_tail
alpha	1.0	3872.	2616.
beta	1.0	3770.	2396.

RStanARM

- RStanARM provides simplified model description with pre-compiled models
 - no need to wait for compilation
 - a restricted set of models

Two group Binomial model:

```
d_bin2 <- data.frame(N = c(674, 680), y = c(39,22), grp2 = c(0,1))  
fit_bin2 <- stan_glm(y/N ~ grp2, family = binomial(), data = d_bin2,  
                    weights = N)
```

RStanARM

- RStanARM provides simplified model description with pre-compiled models
 - no need to wait for compilation
 - a restricted set of models

Two group Binomial model:

```
d_bin2 <- data.frame(N = c(674, 680), y = c(39,22), grp2 = c(0,1))  
fit_bin2 <- stan_glm(y/N ~ grp2, family = binomial(), data = d_bin2,  
                    weights = N)
```

Normal linear model

```
fit_lin <- stan_glm(temp ~ year, data = d_lin)
```

brms

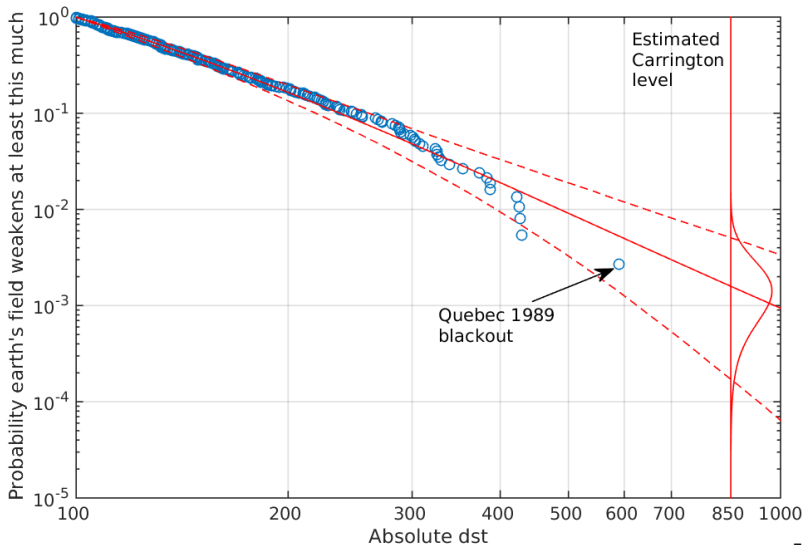
- brms provides simplified model description
 - + a larger set of models than RStanARM, but still restricted
 - need to wait for the compilation

```
fit_bin2 <- brm(y | trials(N) ~ grp2, family = binomial(), data = d_bin2)
```

```
fit_lin_t <- brm(temp ~ year, data = d_lin, family = student())
```

Extreme value analysis

Geomagnetic storms



Extreme value analysis

```
data {  
  int<lower=0> N;  
  vector<lower=0>[N] y;  
  int<lower=0> Nt;  
  vector<lower=0>[Nt] yt;  
}  
transformed data {  
  real ymax = max(y);          // pre-compute a useful quantity  
}  
parameters {  
  real<lower=0> sigma;  
  real<lower=-sigma/ymax> k; // constraint can depend on other parameters  
}  
model {  
  y ~ gpareto(k, sigma);      // user defined distribution  
}  
generated quantities {  
  vector[Nt] predccdf = gpareto_ccdf(yt, k, sigma);  
}
```

Extreme value analysis

```
data {  
  int<lower=0> N;  
  vector<lower=0>[N] y;  
  int<lower=0> Nt;  
  vector<lower=0>[Nt] yt;  
}  
transformed data {  
  real ymax = max(y);           // pre-compute a useful quantity  
}  
parameters {  
  real<lower=0> sigma;  
  real<lower=-sigma/ymax> k; // constraint can depend on other parameters  
}  
model {  
  y ~ gpareto(k, sigma);        // user defined distribution  
}  
generated quantities {  
  vector[Nt] predccdf = gpareto_ccdf(yt, k, sigma);  
}
```

Extreme value analysis

```
data {  
  int<lower=0> N;  
  vector<lower=0>[N] y;  
  int<lower=0> Nt;  
  vector<lower=0>[Nt] yt;  
}  
transformed data {  
  real ymax = max(y);          // pre-compute a useful quantity  
}  
parameters {  
  real<lower=0> sigma;  
  real<lower=-sigma/ymax> k; // constraint can depend on other parameters  
}  
model {  
  y ~ gpareto(k, sigma);      // user defined distribution  
}  
generated quantities {  
  vector[Nt] predccdf = gpareto_ccdf(yt, k, sigma);  
}
```

Extreme value analysis

```
data {  
  int<lower=0> N;  
  vector<lower=0>[N] y;  
  int<lower=0> Nt;  
  vector<lower=0>[Nt] yt;  
}  
transformed data {  
  real ymax = max(y);          // pre-compute a useful quantity  
}  
parameters {  
  real<lower=0> sigma;  
  real<lower=-sigma/ymax> k; // constraint can depend on other parameters  
}  
model {  
  y ~ gpareto(k, sigma);      // user defined distribution  
}  
generated quantities {  
  vector[Nt] predccdf = gpareto_ccdf(yt, k, sigma);  
}
```

User defined functions

```
functions {  
  real gpareto_lpdf(vector y, real k, real sigma) {  
    // generalised Pareto log pdf with mu=0  
    // should check and give error if k<0  
    // and max(y)/sigma > -1/k  
    int N;  
    N <- dims(y)[1];  
    if (abs(k) > 1e-15)  
      return -(1+1/k)*sum(log1pv(y*k/sigma)) -N*log(sigma);  
    else  
      return -sum(y/sigma) -N*log(sigma); // limit k->0  
  }  
  vector gpareto_ccdf(vector y, real k, real sigma) {  
    // generalised Pareto log ccdf with mu=0  
    // should check and give error if k<0  
    // and max(y)/sigma < -1/k  
    if (abs(k) > 1e-15)  
      return exp((-1/k)*log1pv(y/sigma*k));  
    else  
      return exp(-y/sigma); // limit k->0  
  }  
}
```

User defined functions

```
functions {  
  real gpareto_lpdf(vector y, real k, real sigma) {  
    // generalised Pareto log pdf with mu=0  
    // should check and give error if k<0  
    // and max(y)/sigma > -1/k  
    int N;  
    N <- dims(y)[1];  
    if (abs(k) > 1e-15)  
      return -(1+1/k)*sum(log1pv(y*k/sigma)) -N*log(sigma);  
    else  
      return -sum(y/sigma) -N*log(sigma); // limit k->0  
  }  
  vector gpareto_ccdf(vector y, real k, real sigma) {  
    // generalised Pareto log ccdf with mu=0  
    // should check and give error if k<0  
    // and max(y)/sigma < -1/k  
    if (abs(k) > 1e-15)  
      return exp((-1/k)*log1pv(y/sigma*k));  
    else  
      return exp(-y/sigma); // limit k->0  
  }  
}
```

Different interfaces

- CmdStanR / CmdStanPy
 - Interface on top of command-line program CmdStan
- RStan / PyStan
 - C++ functions of Stan are called directly from R / Python
 - Higher integration between R/Python and Stan, but maybe more difficult to install due to more requirements of compatible C++ compilers and libraries

Other packages

- R
 - posterior — posterior handling and diagnostics (Lectures 5 and 6)
 - bayesplot — visualization and model checking (Lectures 5, 6, and 8)
 - tidybayes and ggdist — more posterior and prediction visualization (Lecture 6)
 - marginalesffects — prediction and comparison visualization
 - loo — cross-validation model assessment and comparison (Lecture 9)
 - projpred — projection predictive variable selection (Lecture 12)
 - priorsense — prior and likelihood sensitivity diagnostics (Lecture 12)
- Python
 - ArviZ — visualization, and model checking and assessment