Hamiltonian Monte Carlo and Stan

- Hamiltonian Monte Carlo uses gradient information and dynamic simulation to reduce random-walk and increase acceptance rate
  - 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_jebs_2.pdf
- Carpenter et al (2017). Stan: A probabilistic programming language. Journal of Statistical Software 76(1). https://dox.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/

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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/

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- Uses gradient of log density for more efficient sampling

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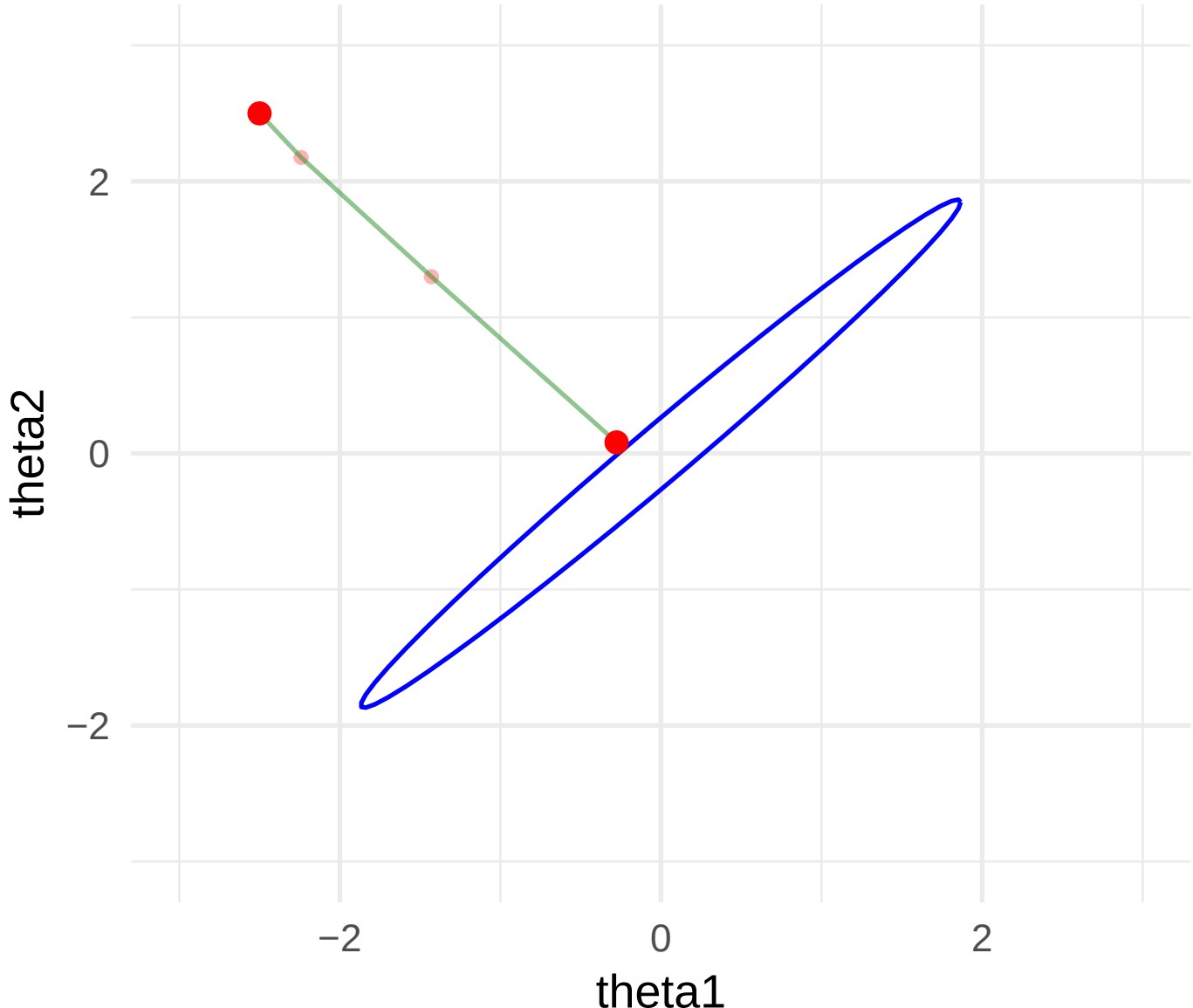

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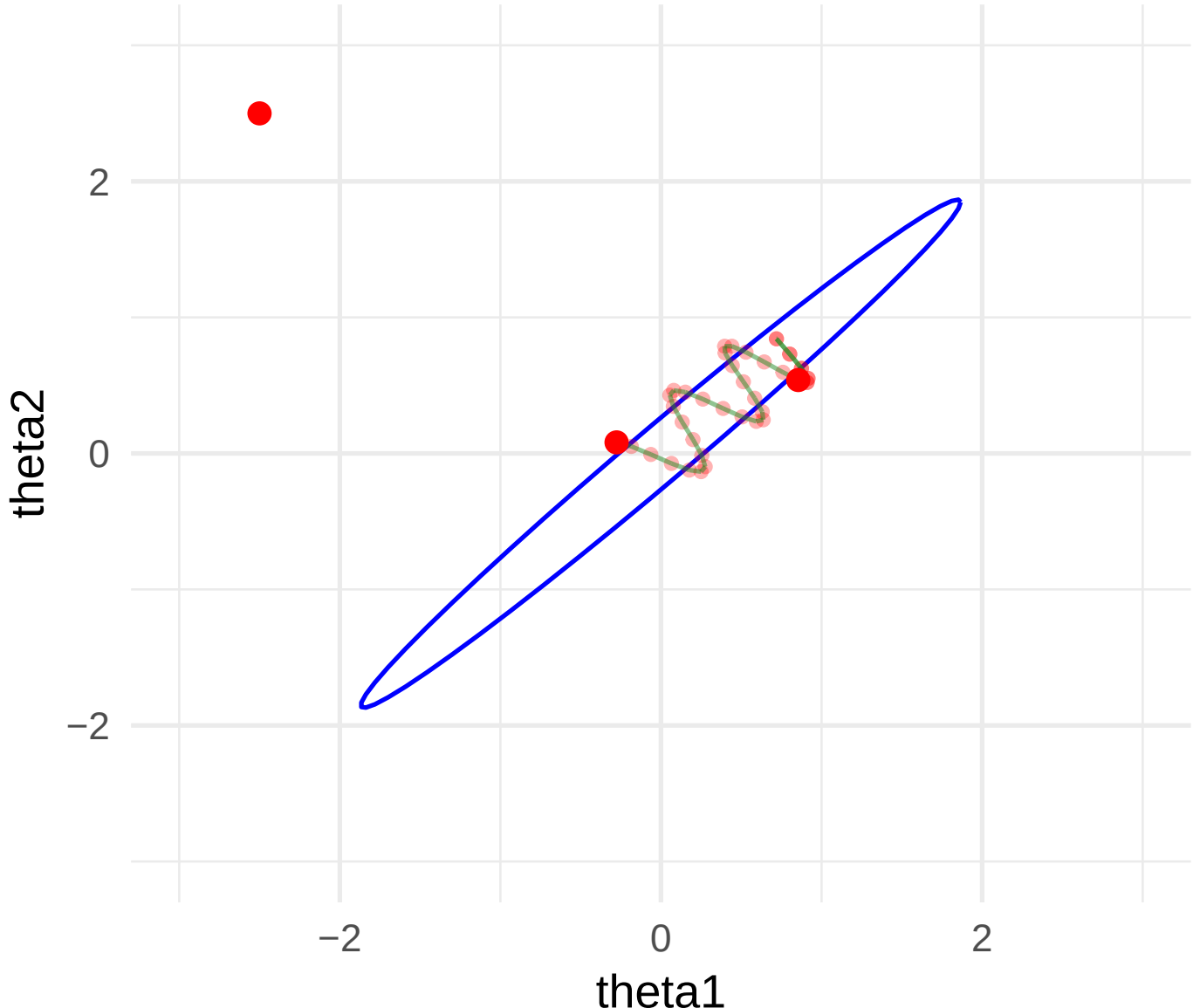

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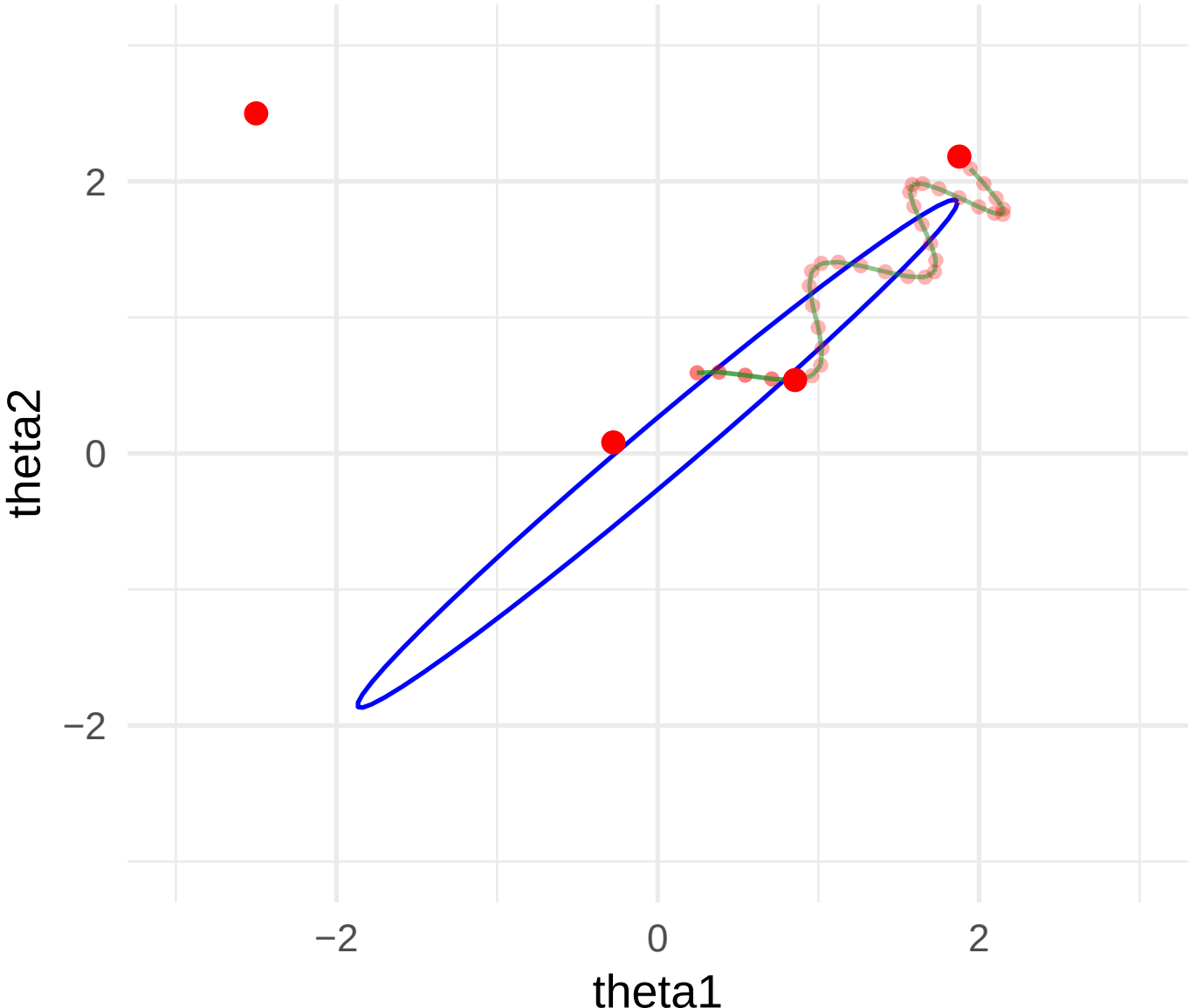

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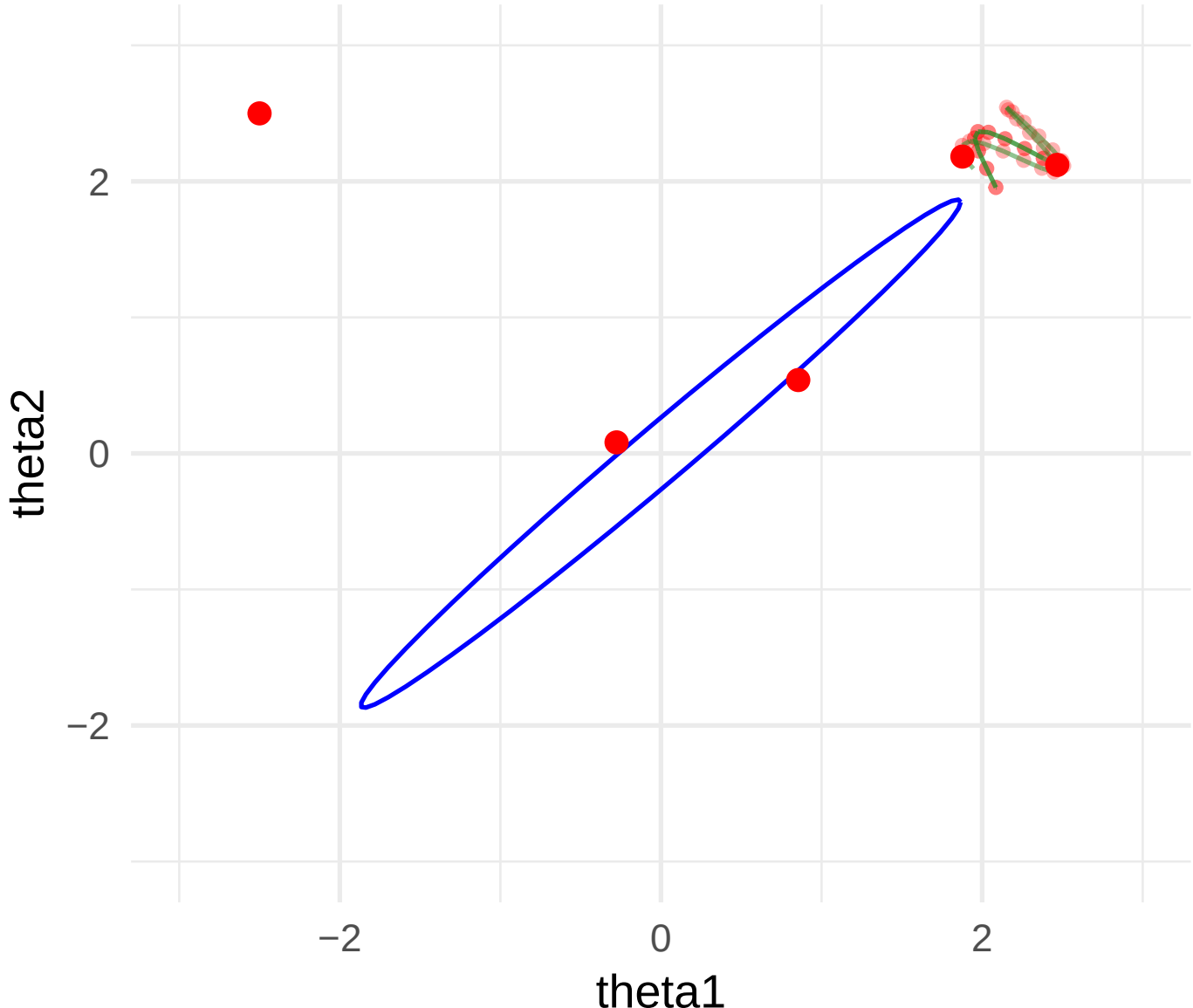

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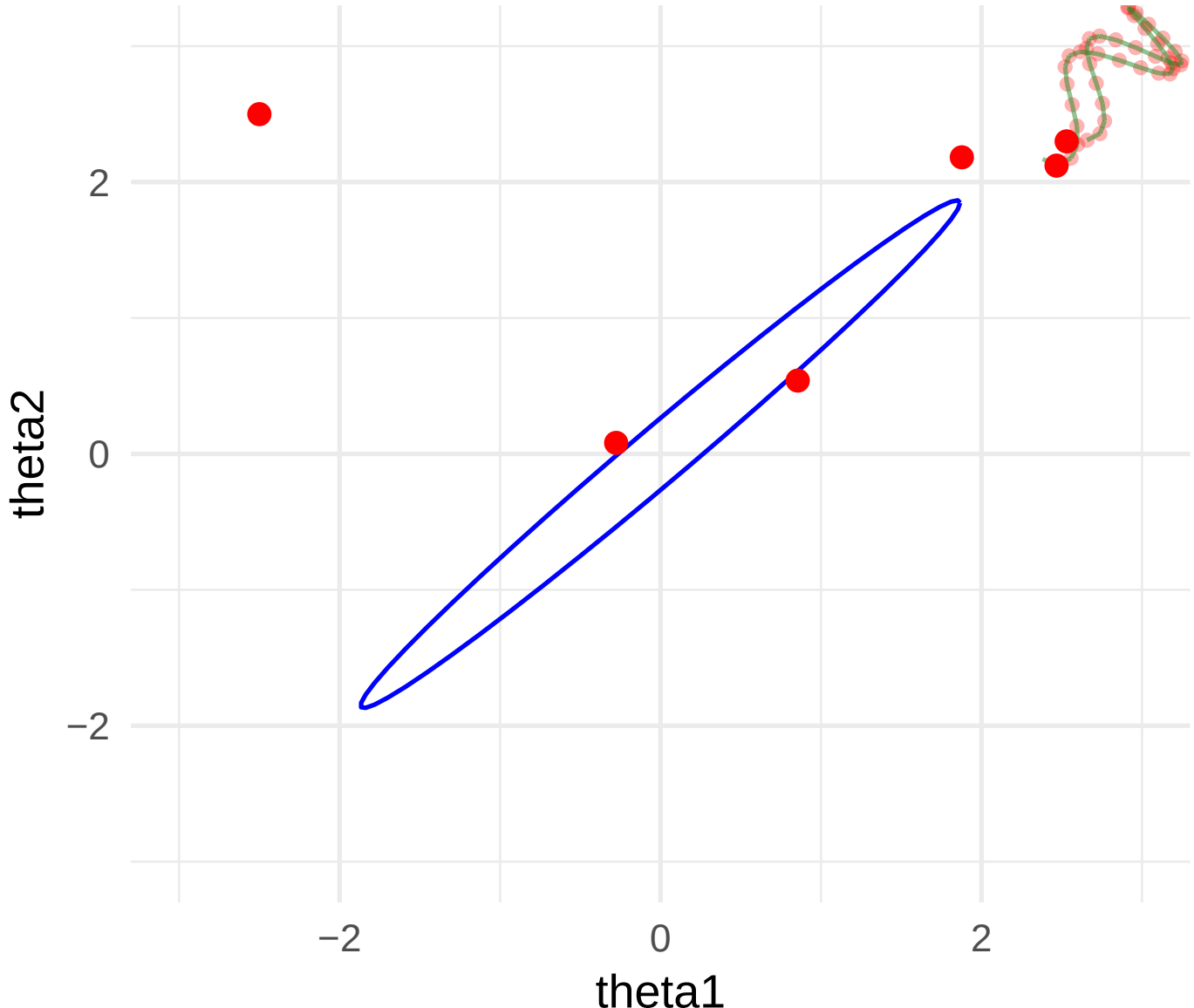

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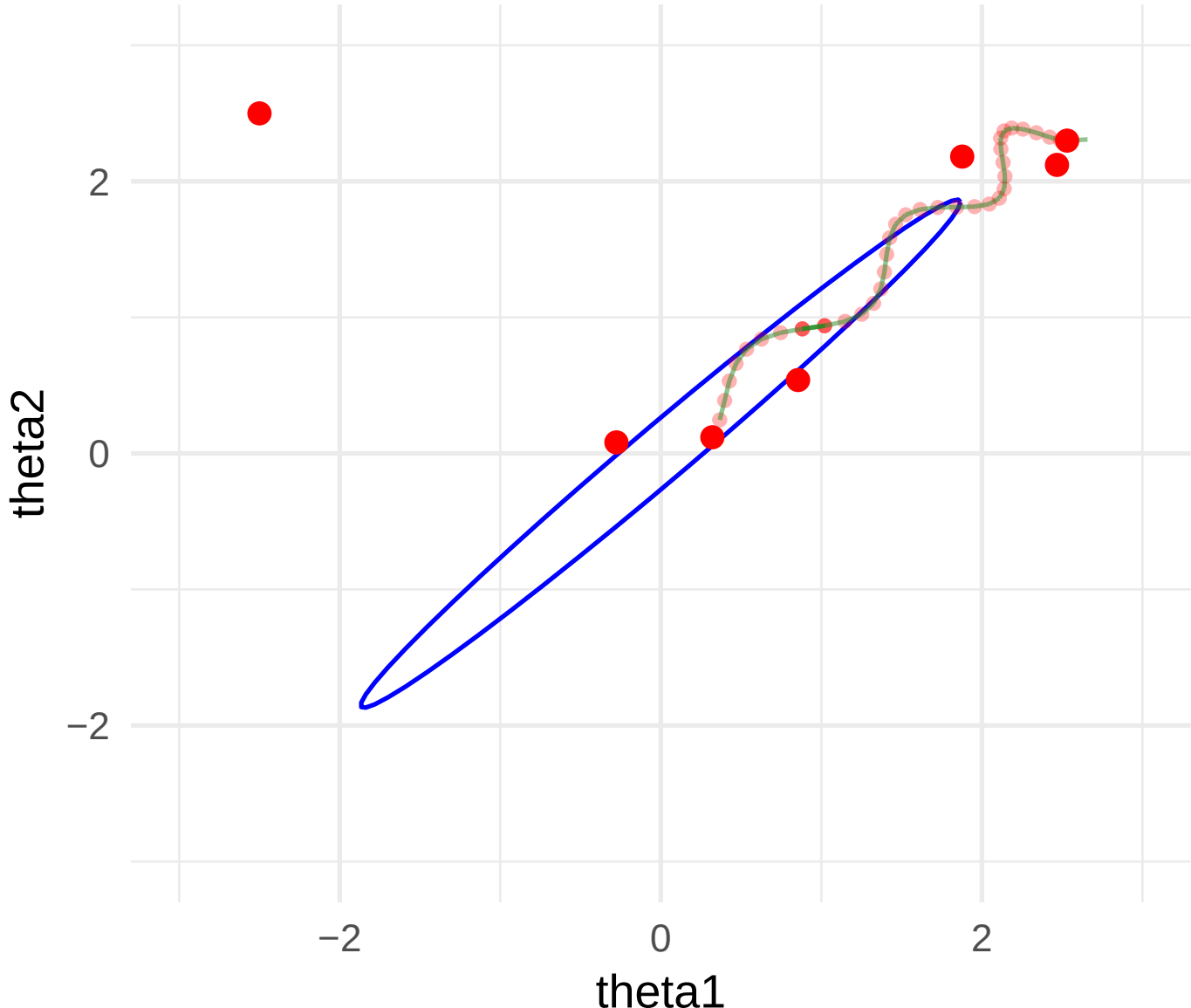

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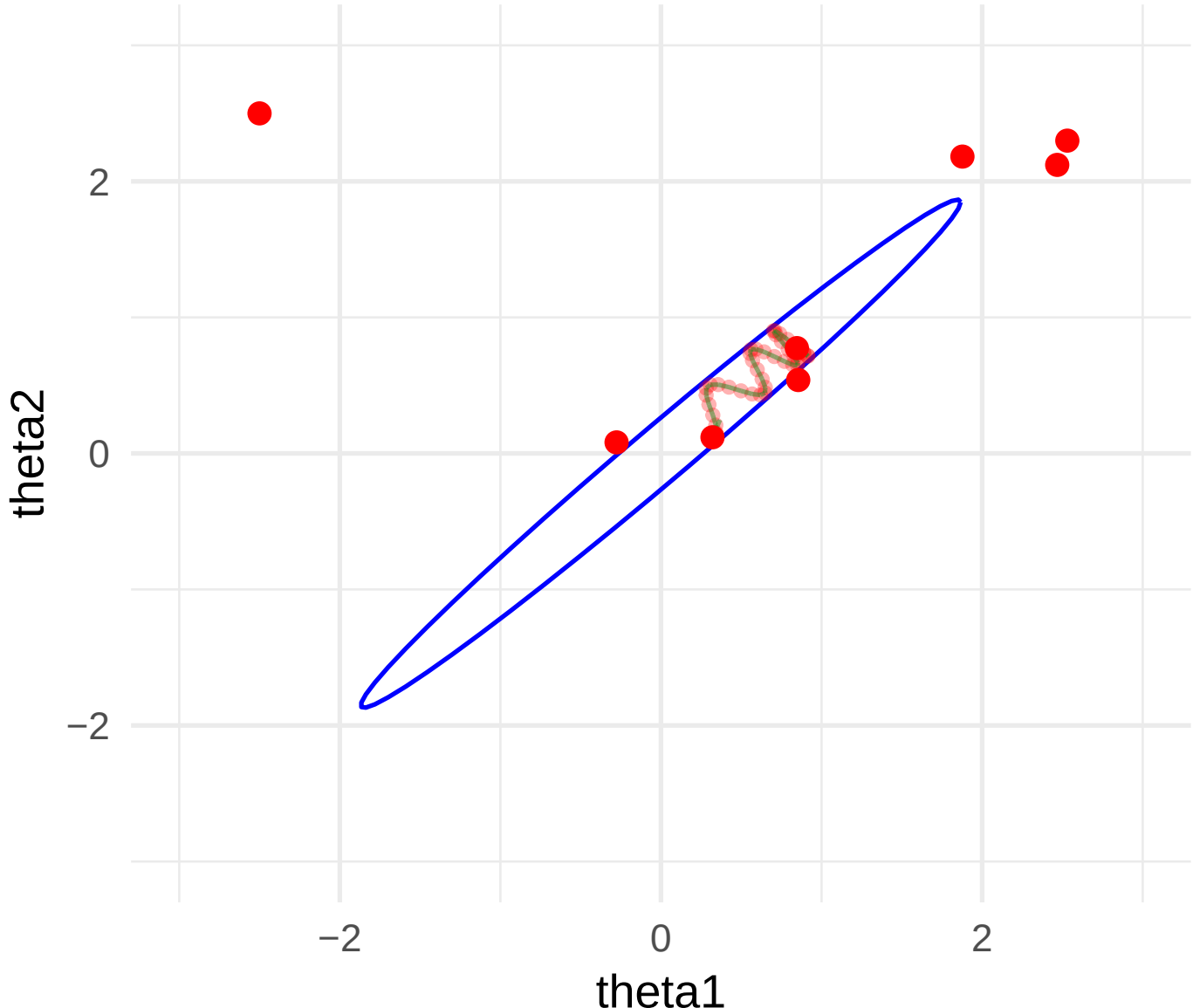

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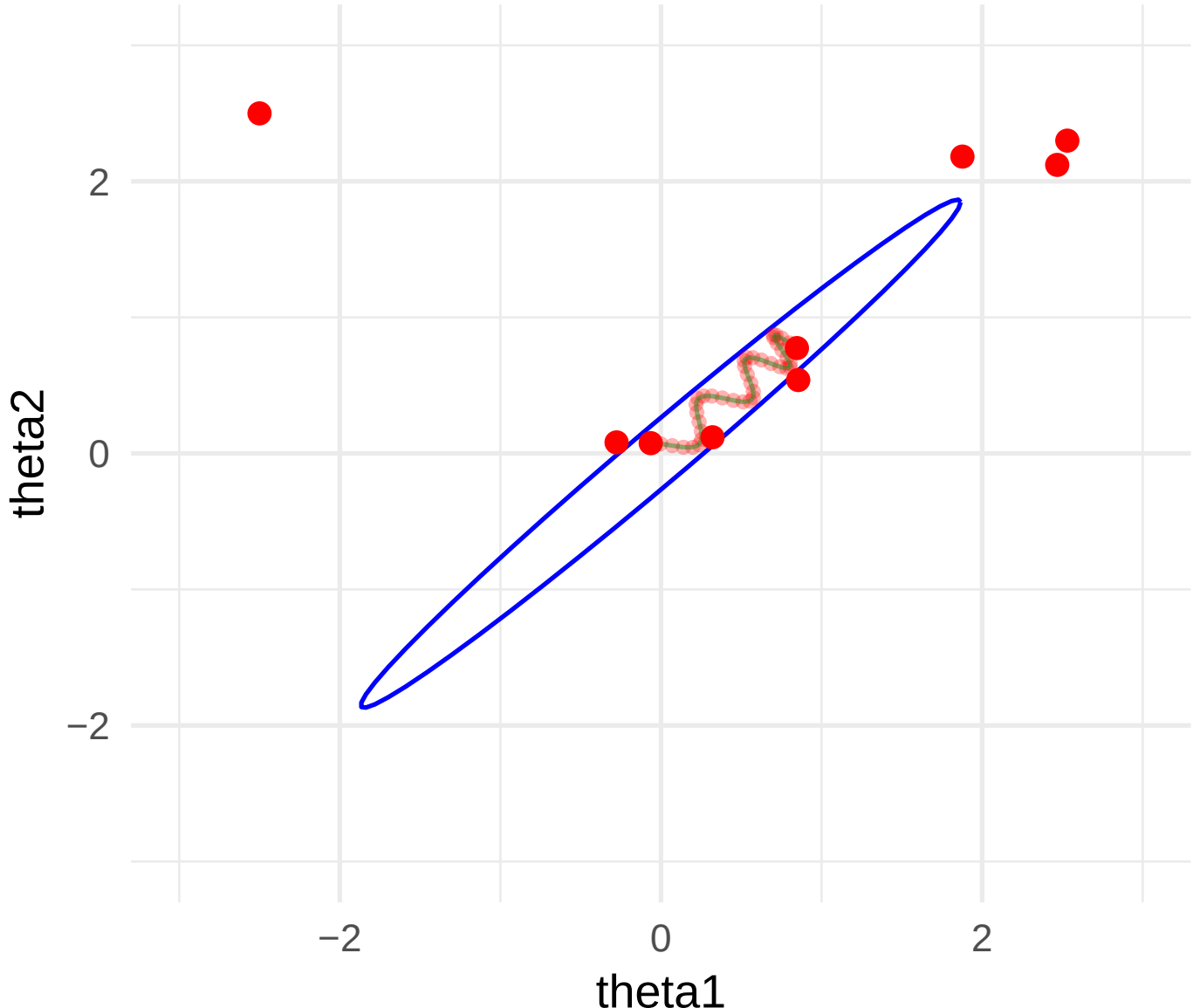

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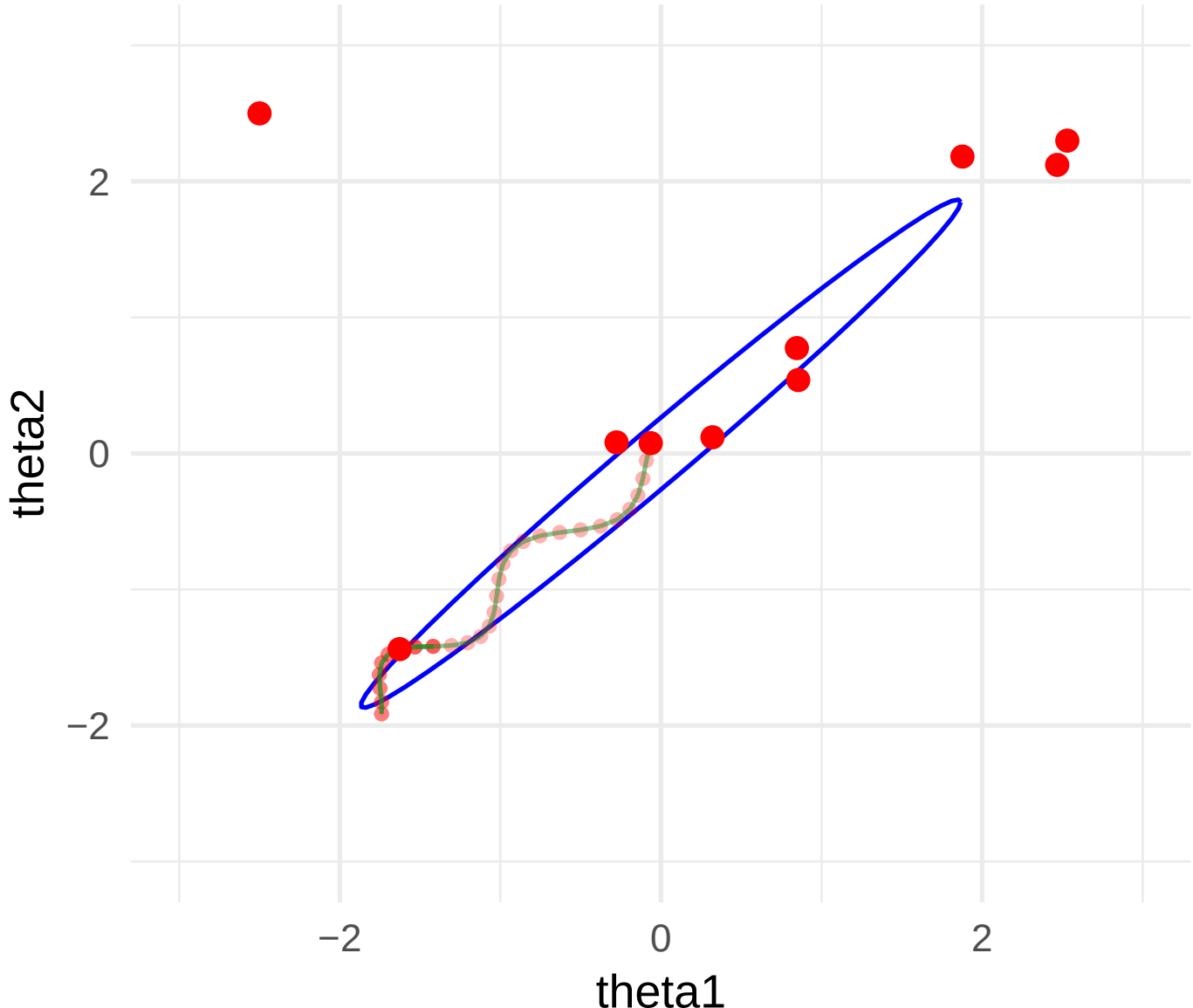

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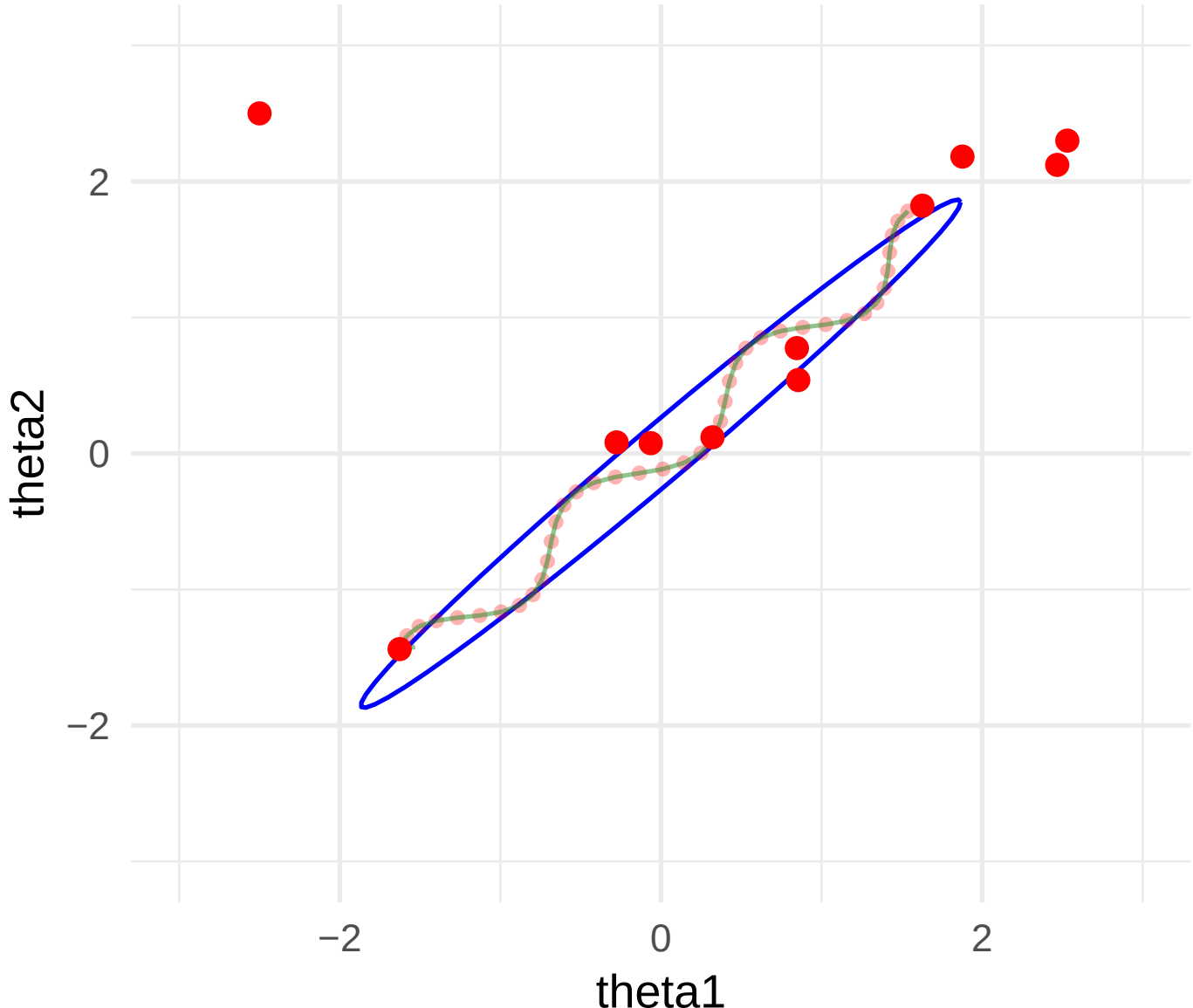

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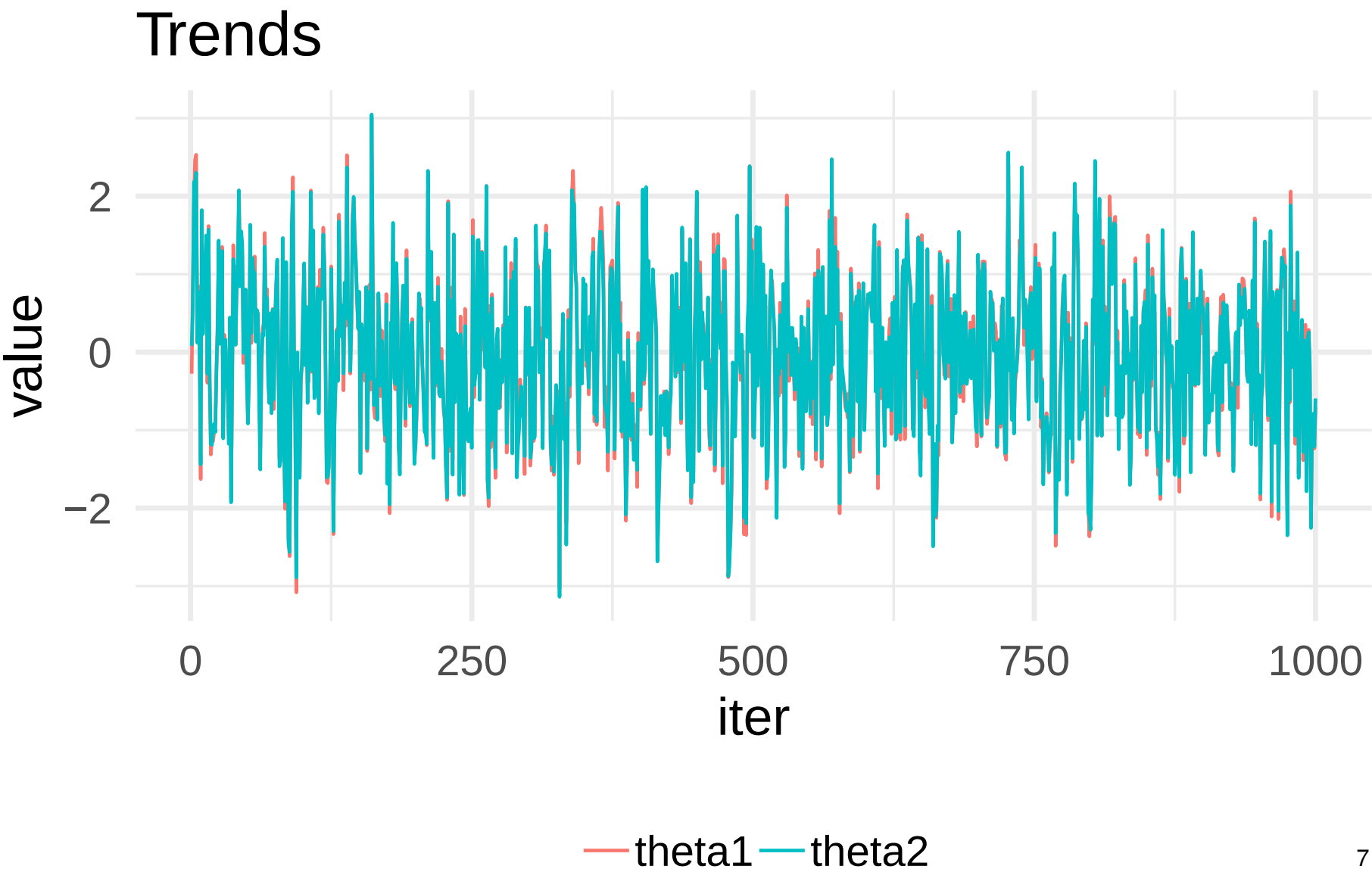

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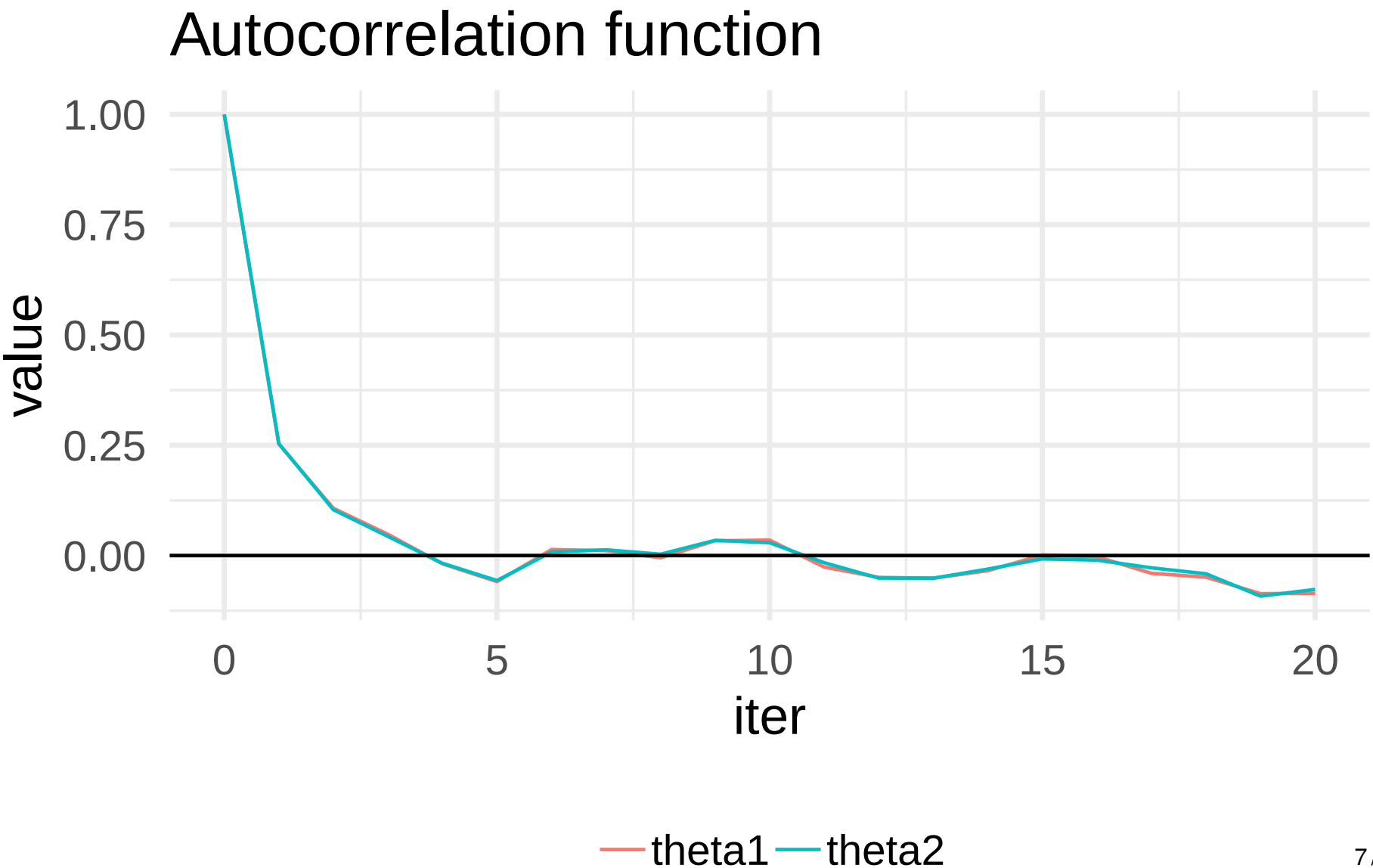

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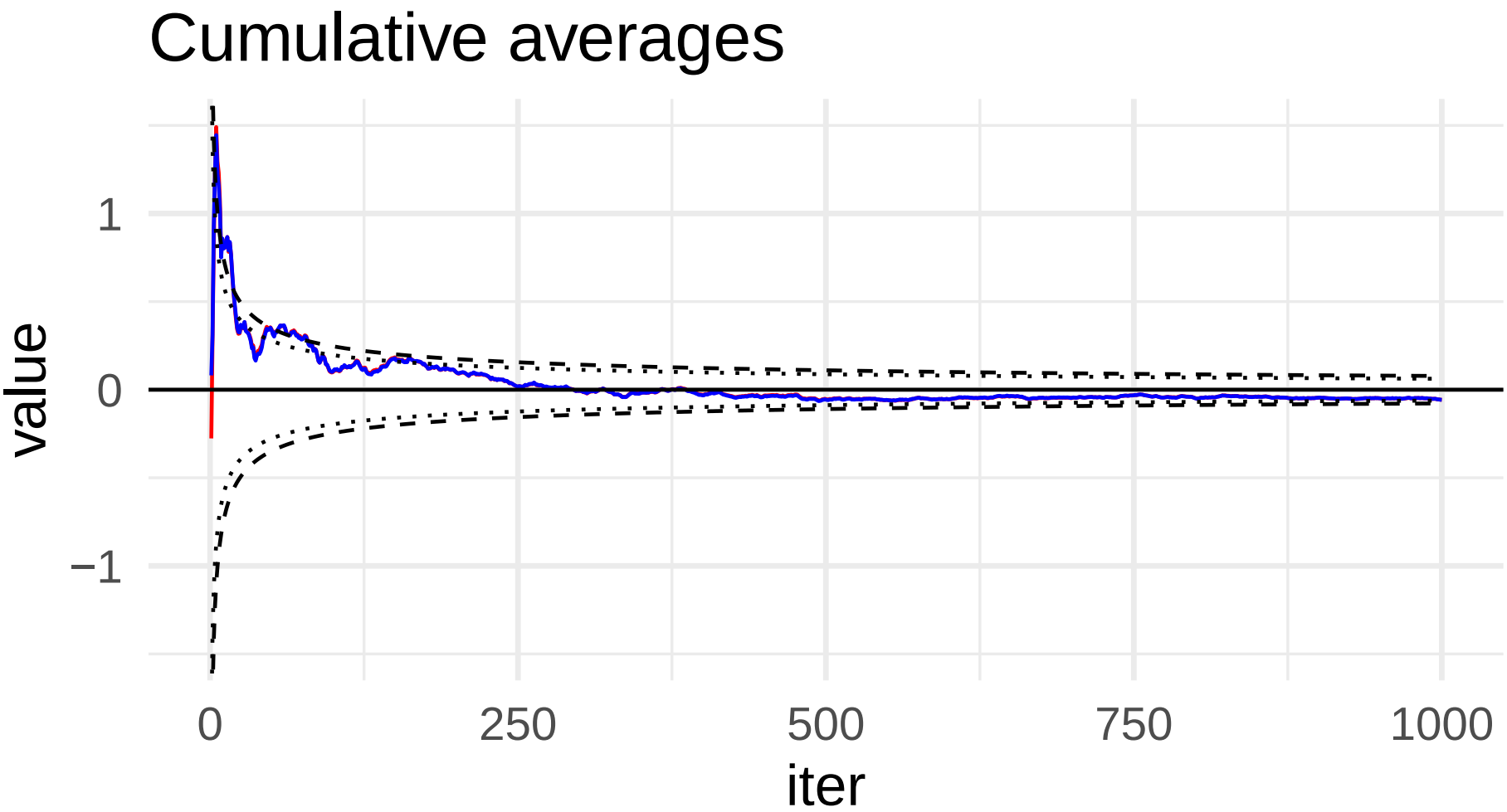

Hamiltonian Monte Carlo / No-U-Turn sampling

1. HMC basics (static HMC)

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4. NUTS + multinomial (dynamic HMC)
    - Betancourt (2018)

Hamiltonian Monte Carlo

- Related methods
  - Factorizing $p(\theta_1, \theta_2) = p(\theta_1 \mid \theta_2)p(\theta_2)$: sample from
    1) $p(\theta_2)$,
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- 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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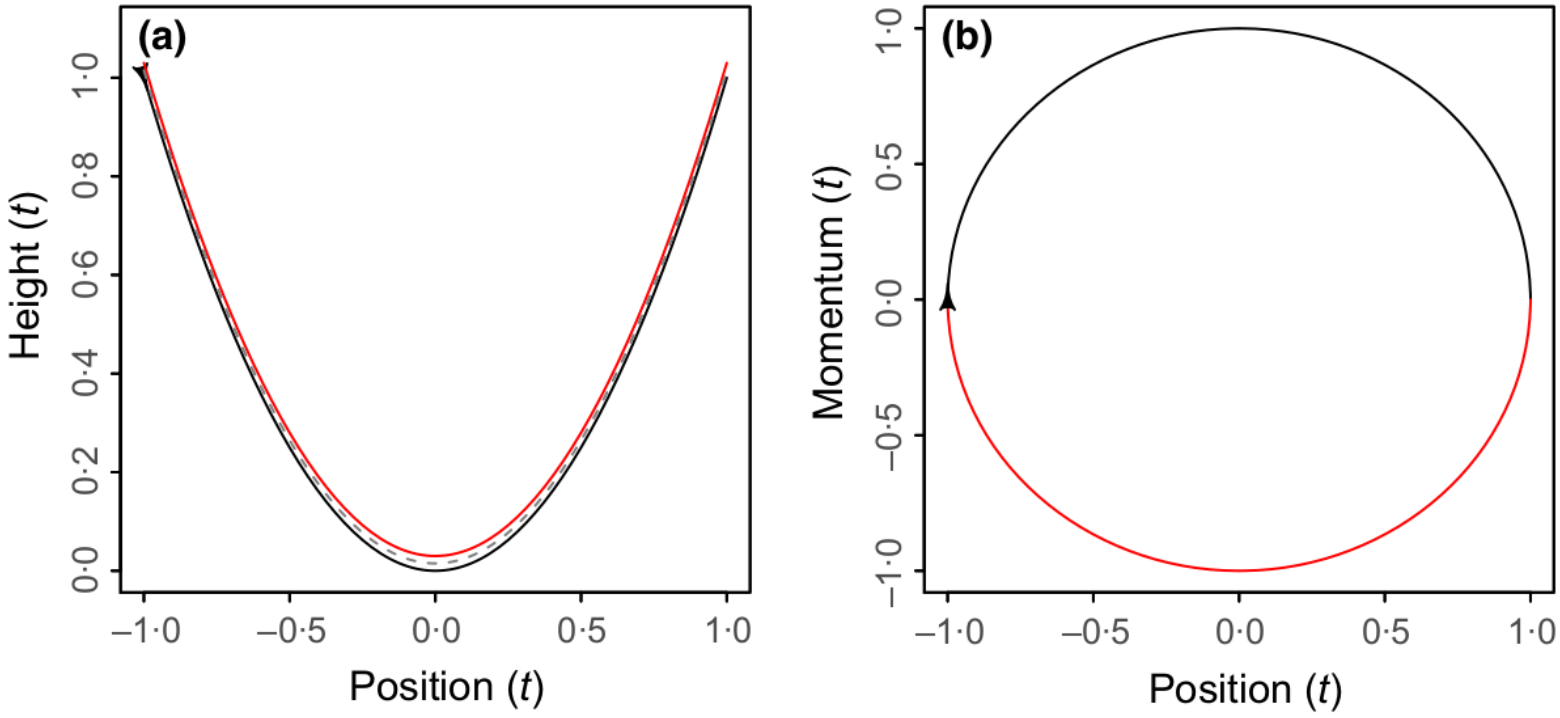
  - ϕ is called a momentum variable
- The potential energy is the negative log density $U(\theta) = -\log(p(\theta)) + C$

Hamiltonian dynamic simulation

Equations of motion, use also the gradient

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



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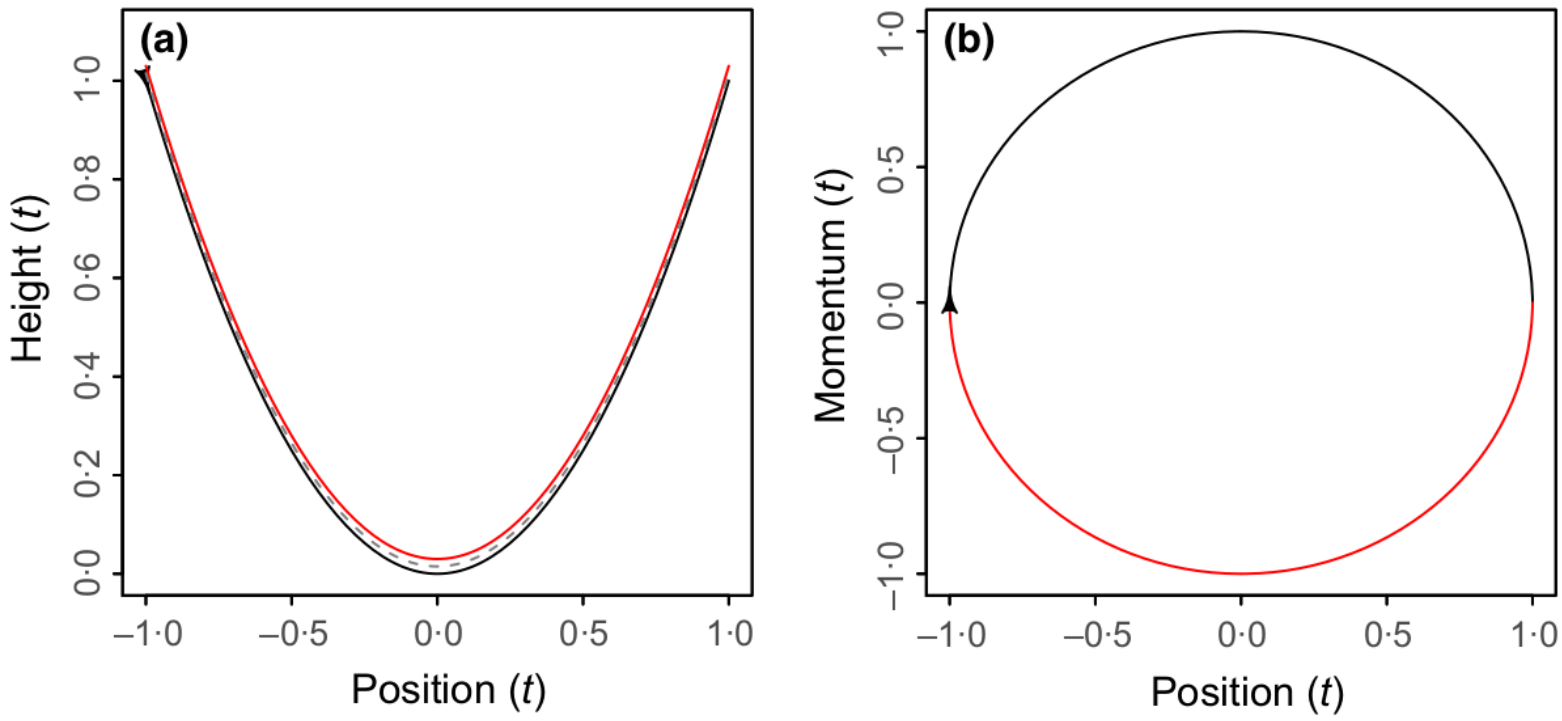

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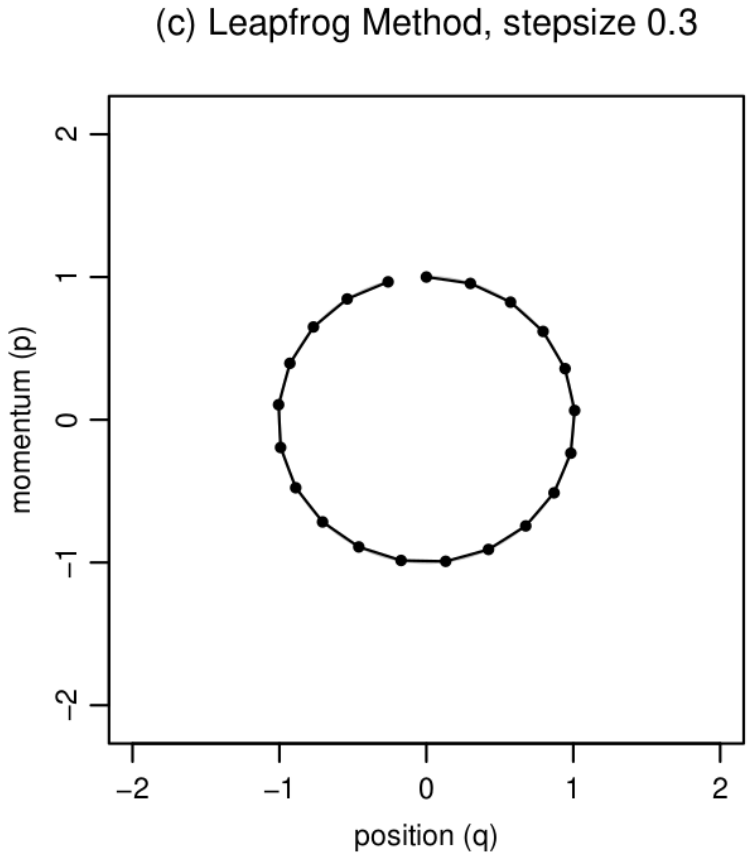
Leapfrog discretization

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



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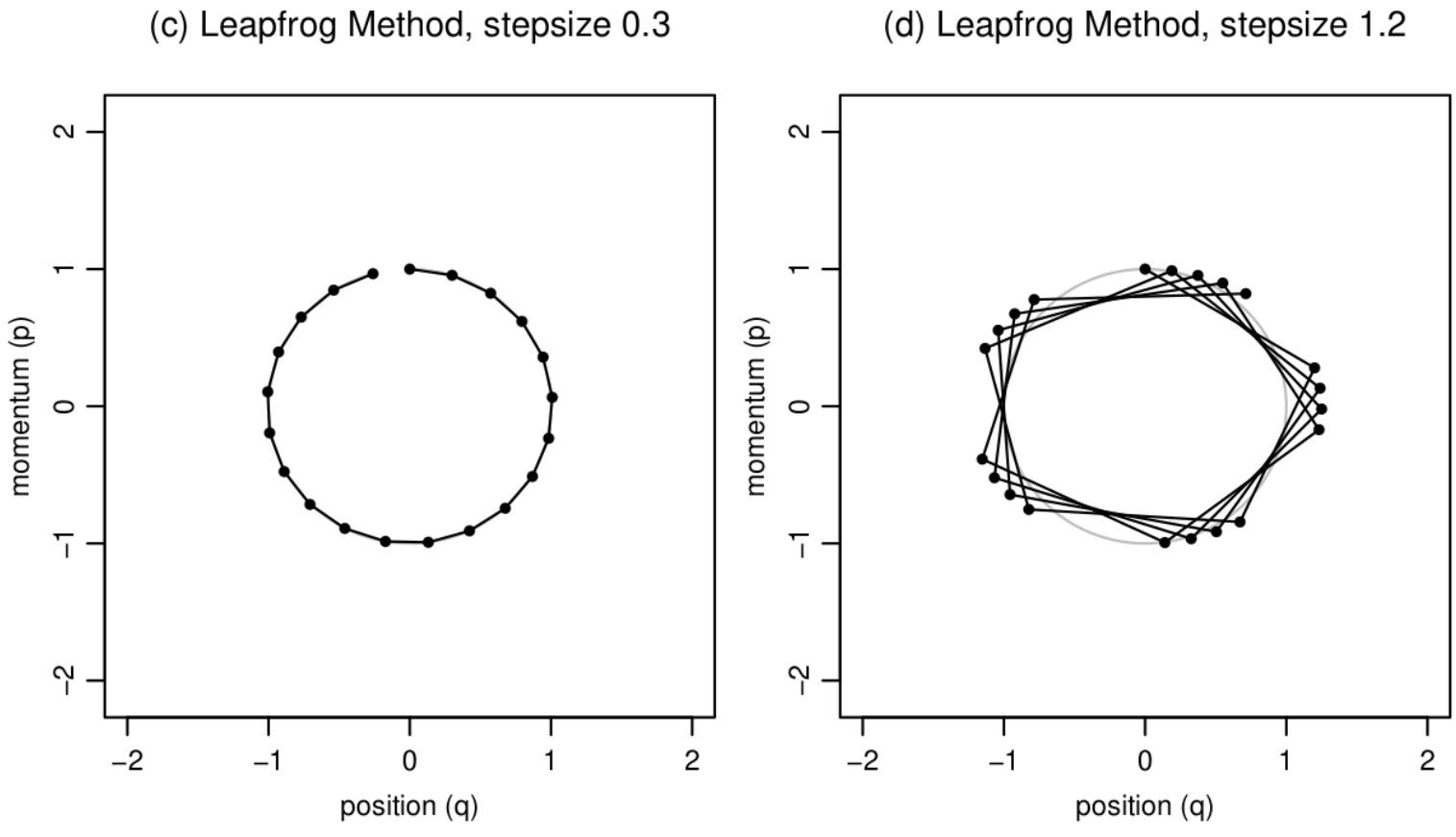

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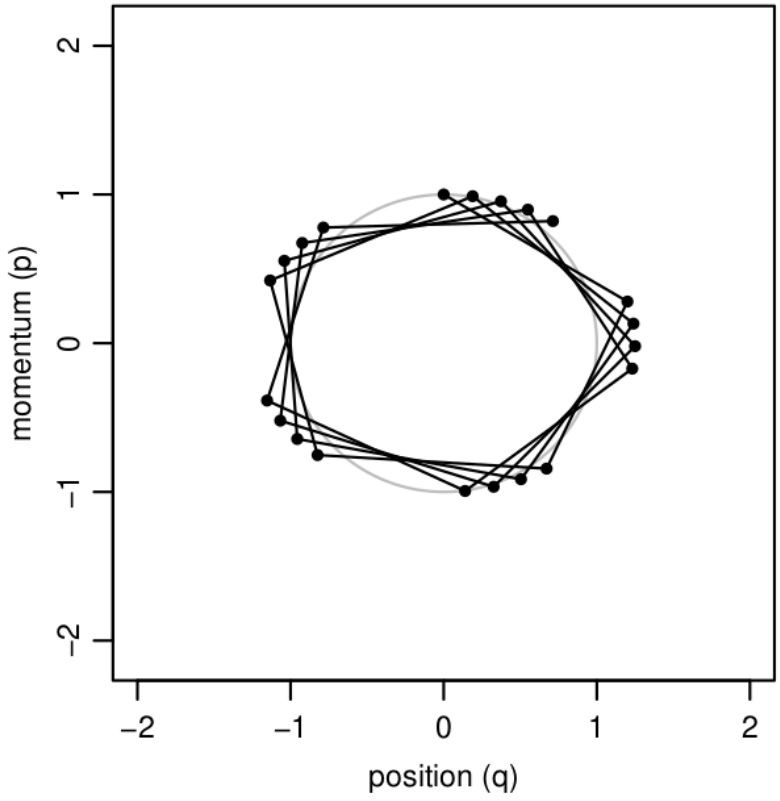

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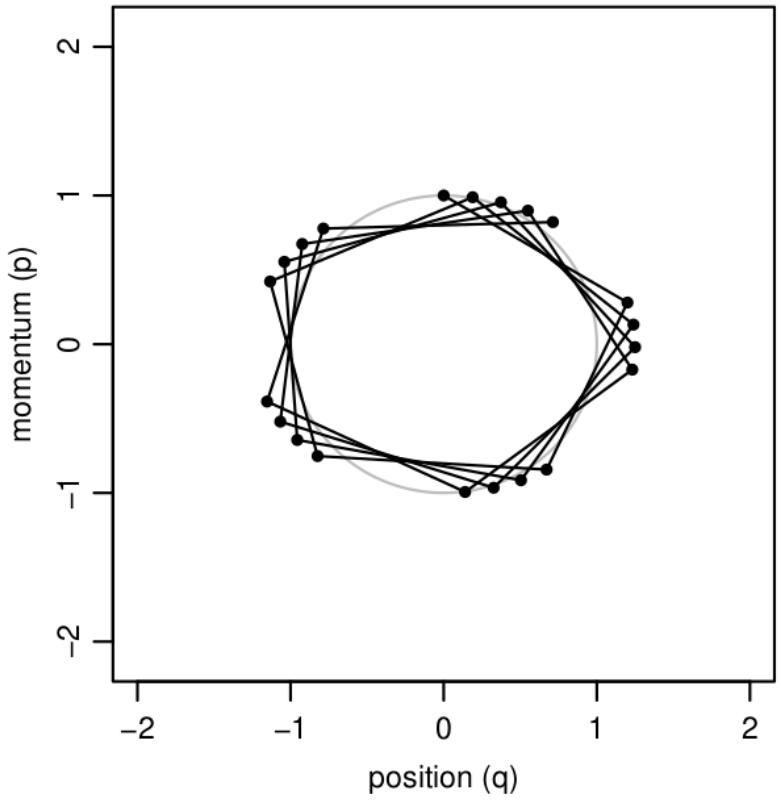
- Metropolis step with $r = \exp\left(-H(\theta^*, \phi^*) + H(\theta^{(t-1)}, \phi^{(t-1)})\right)$
  - accept if the Hamiltonian energy in the end is higher
  - accept with some probability if the Hamiltonian energy in the end is lower



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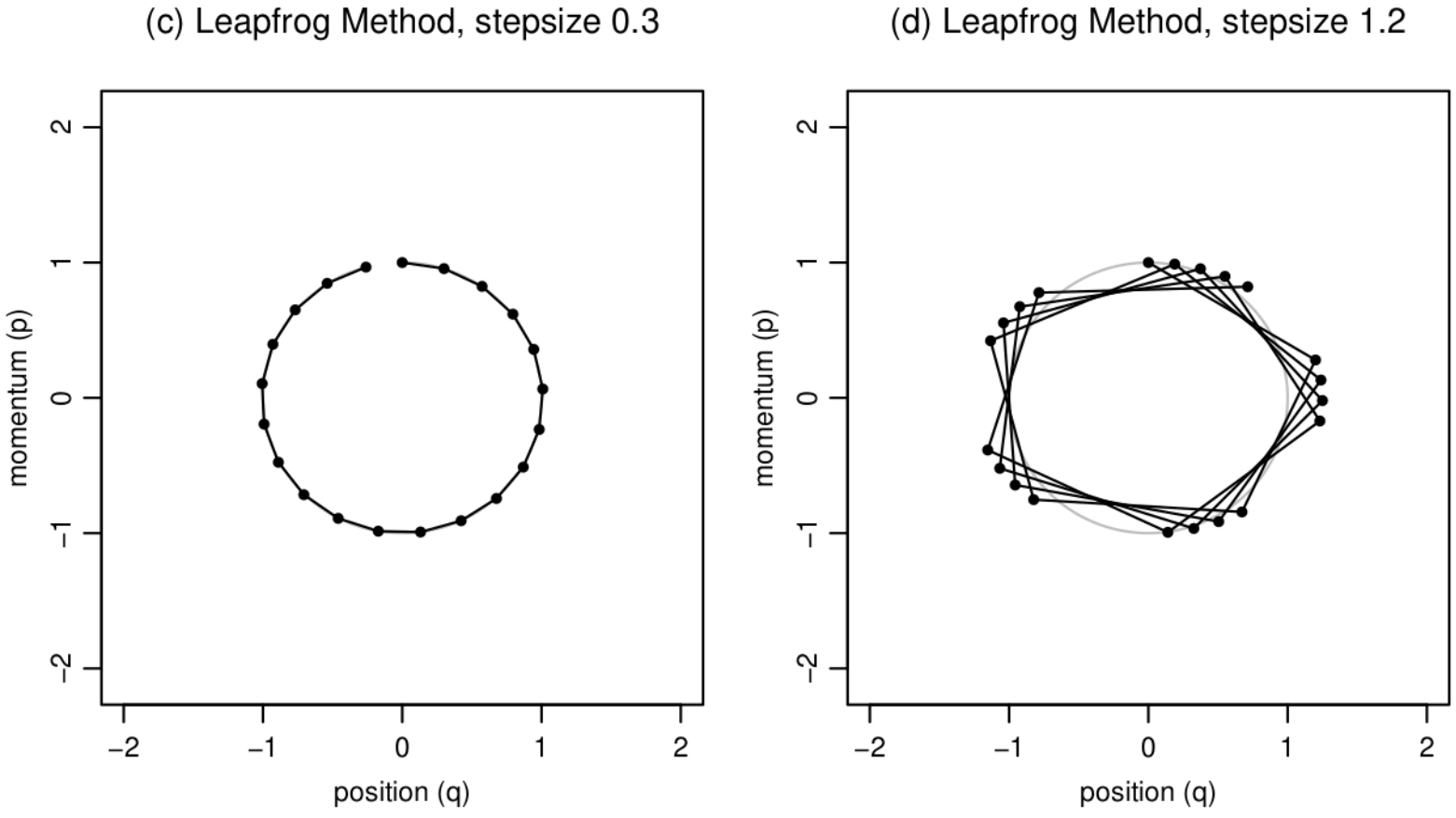
Two steps of Hamiltonian Monte Carlo

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



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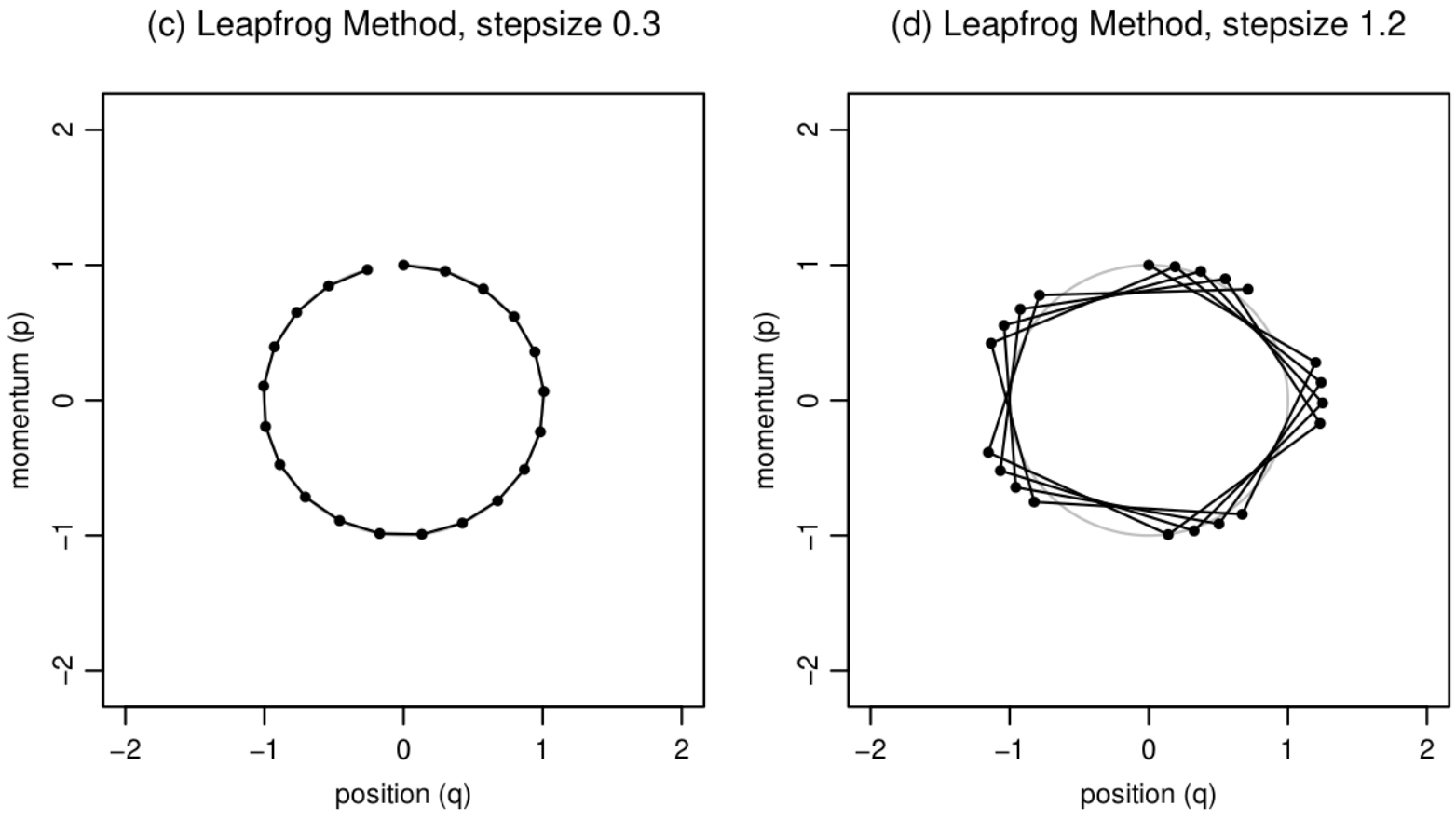

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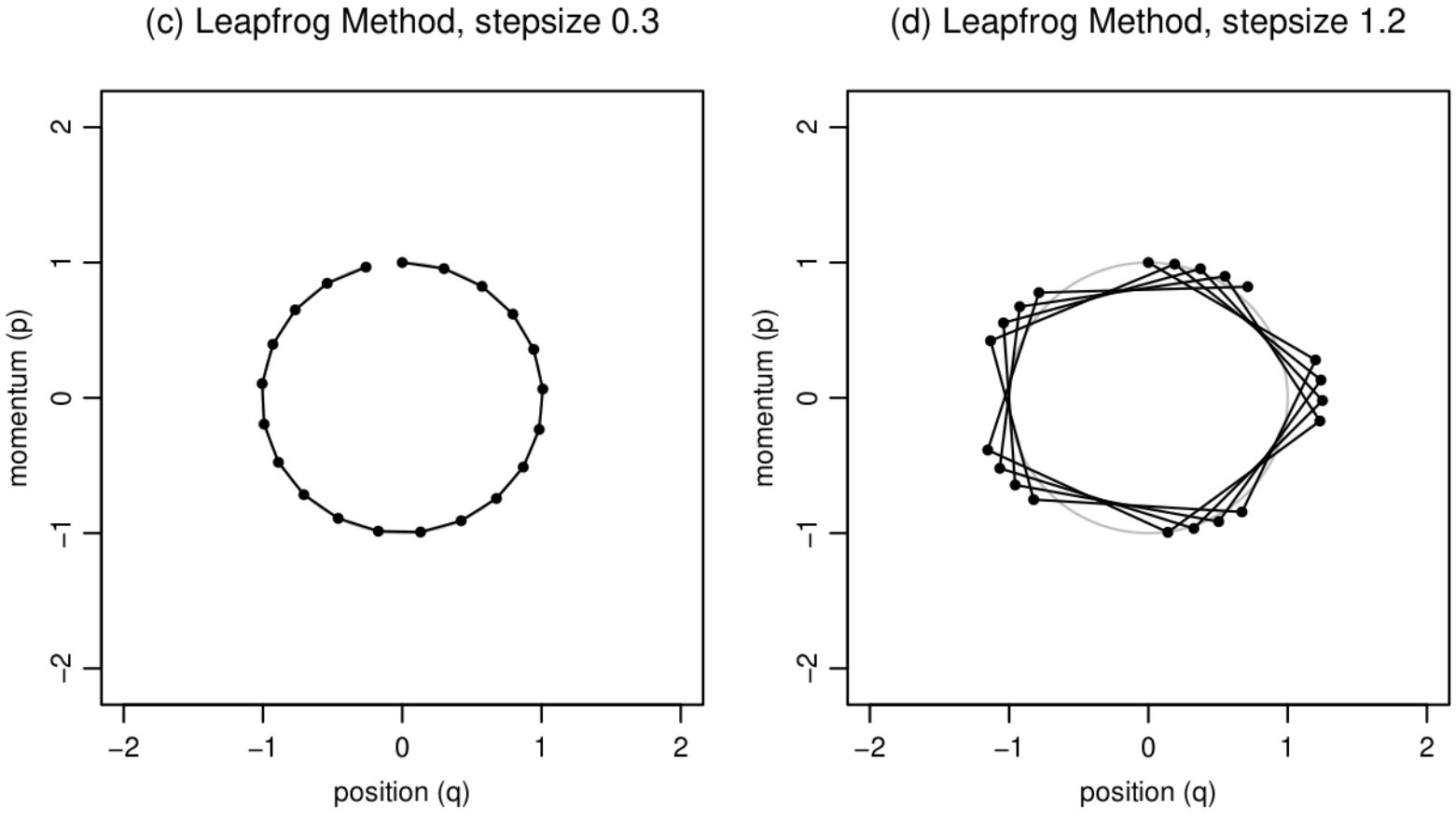
- Alternating sampling from $p(\phi)$ is crucial for moving to (θ, ϕ) points with different joint density



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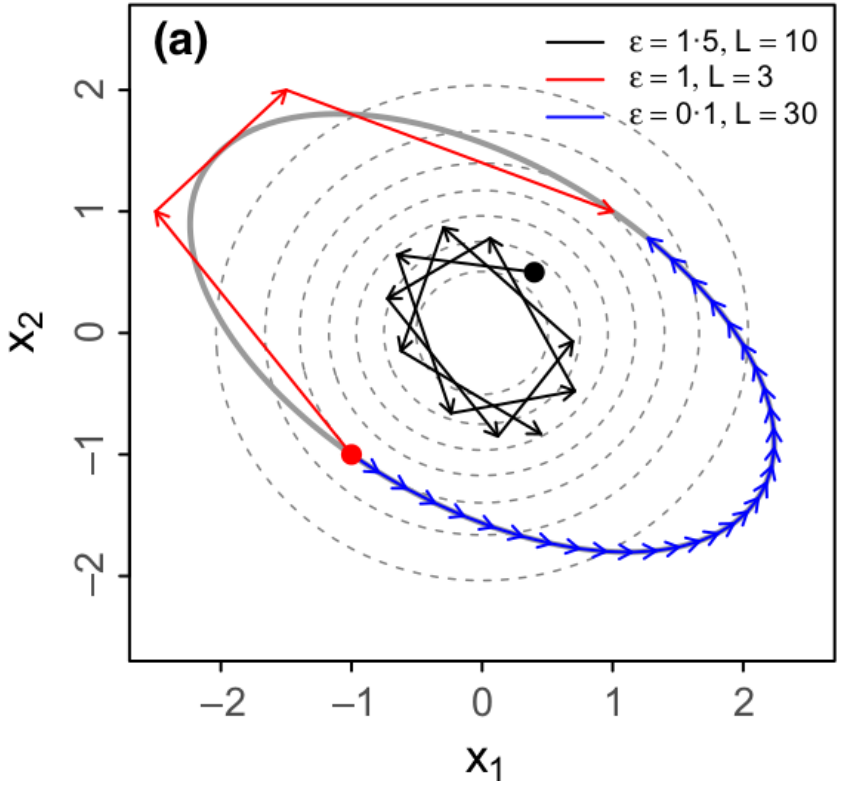

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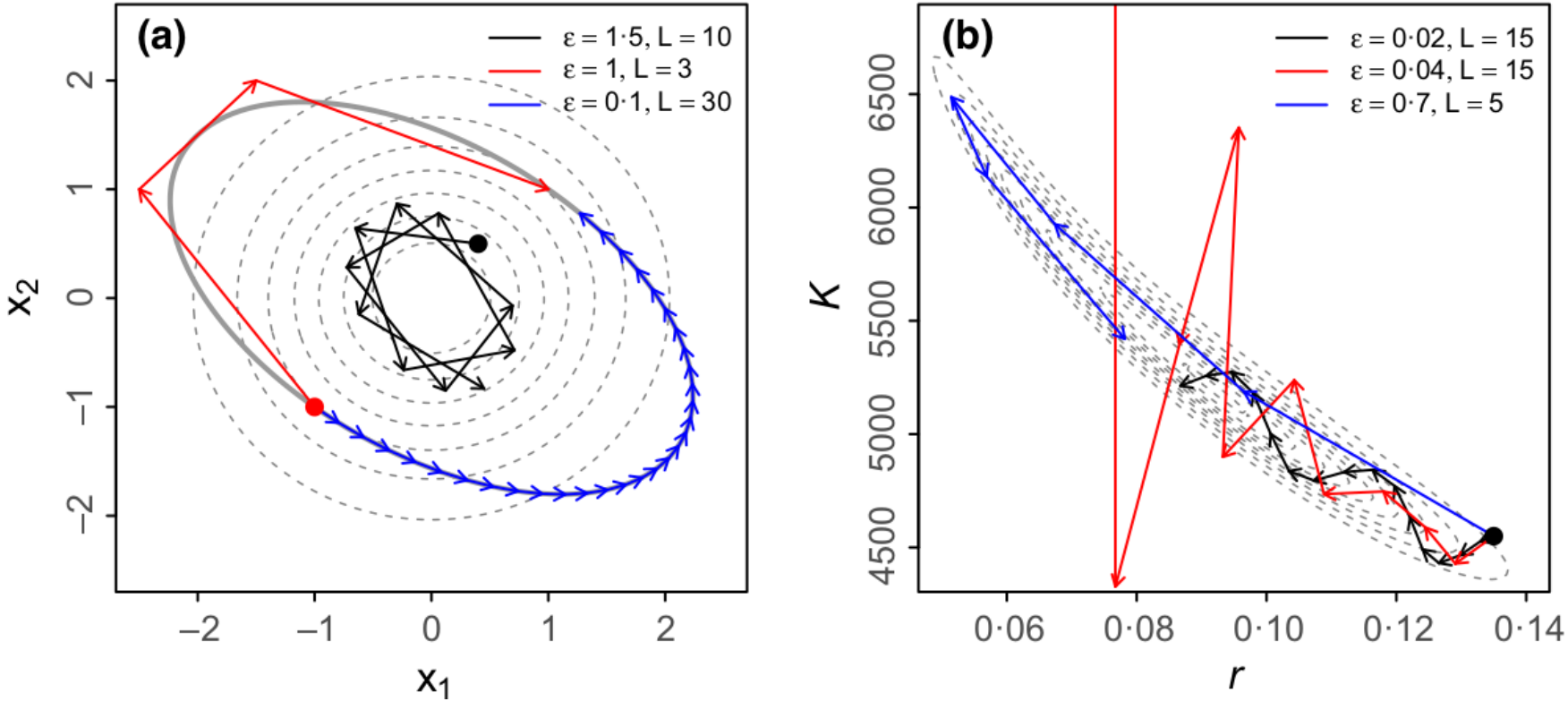
- Big step size → less log density and gradient evaluations, but lower acceptance rate and the simulation may diverge



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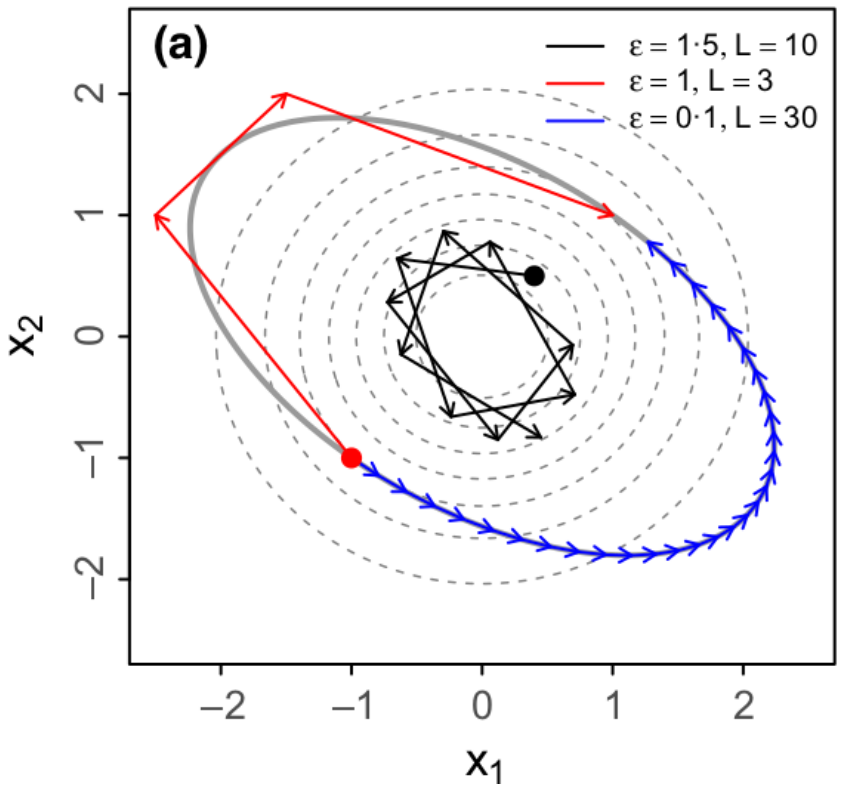
Leapfrog discretization, the number of steps

- 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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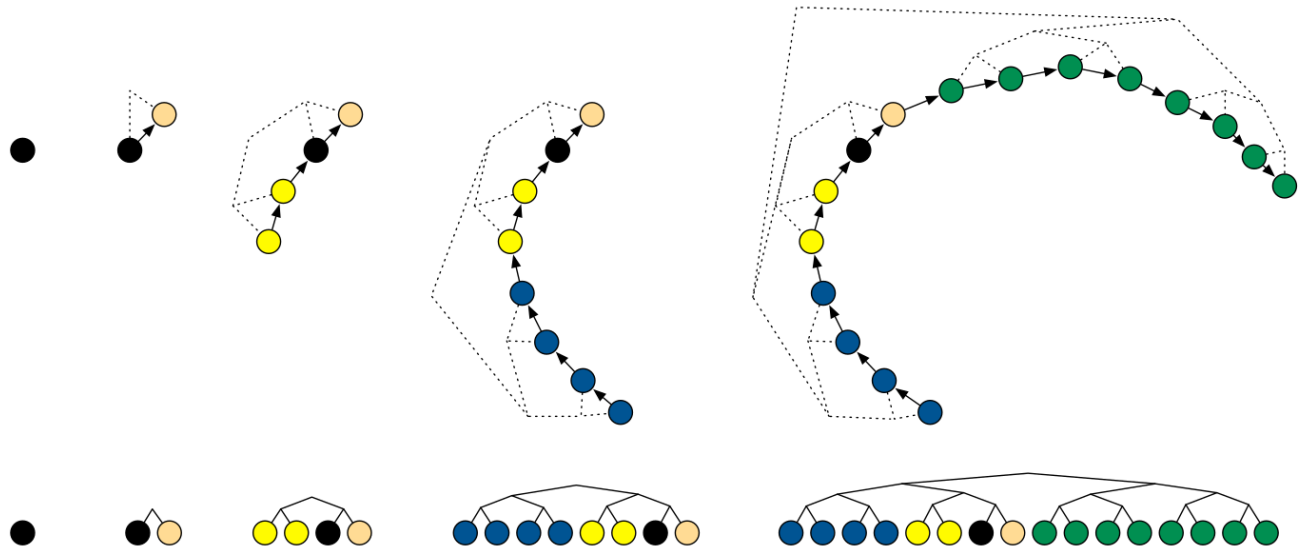

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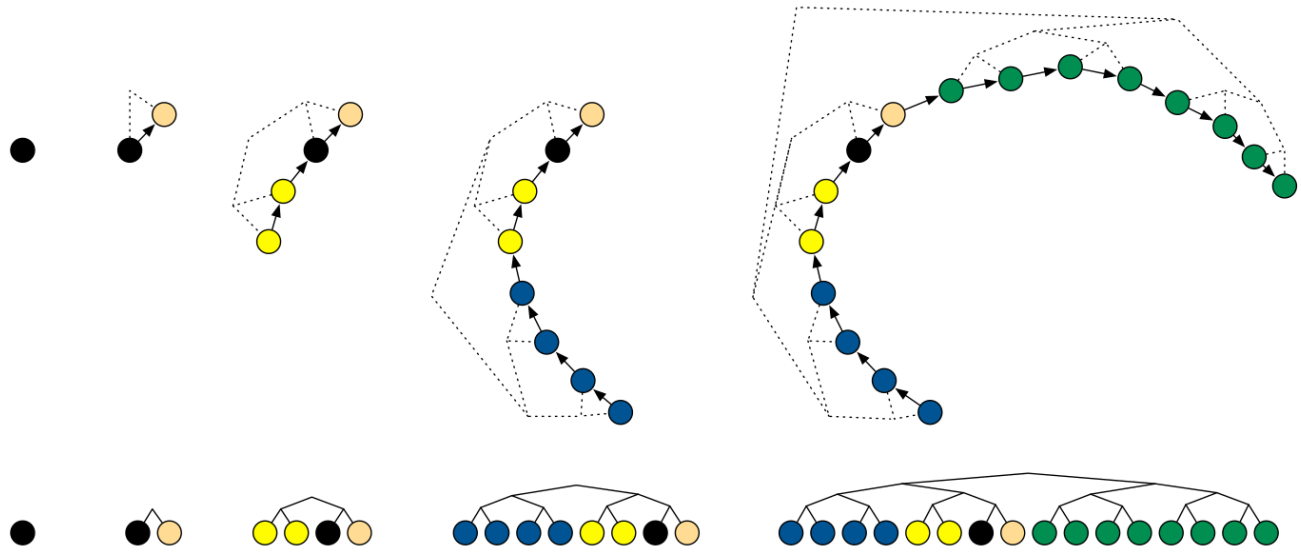

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- For further efficiency
  - simulation path parts further away from the starting point can have higher probability
  - max treedepth to keep computation in control

No-U-Turn sampler

- Adaptively selects number of steps
  - NUTS is a dynamic HMC algorithm, where dynamic refers to the dynamic trajectory length
  - simulate until a U-turn is detected
  - the number of simulation steps doubled if no U-turn yet
- To keep reversibility of Markov chain
  - need to simulate in two directions
  - choose a point along the simulation path with slice sampling
  - Metropolis acceptance step for the selected point
- For further efficiency
  - simulation path parts further away from the starting point can have higher probability
  - max treedepth to keep computation in control
- Demo https://chi-feng.github.io/mcmc-demo/

No-U-Turn sampler with multinomial sampling

- Original NUTS
  - choose a point along the simulation path with slice sampling
  - possibly with bigger weighting for further points
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Mass matrix and the step size adaptation

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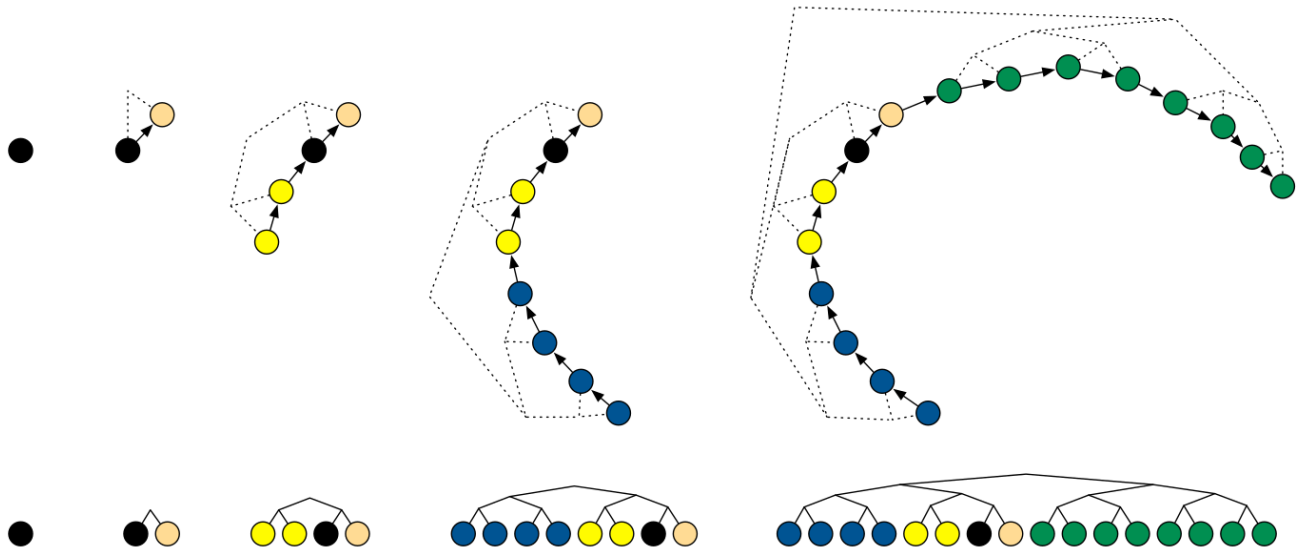
- After adaptation the algorithm parameters are fixed and some more iterations run to finish the warmup

Max tree depth diagnostic

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



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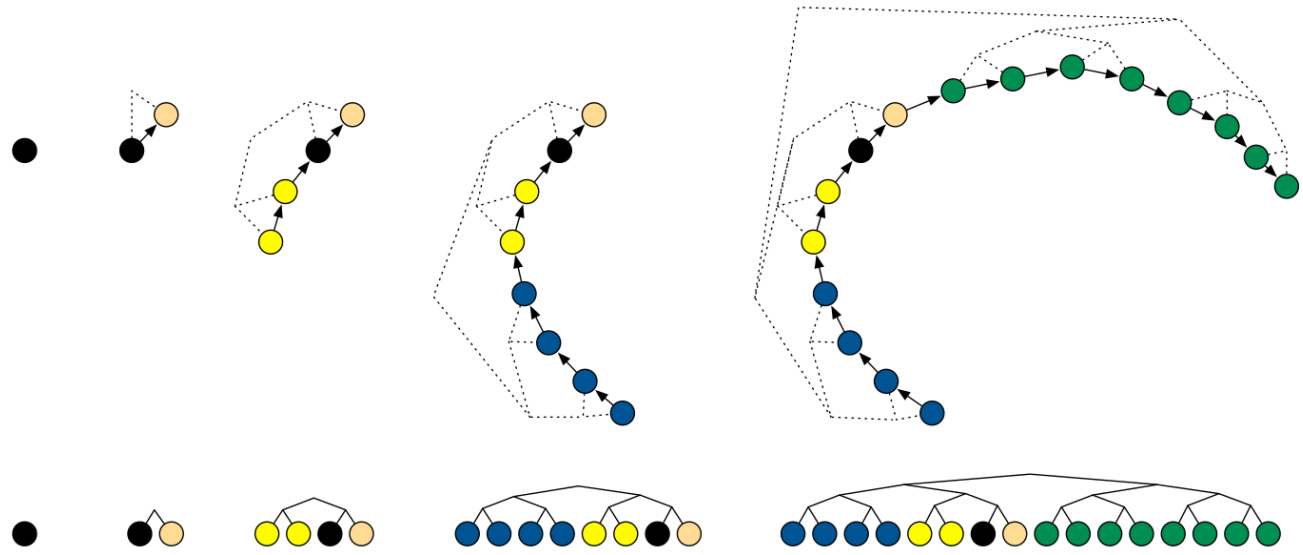

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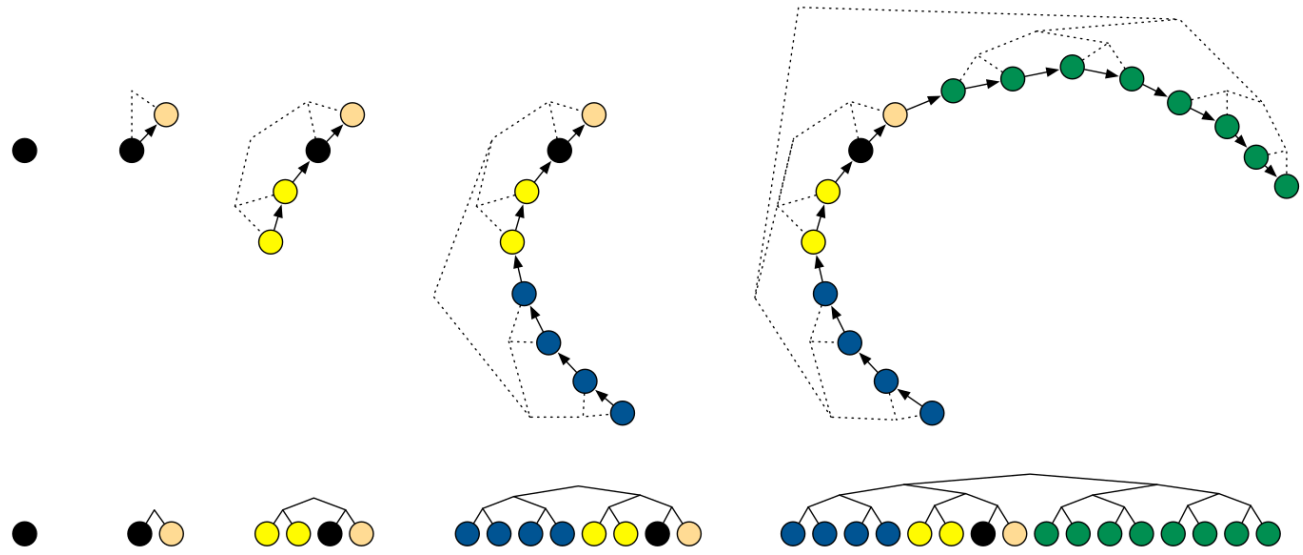

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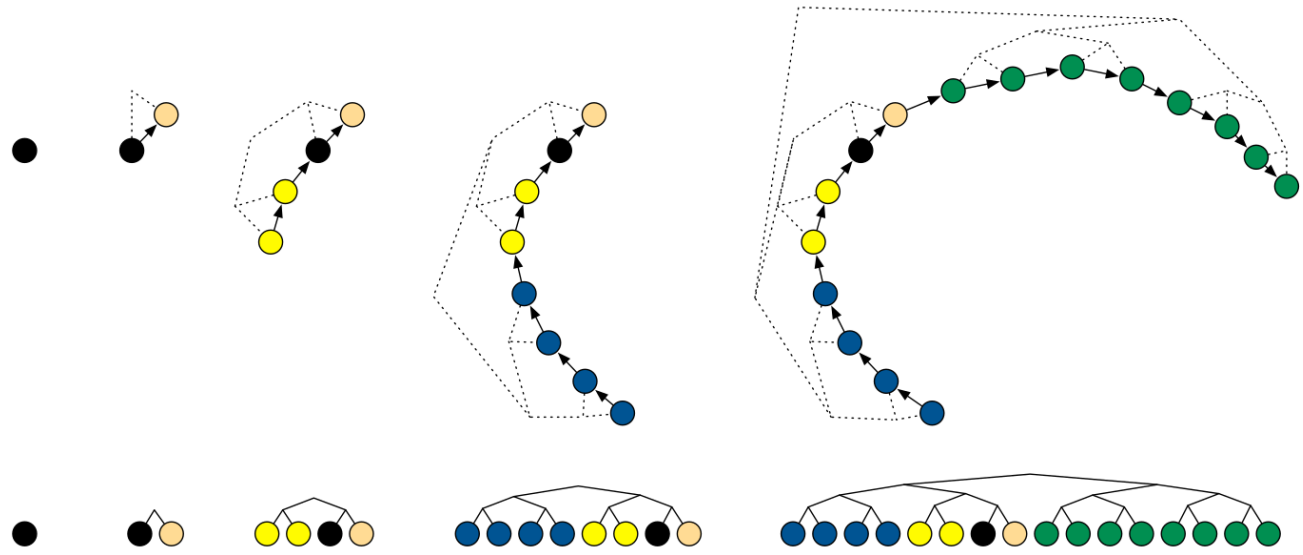

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Divergences

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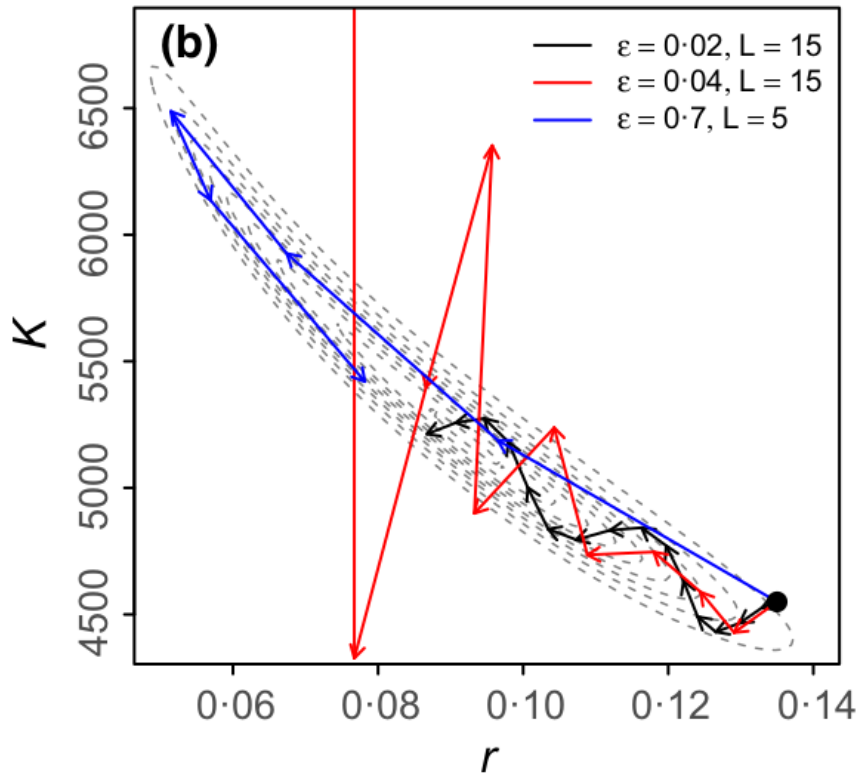

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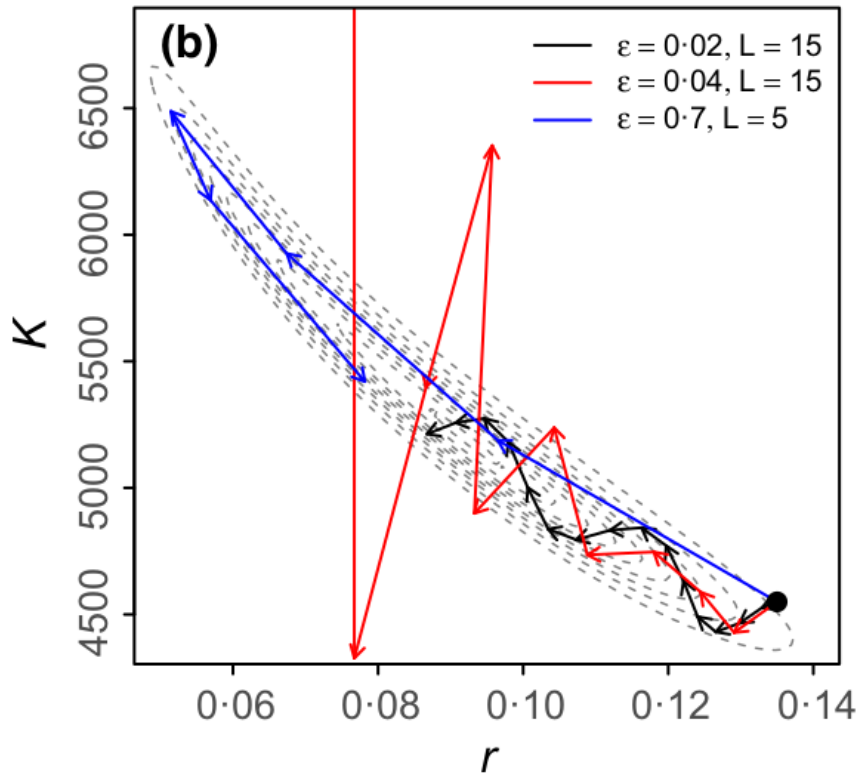

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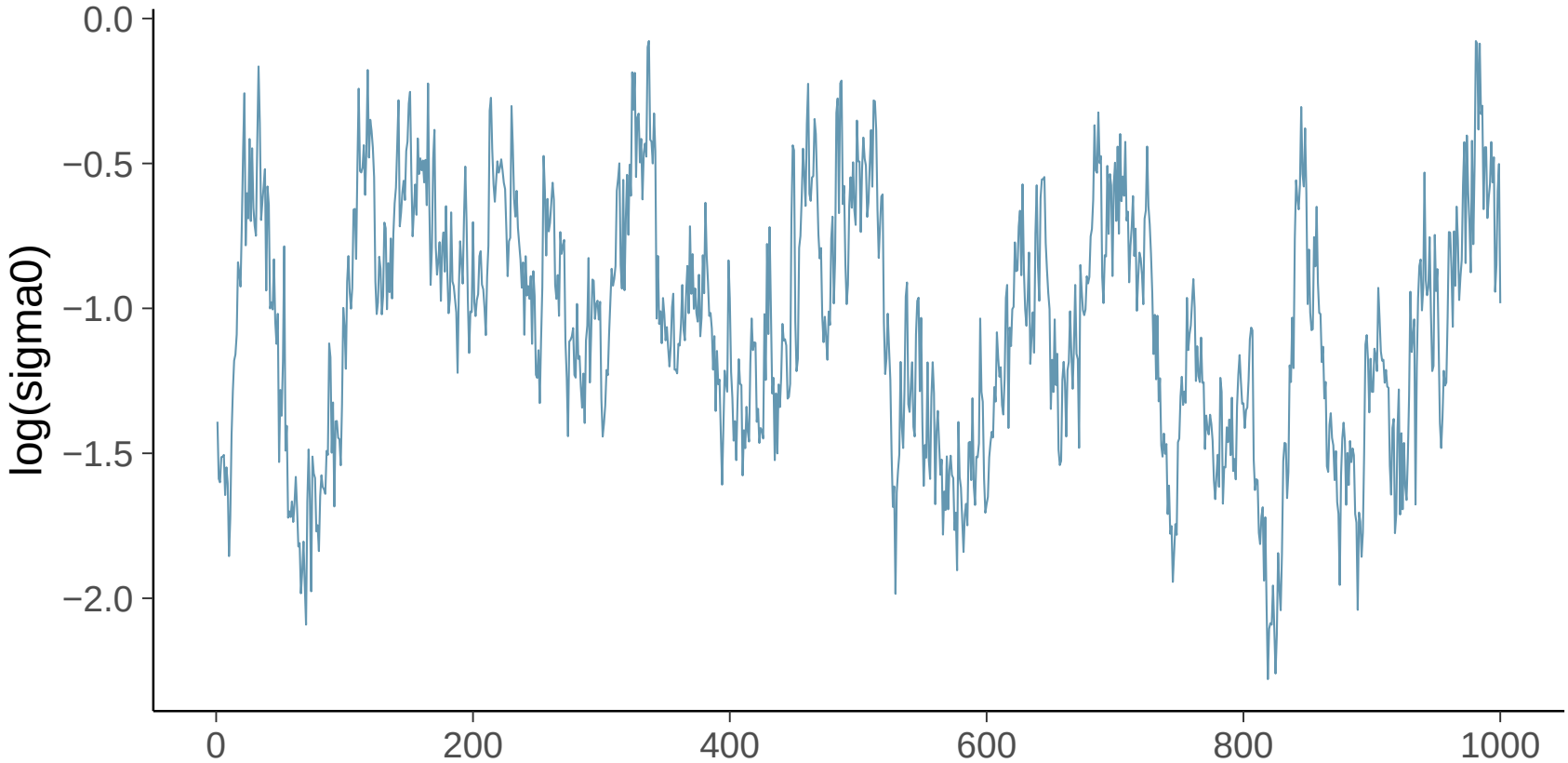

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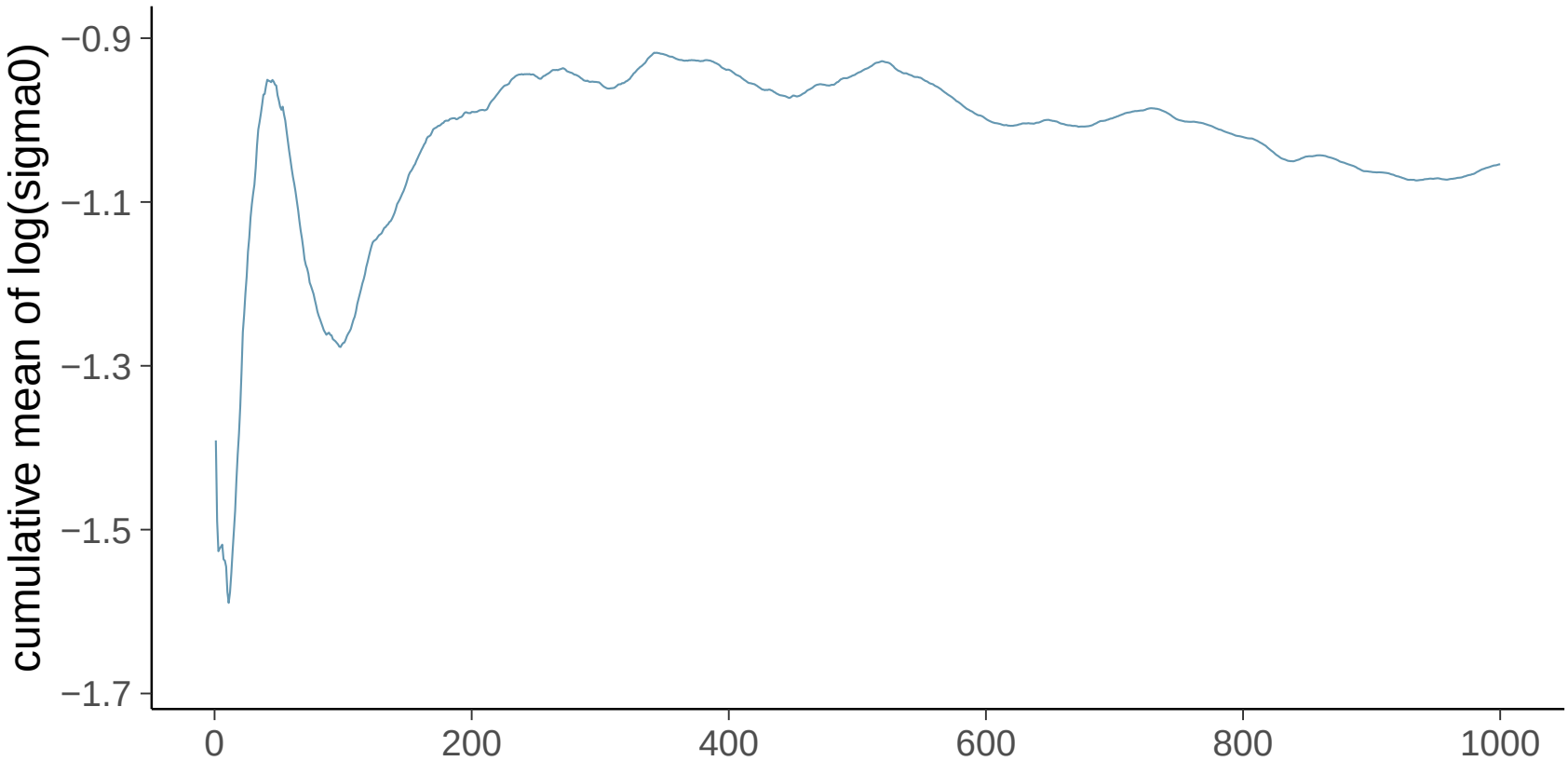

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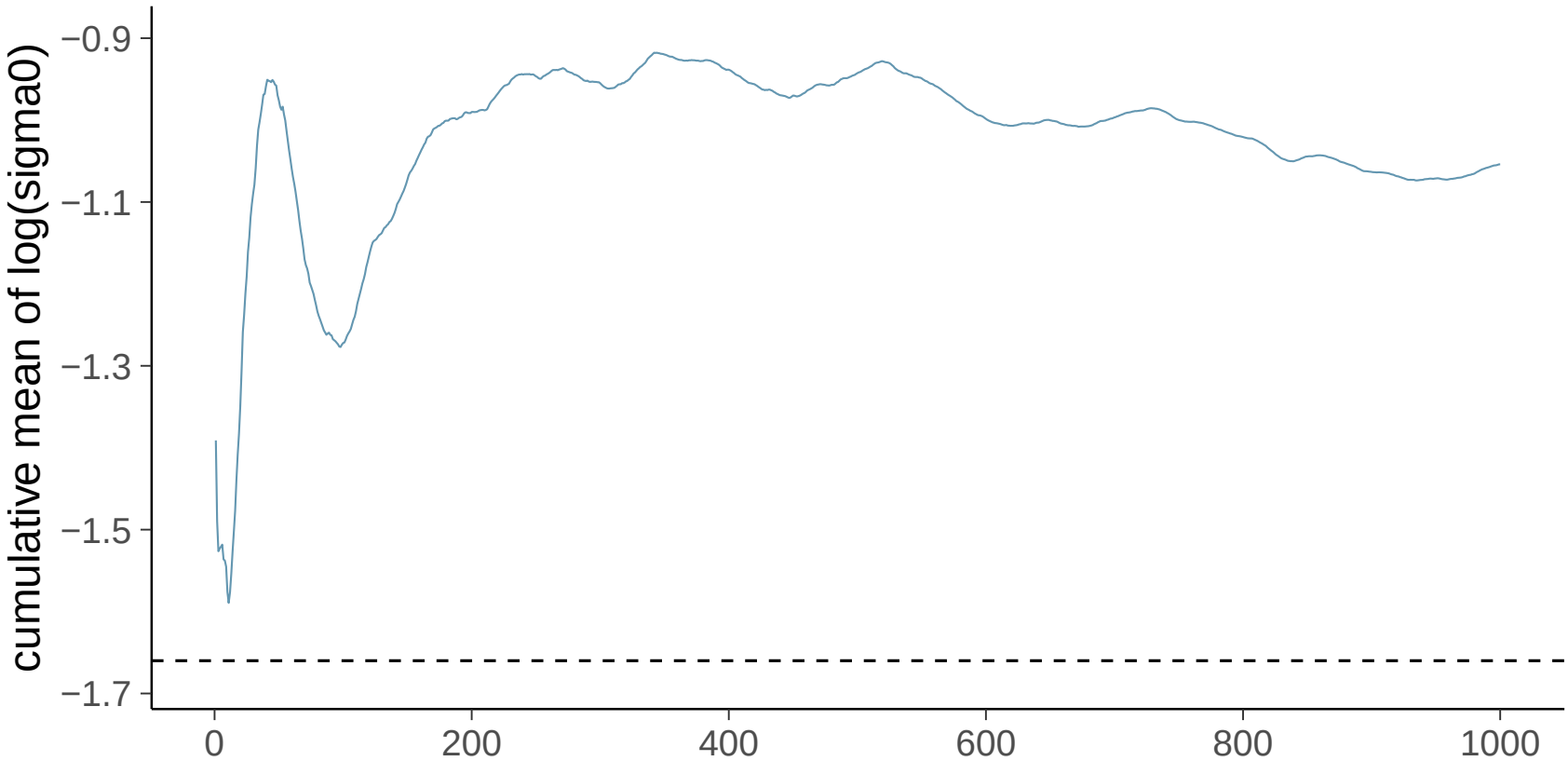

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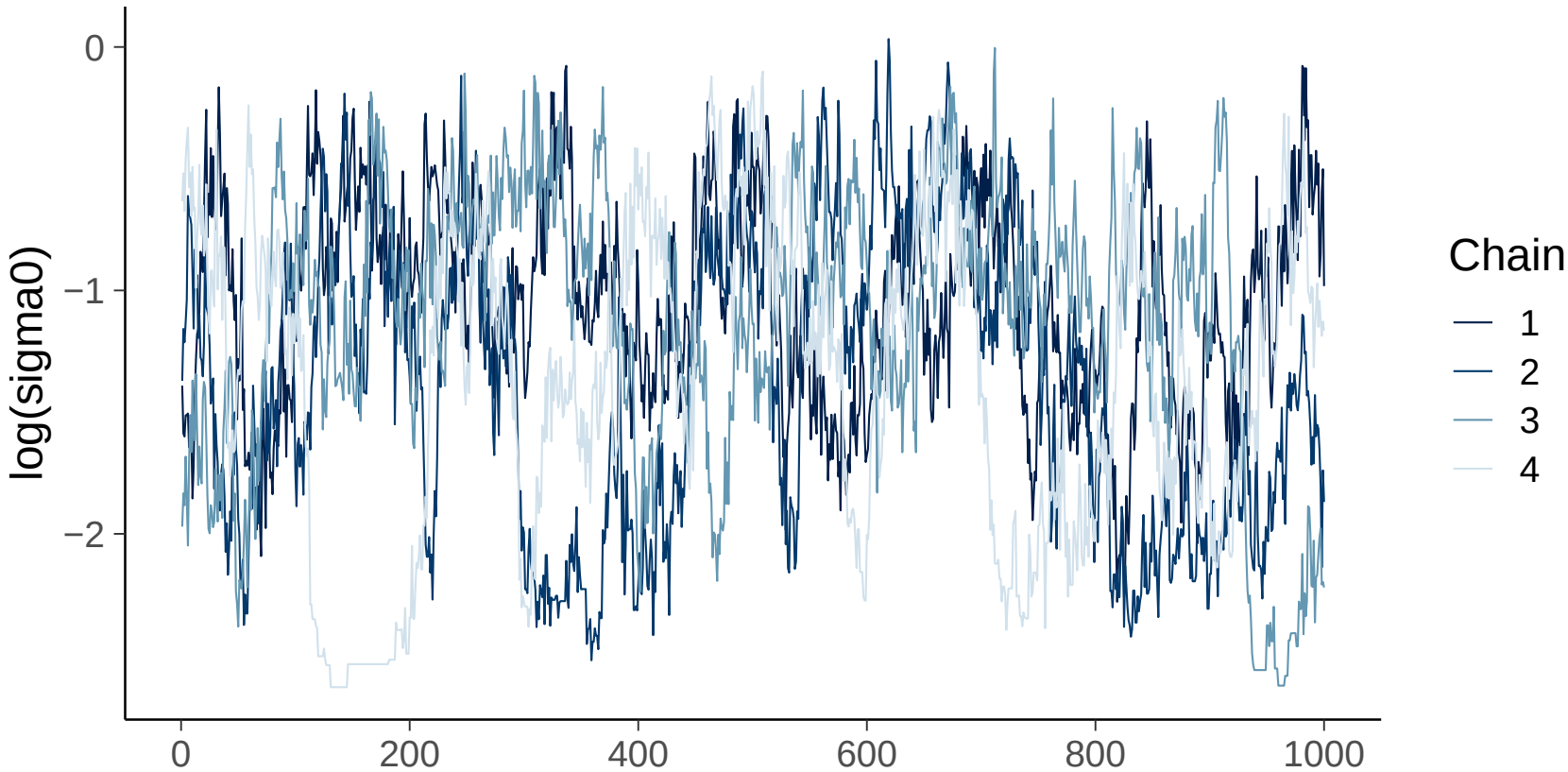

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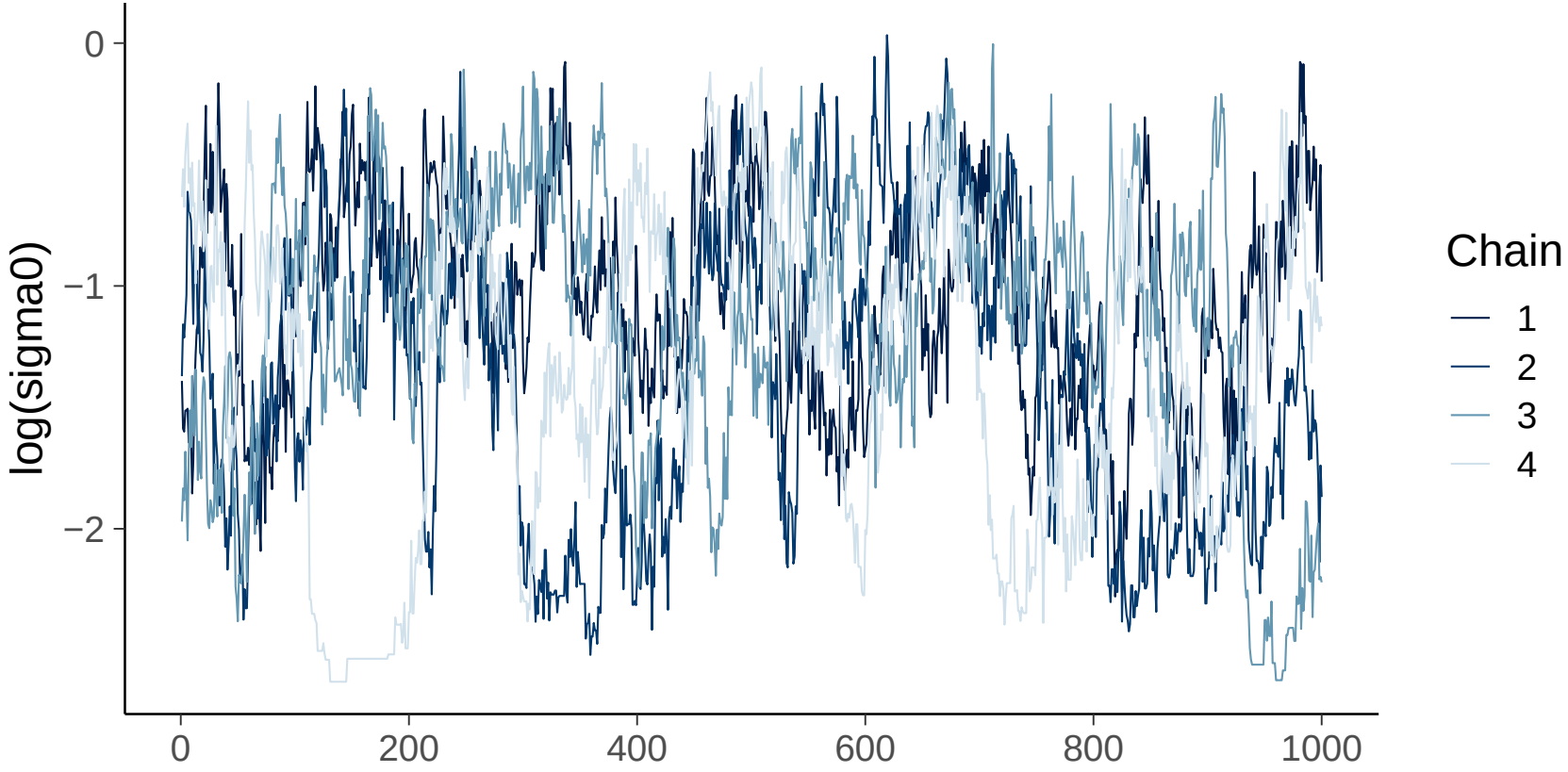

variable	mean	median	sd	mad	q5	q95	rhat	ess_bulk	ess_tail
lsigma0	-1.0	-1.0	0.10	0.070	-1.2	-0.93	1.2	7.2	19.

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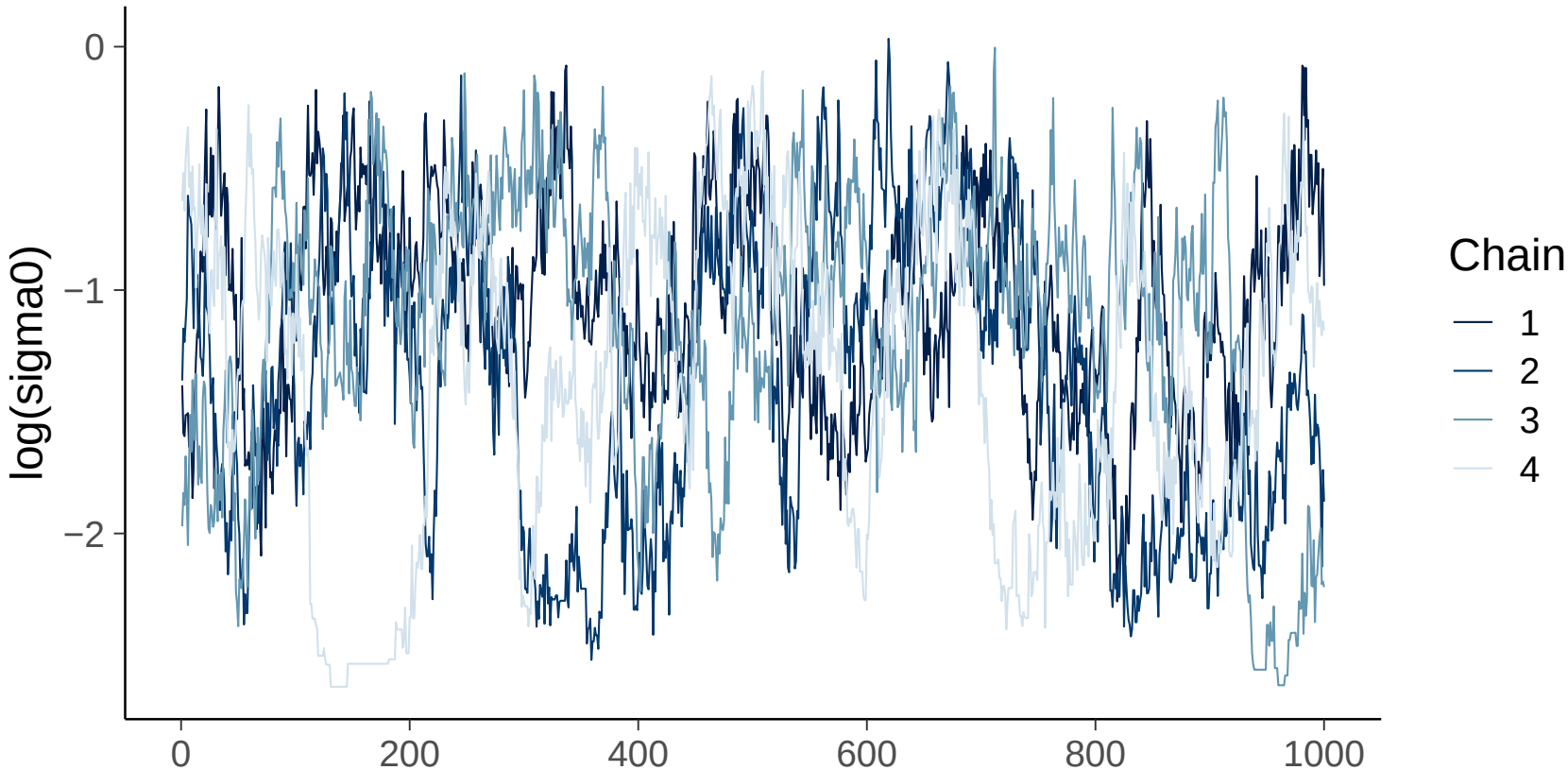


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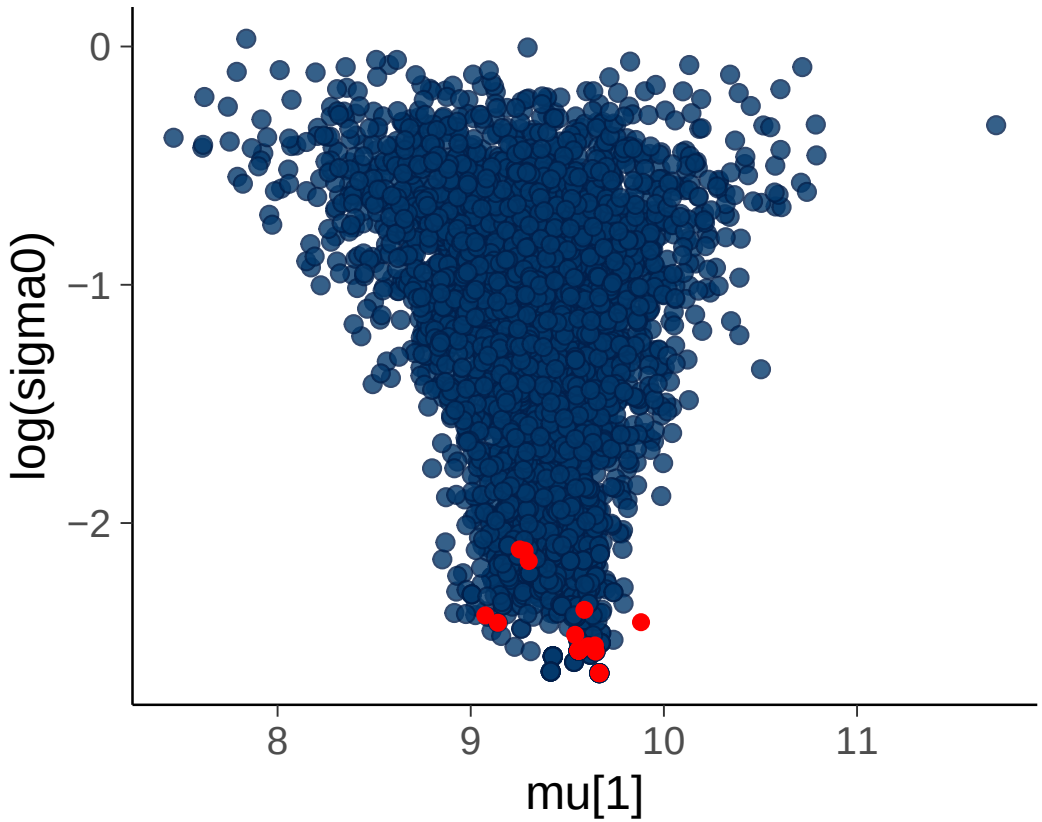


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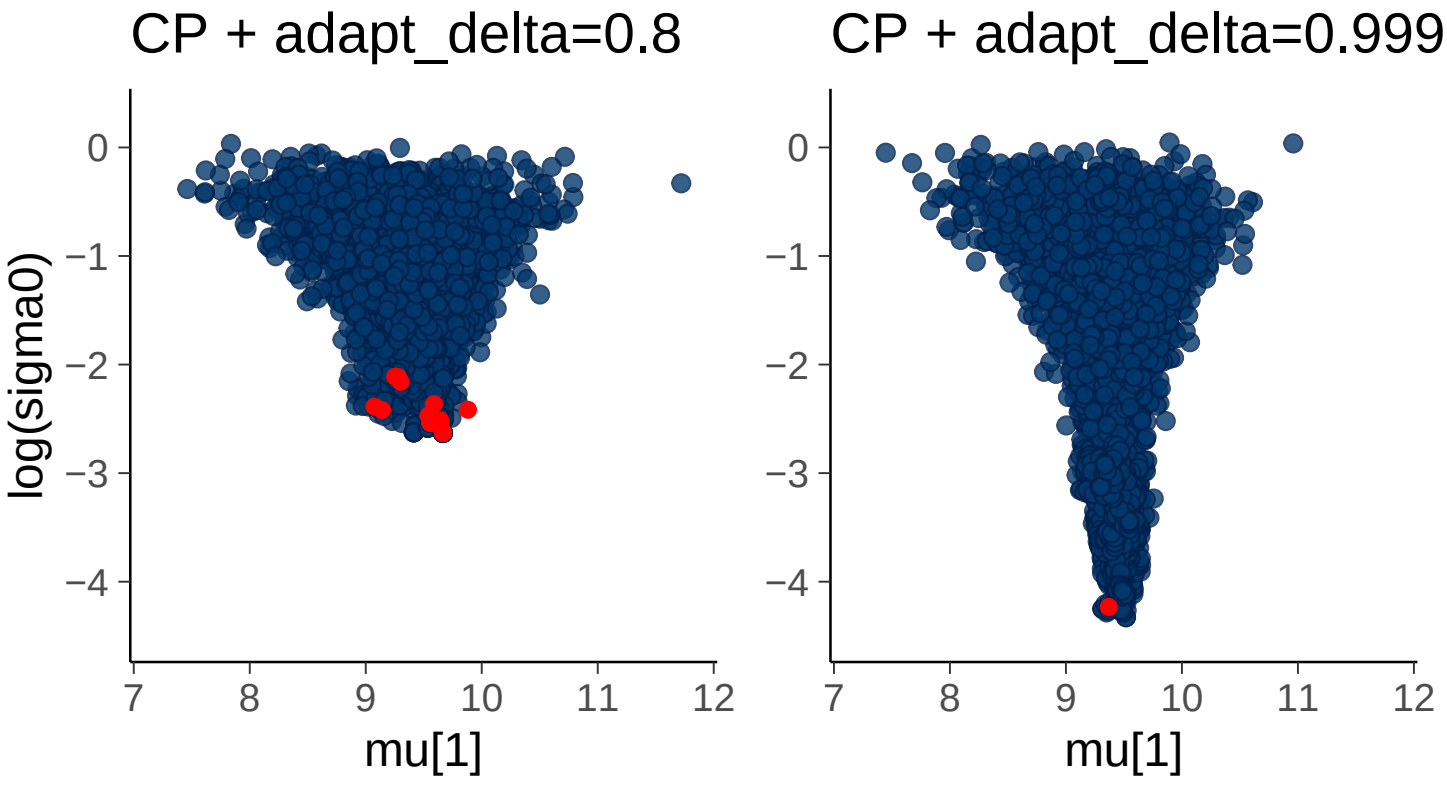

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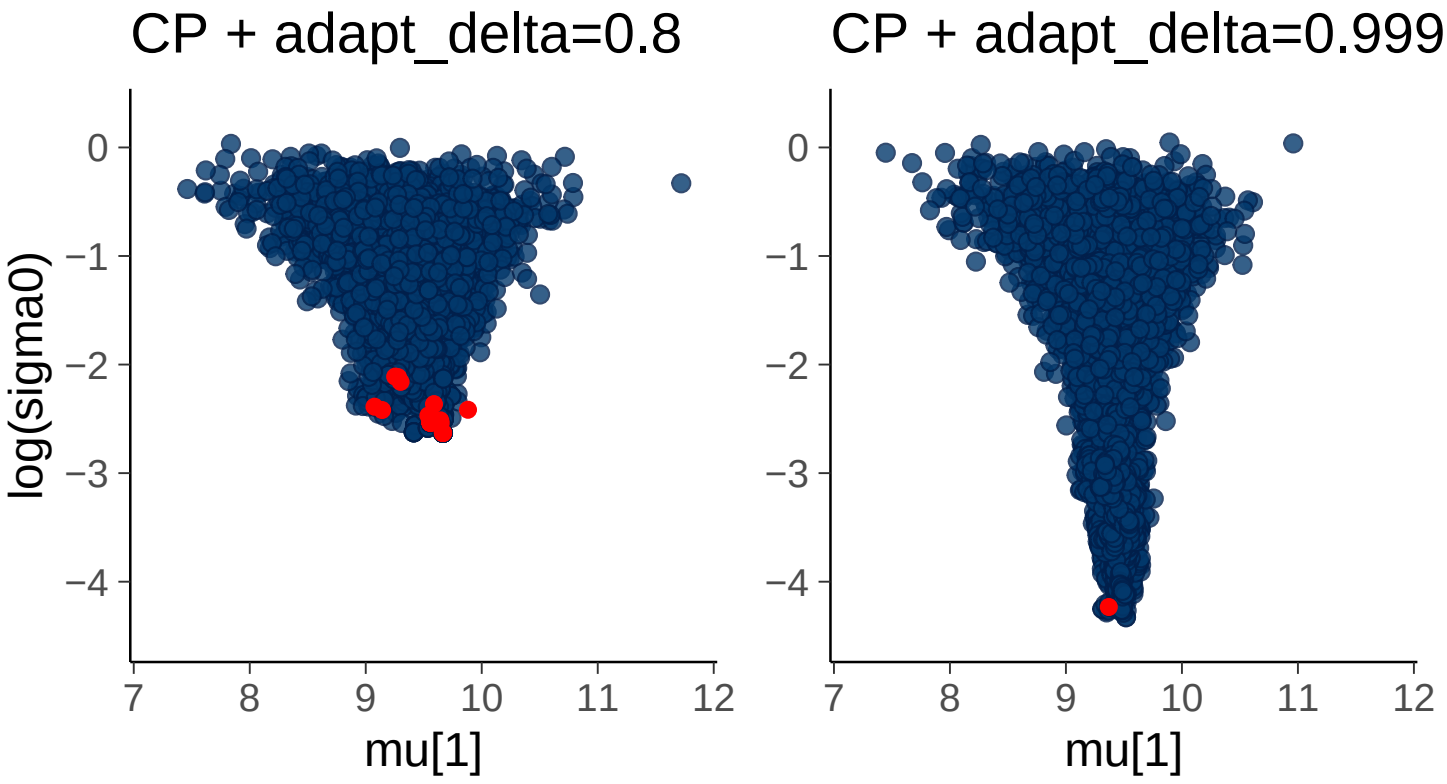

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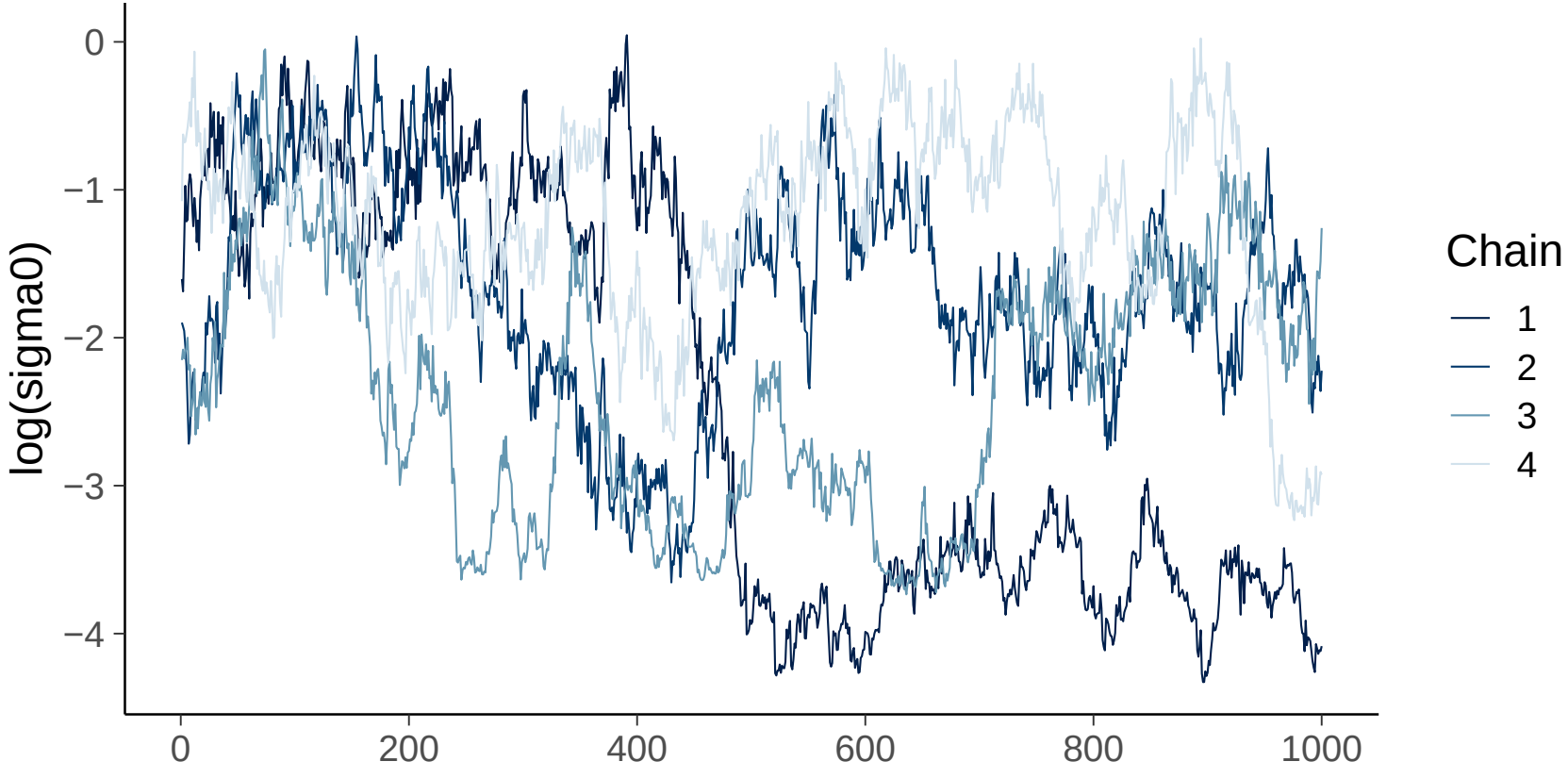

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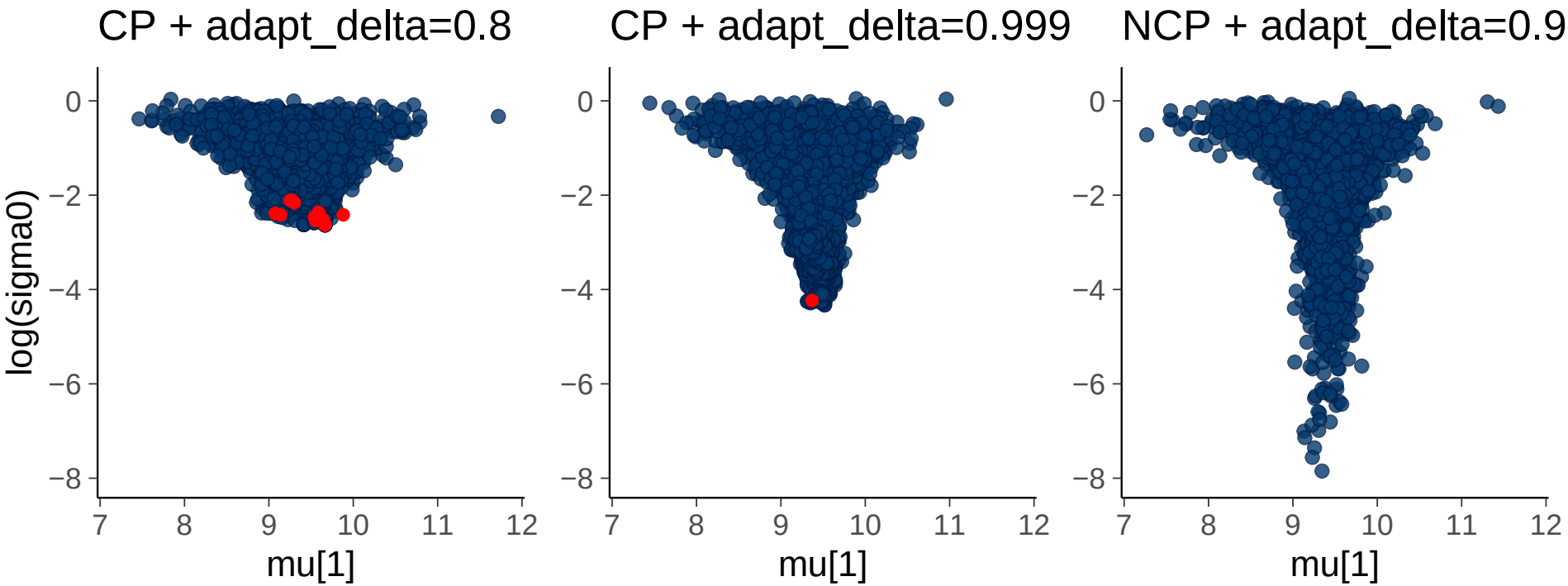

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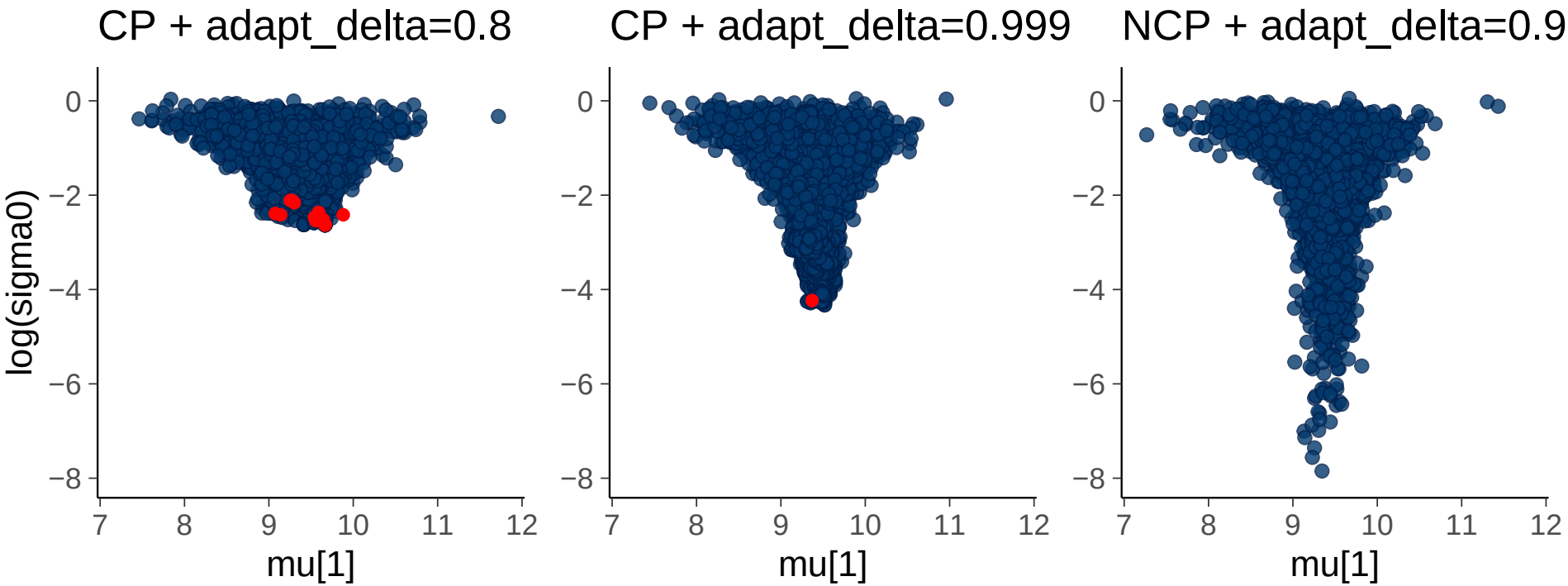

With NCP parameterization

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

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- 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.

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- Language, inference engine, user interfaces, documentation, case studies, diagnostics, packages, ...
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- 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
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model {
  theta ~ beta(1, 1);       // prior
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  - 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

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model {
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- for Stan sampler there is no difference between prior and likelihood, all that matters is the final `target`

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- 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 (transplies) 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

CmdStanR is an R interface for Stan

```
# Load CmdStanR
library(cmdstanr)
options(mc.cores = 1)

# Compile Stan model
mod_bin <- cmdstan_model(stan_file = 'binom.stan')

# Sample from the posterior given the model and data
d_bin <- list(N = 10, y = 7)
fit_bin <- mod_bin$sample(data = d_bin)

# Show summary and access draws
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# Compile Stan model
mod_bin <- cmdstan_model(stan_file = 'binom.stan')

# Sample from the posterior given the model and data
d_bin <- list(N = 10, y = 7)
fit_bin <- mod_bin$sample(data = d_bin)

# Show summary and access draws
fit_bin$summary()
draws <- fit_bin$draws(format = "df")
```

CmdStanR

CmdStanR is an R interface for Stan

```
# Load CmdStanR
library(cmdstanr)
options(mc.cores = 1)

# Compile Stan model
mod_bin <- cmdstan_model(stan_file = 'binom.stan')

# Sample from the posterior given the model and data
d_bin <- list(N = 10, y = 7)
fit_bin <- mod_bin$sample(data = d_bin)

# Show summary and access draws
fit_bin$summary()
draws <- fit_bin$draws(format = "df")
```

Stan

- Compilation (unless previously compiled model available)
- Pick random initial values for MCMC chains
- Run warm-up iterations including adaptation of mass matrix and step-size
- Sampling
- Generated quantities
- Save posterior draws
- Report divergences, ESS, $\widehat{R}$

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);
  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);
  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);
  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

```
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))
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.
```

- `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",
                                            "treedepth"))
```

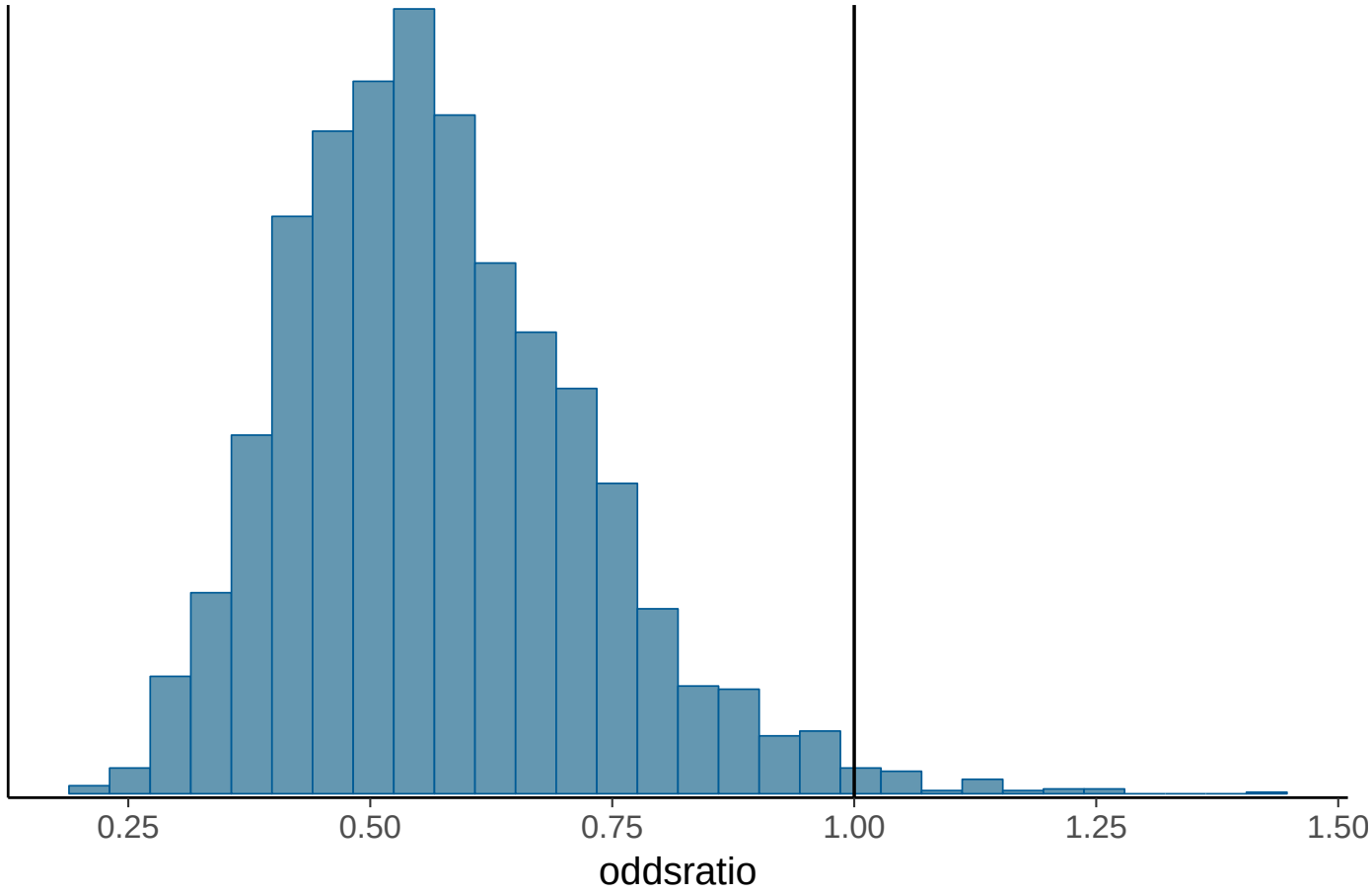
```
$num_divergent
[1] 0 0 0 0

$num_max_treedepth
[1] 0 0 0 0
```

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

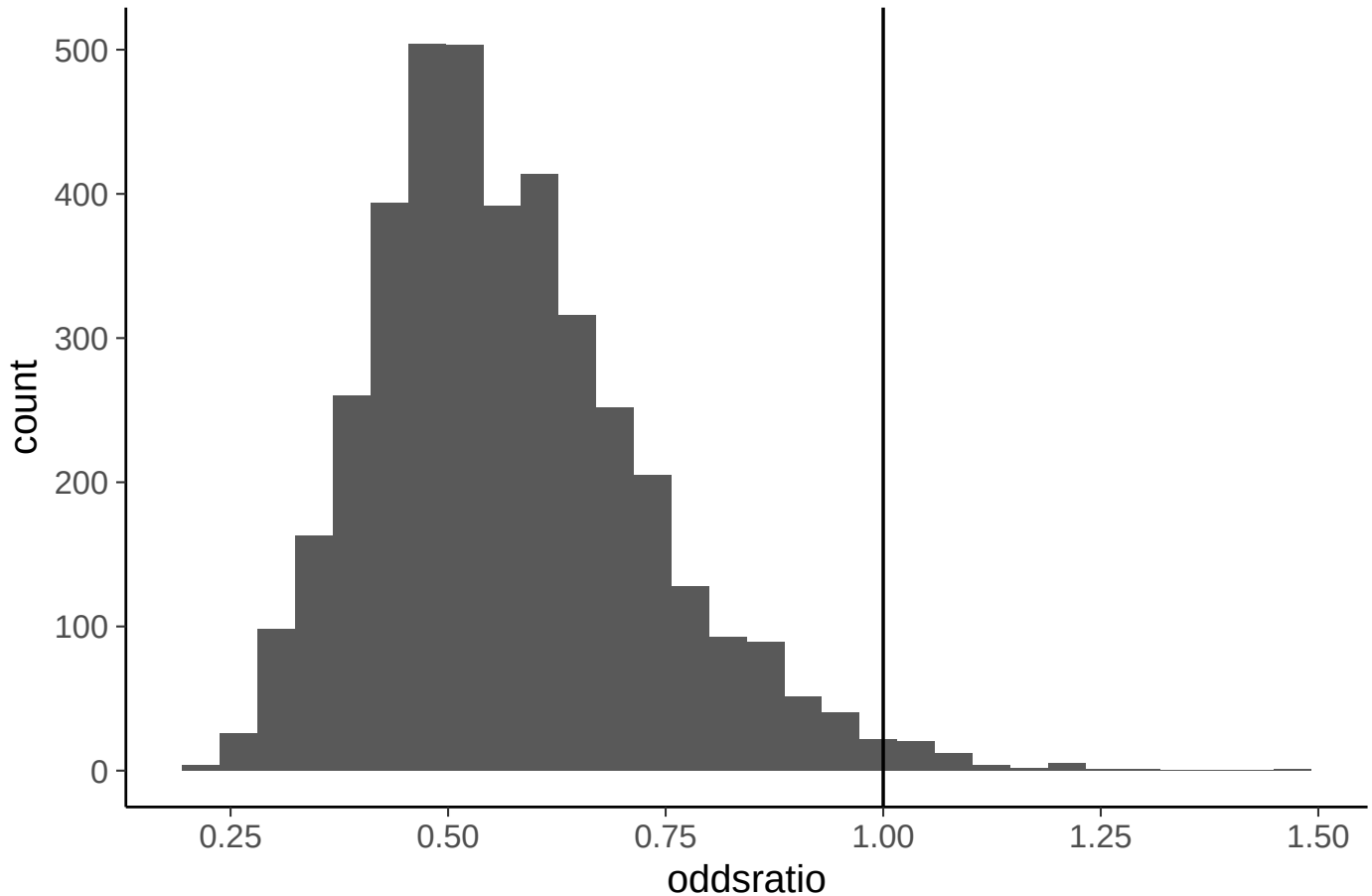
Difference between proportions (bayesplot)

```
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)))
```



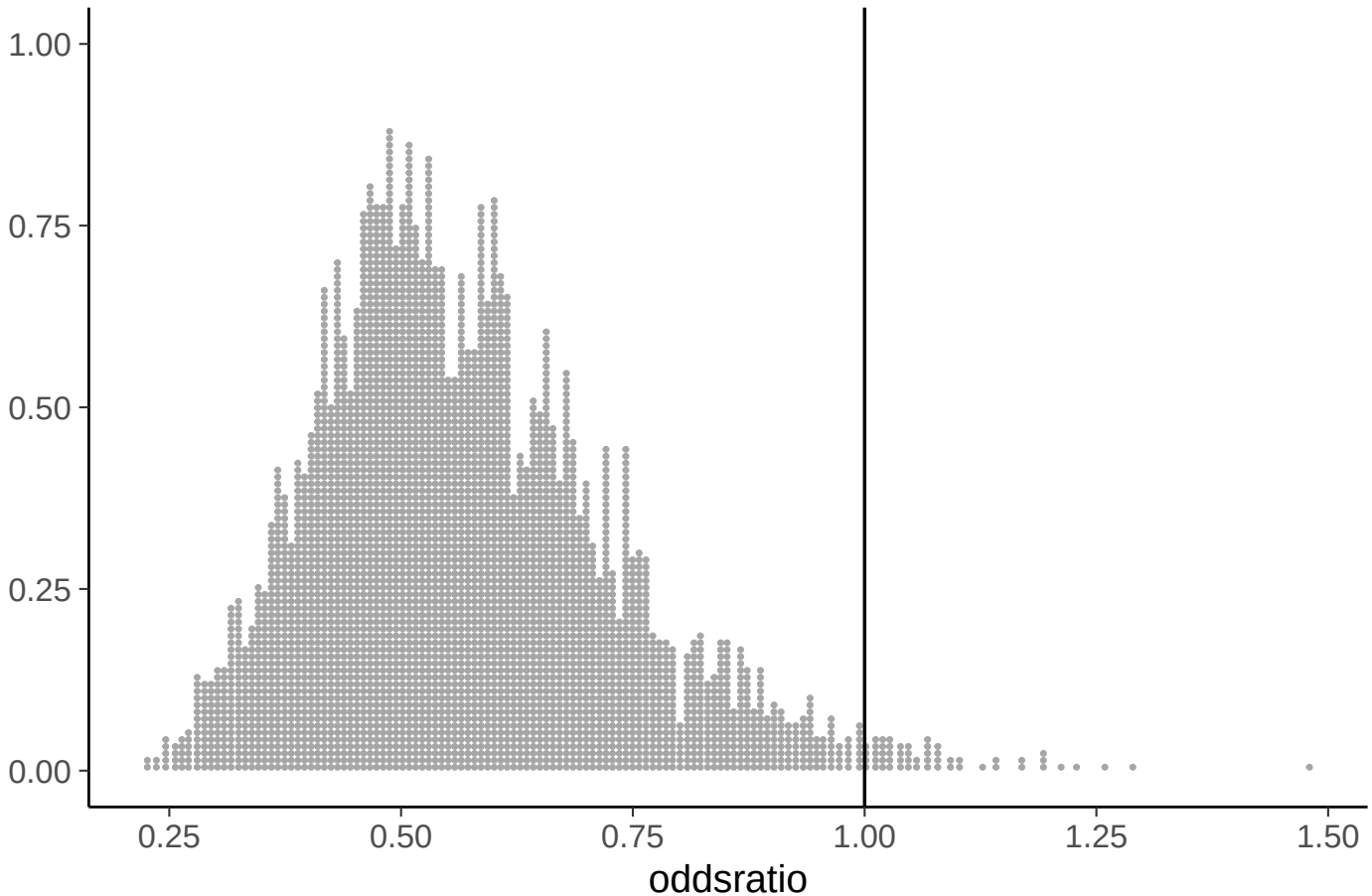
Difference between proportions (ggplot2)

```
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 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

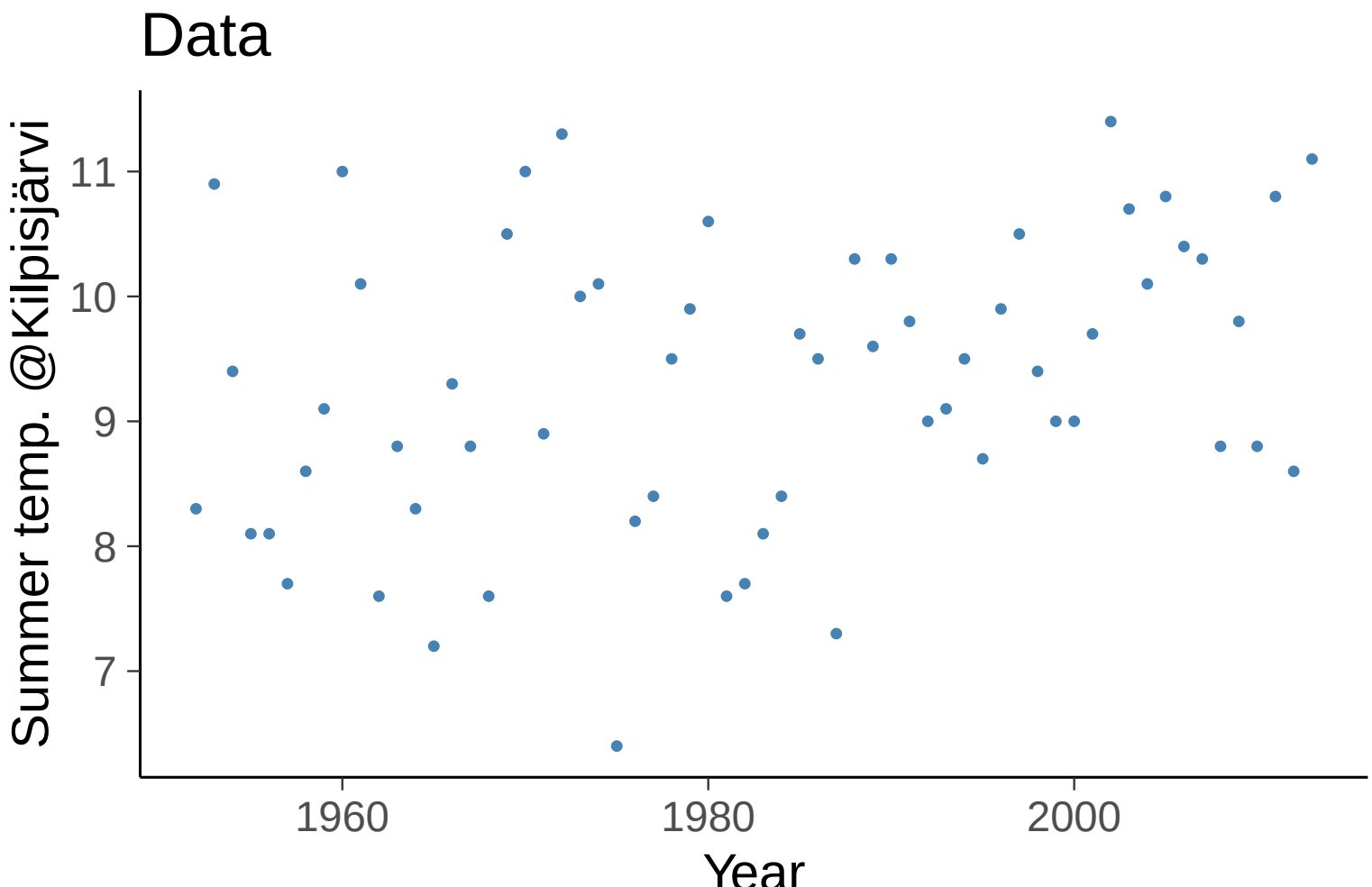
$oddsratio: rvar<1000,4>[1] mean ± sd:
[1] 0.57 ± 0.16

> 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

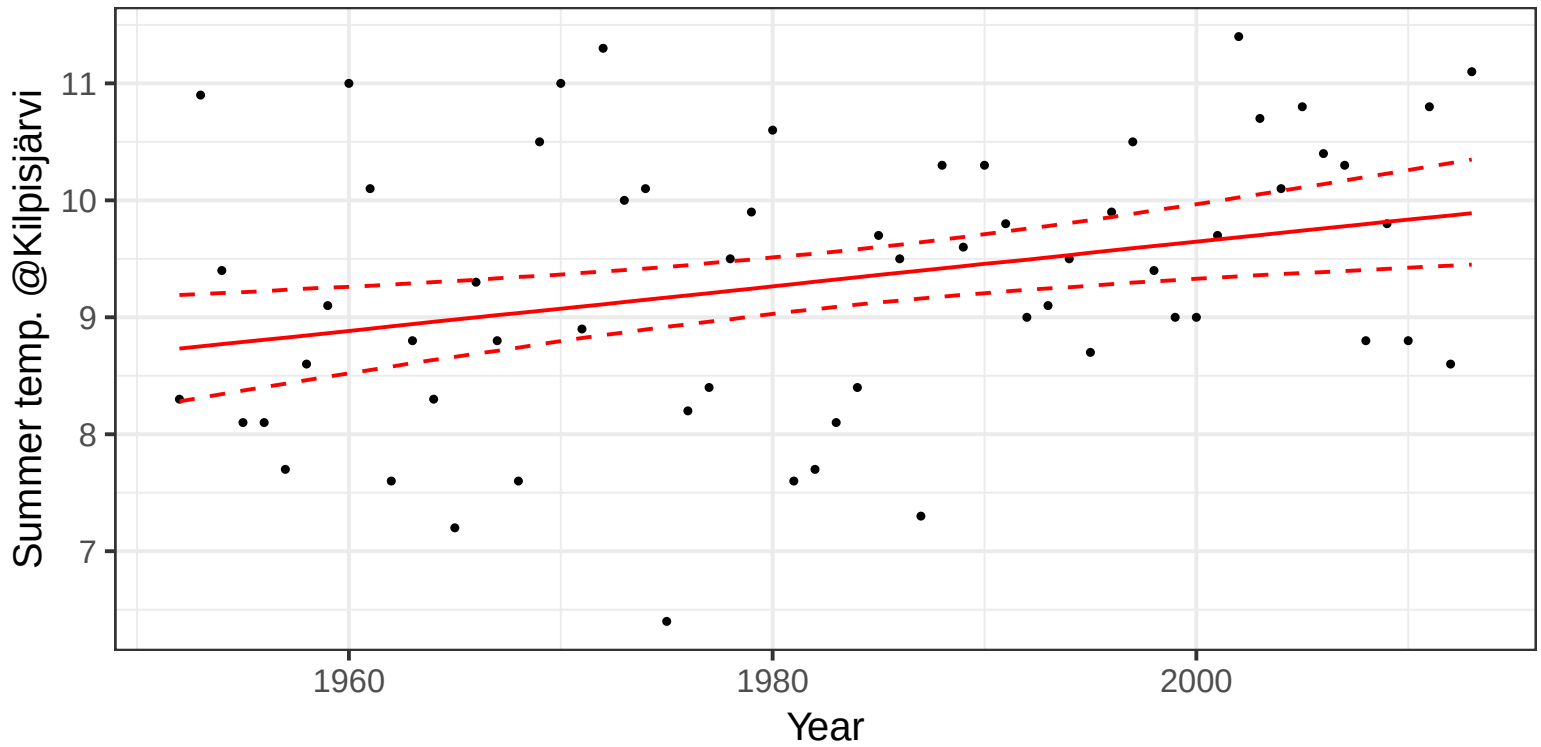
```
data {
    int<lower=0> N; // number of observations
    vector[N] x; //
    vector[N] y; //
    real pmualpha; // prior mean for alpha
    real psalpha;  // prior std for alpha
    real pmubeta;  // prior mean for beta
    real psbeta;   // prior std for beta
}
...
transformed parameters {
    vector[N] 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?

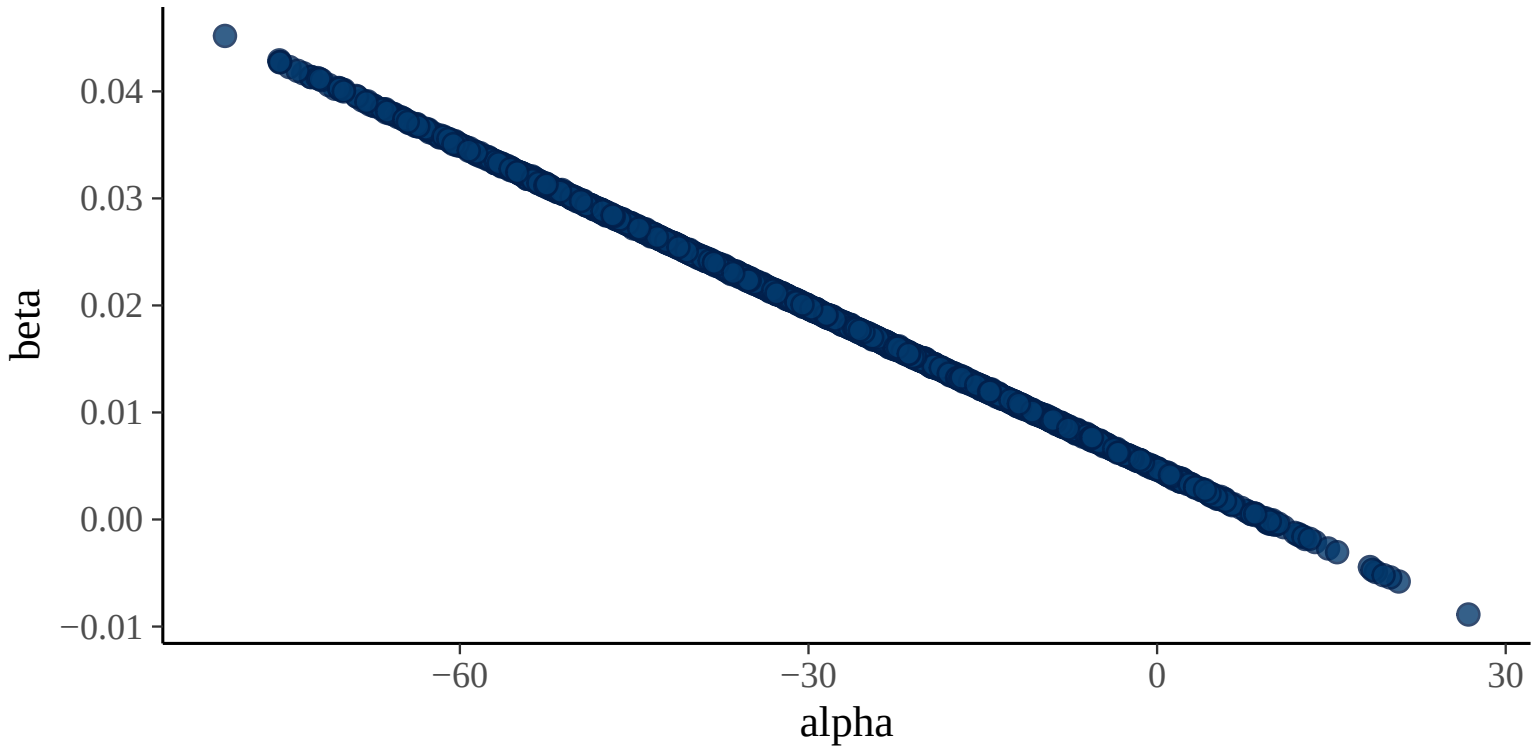
Kilpisjärvi summer temperature

Posterior fit



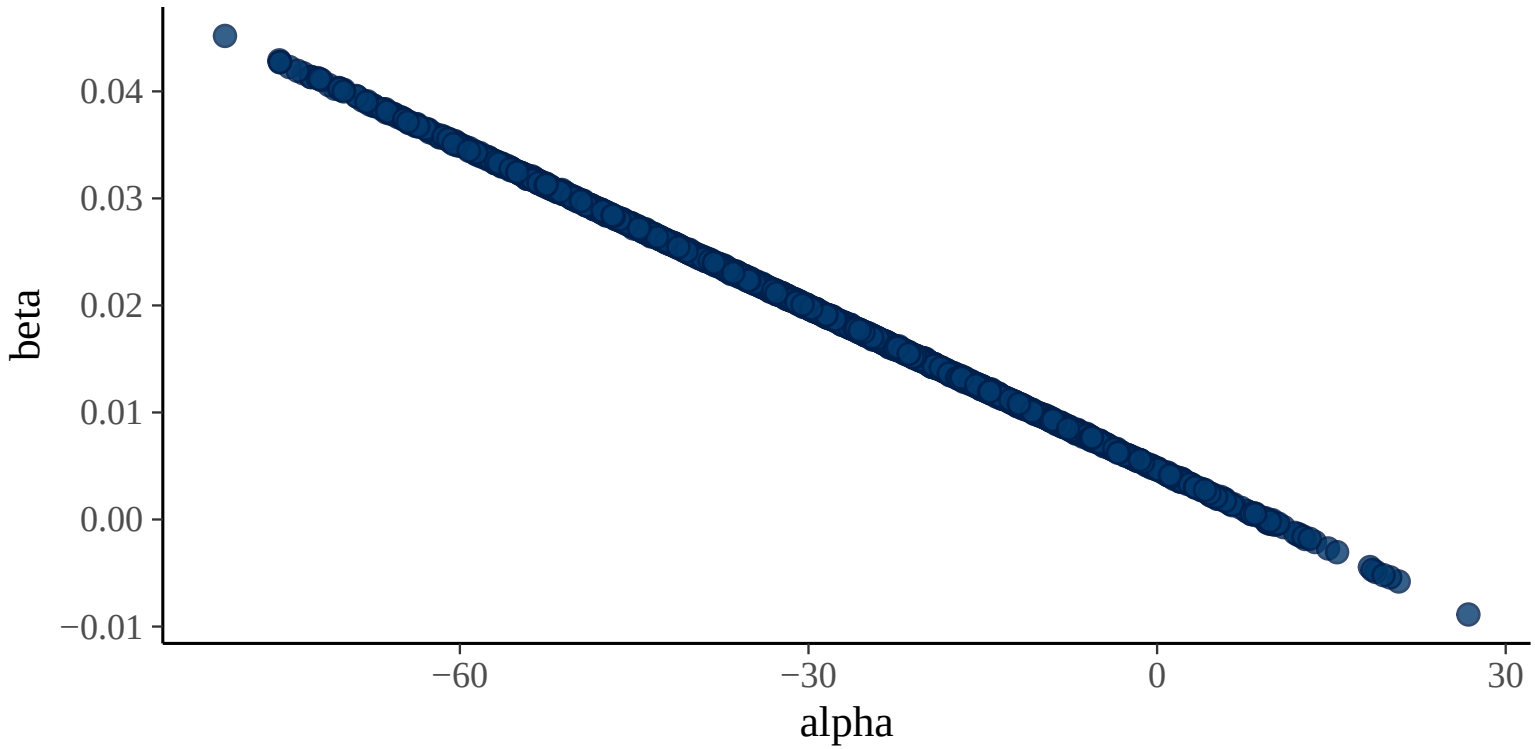
Kilpisjärvi summer temperature

Posterior draws of alpha and beta



Kilpisjärvi summer temperature

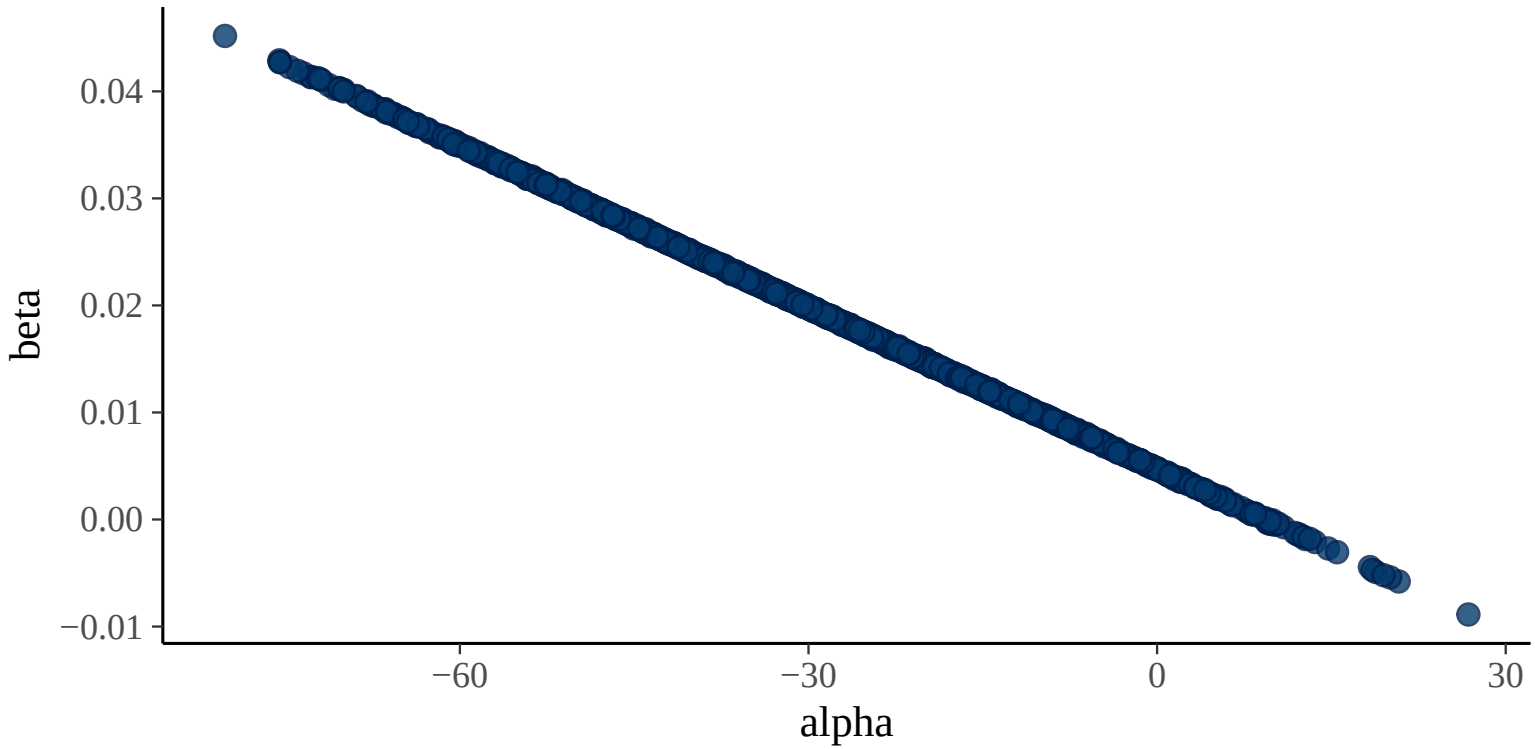
Posterior draws of alpha and beta




```
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

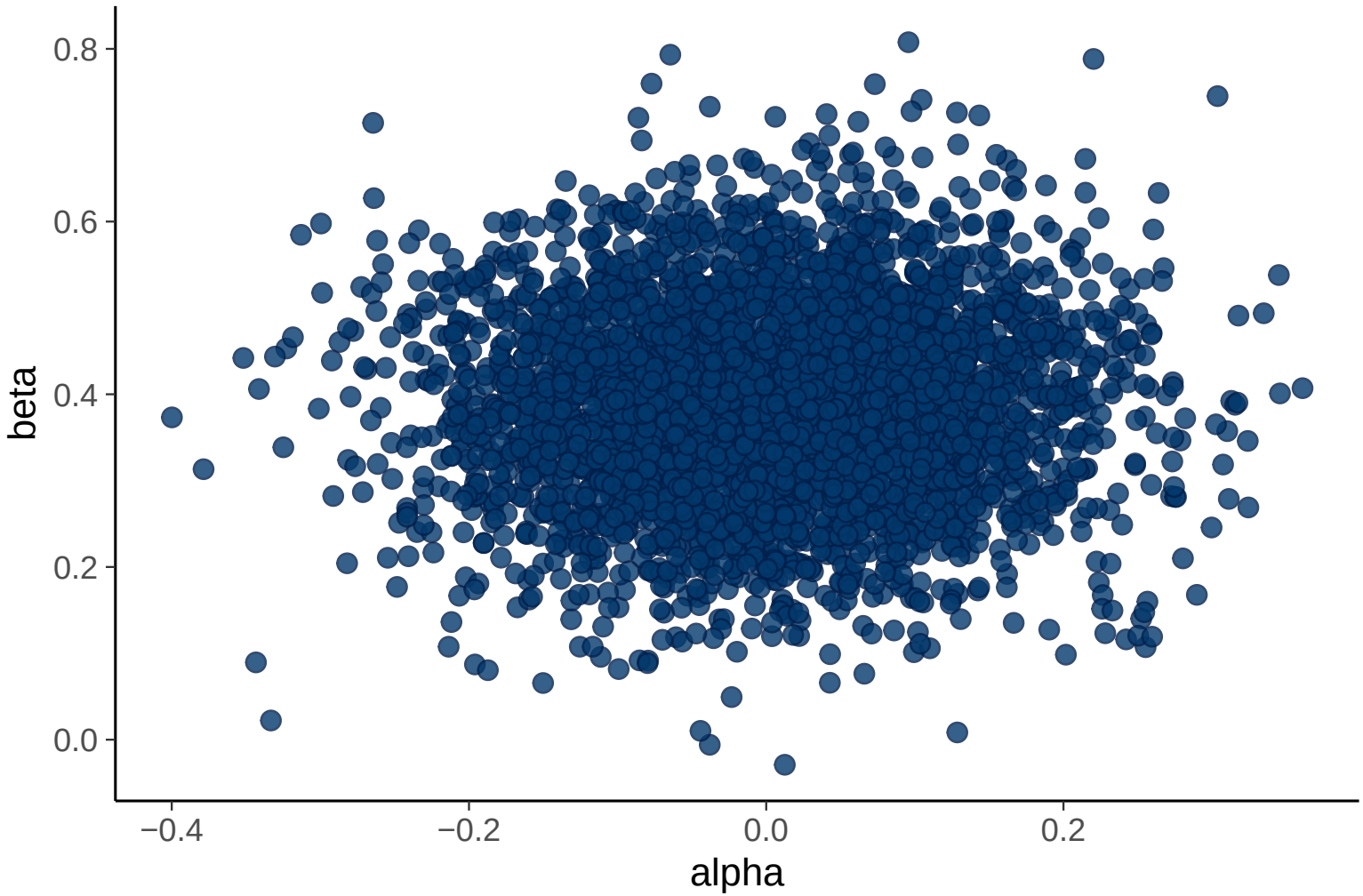
Center the data inside the model code

```
data {
  int<lower=0> N; // number of observations
  vector[N] x;
  vector[N] y;
  real xpred;     // covarite 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,
                     weights = N,
                     family = binomial(),
                     data = d_bin2)
```

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,
                     weights = N,
                     family = binomial(),
                     data = d_bin2)
```

Normal linear model

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

brms

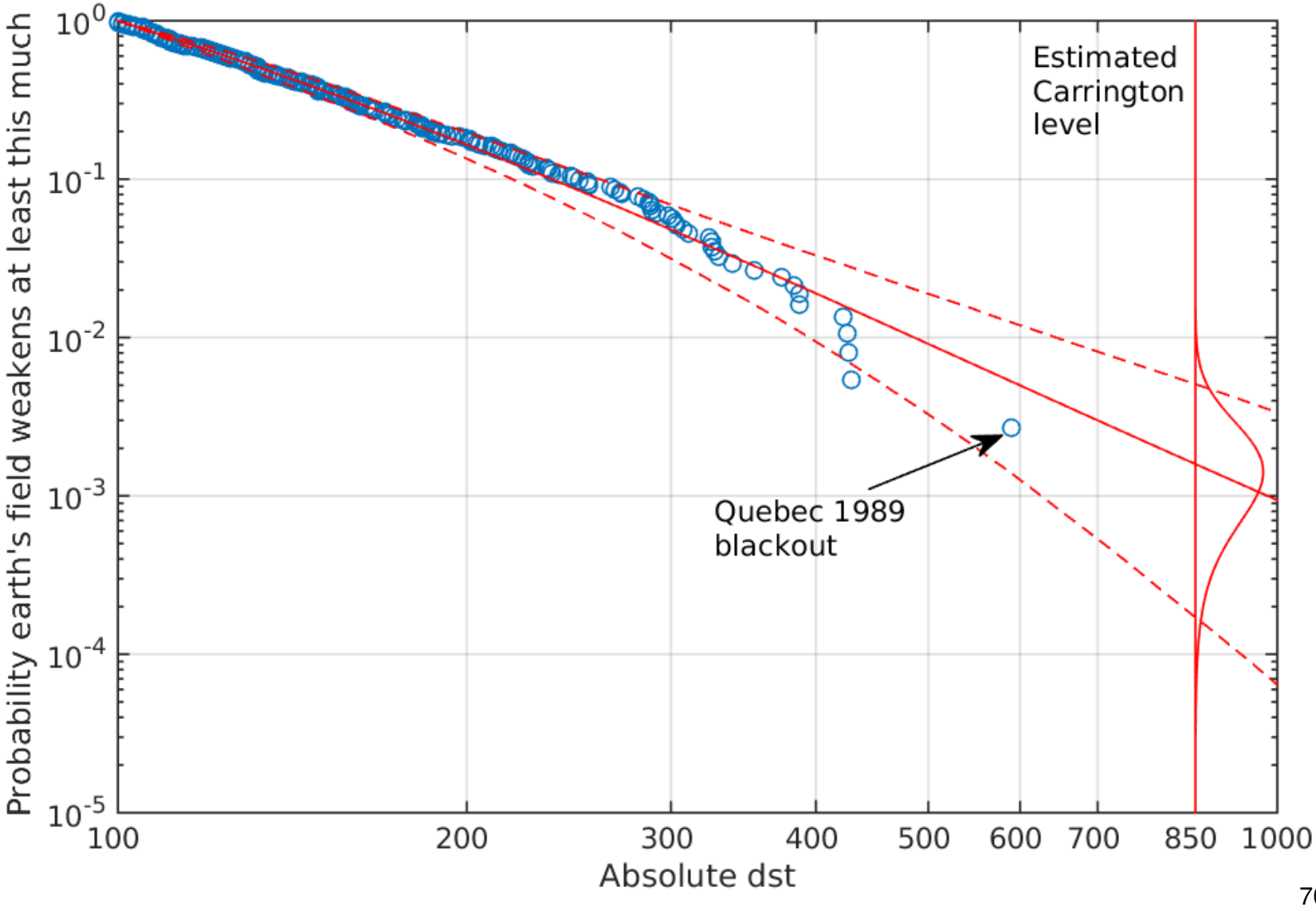
- `brms` provides simplified model description
  - \+ a larger set of models than `RStanARM`, but still restricted
  - \- need to wait for the compilation

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

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

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)
  - `marginaleffects` — 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