# 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 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=ZRpo41I02KQ&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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- 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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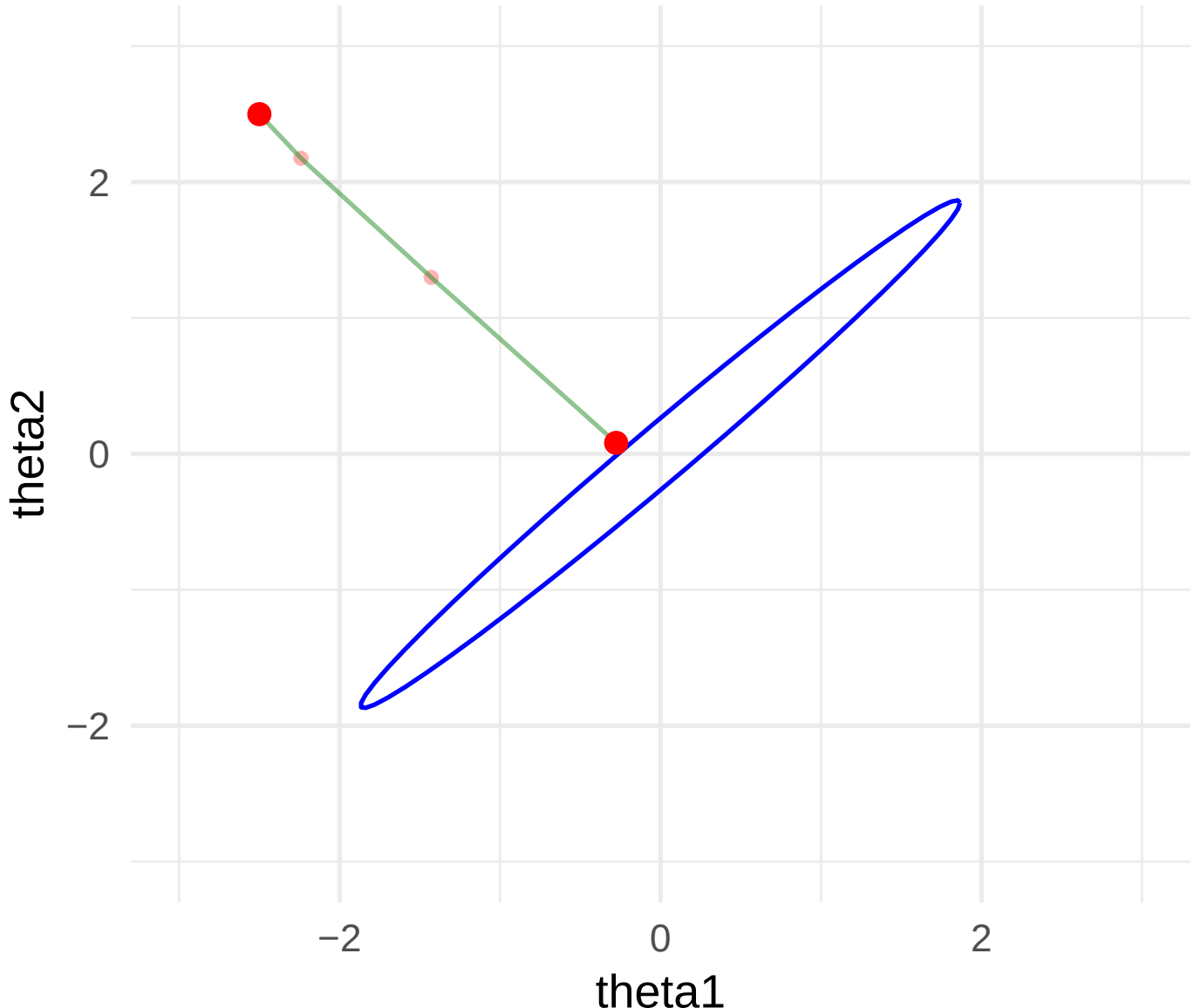

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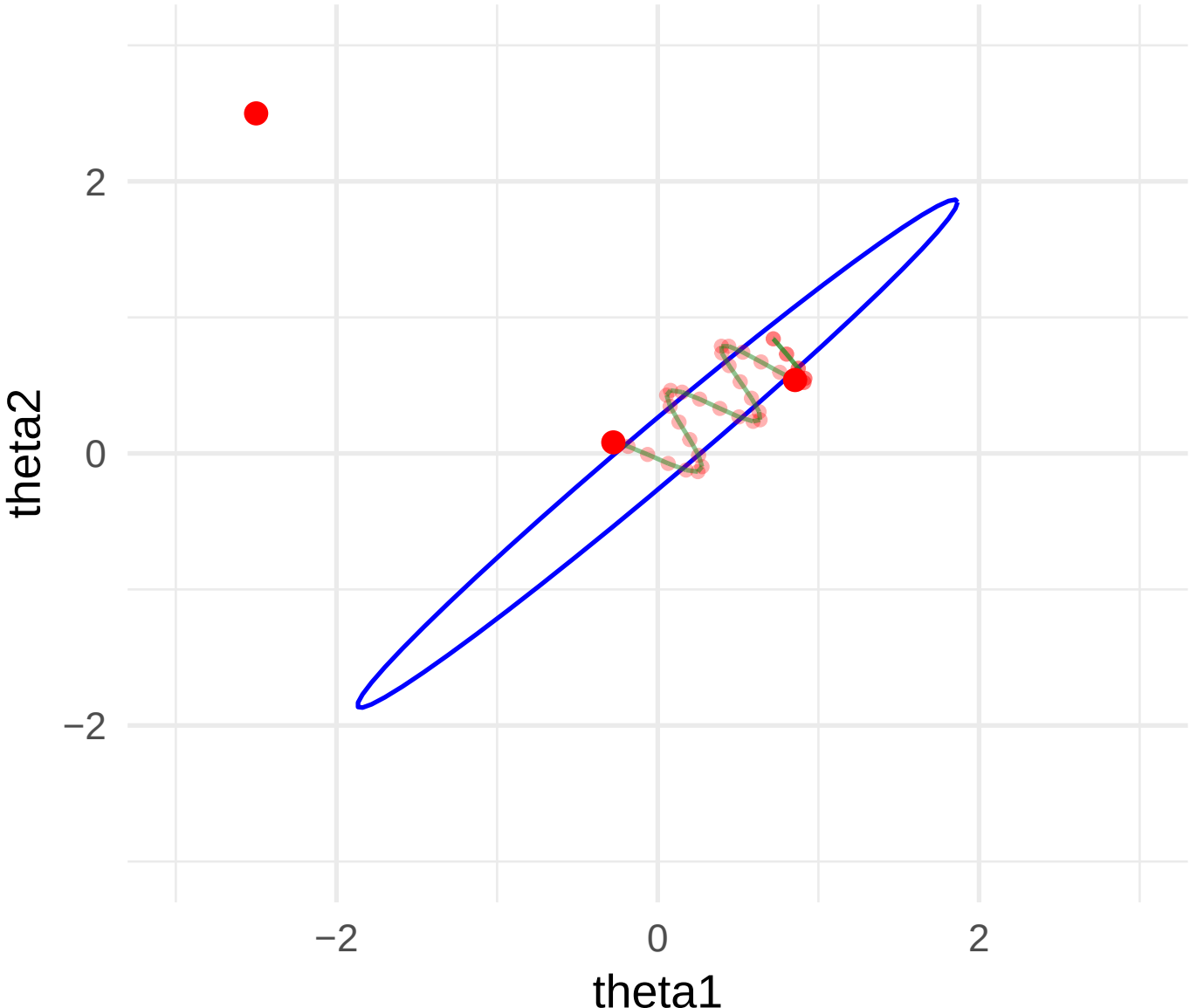

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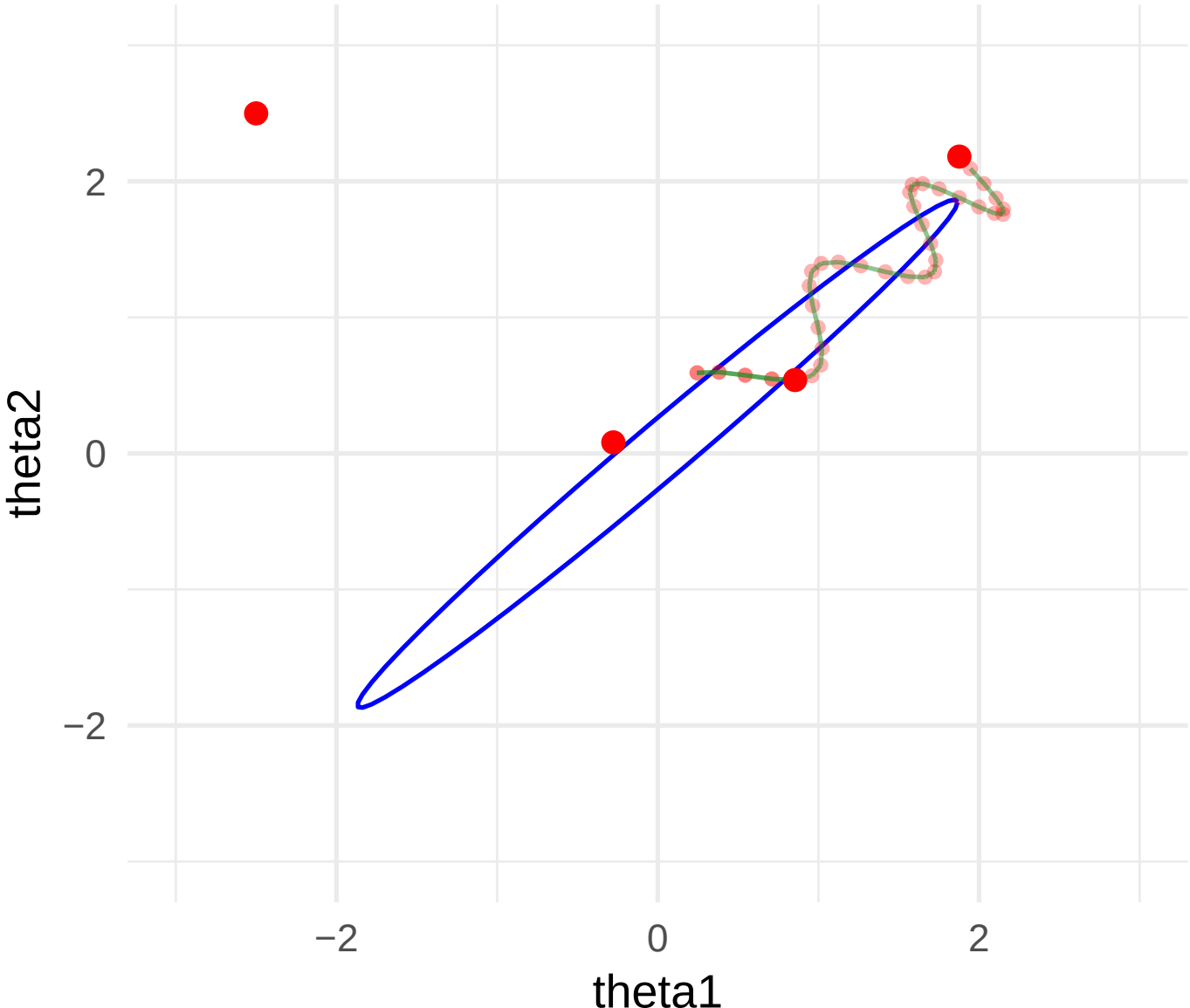

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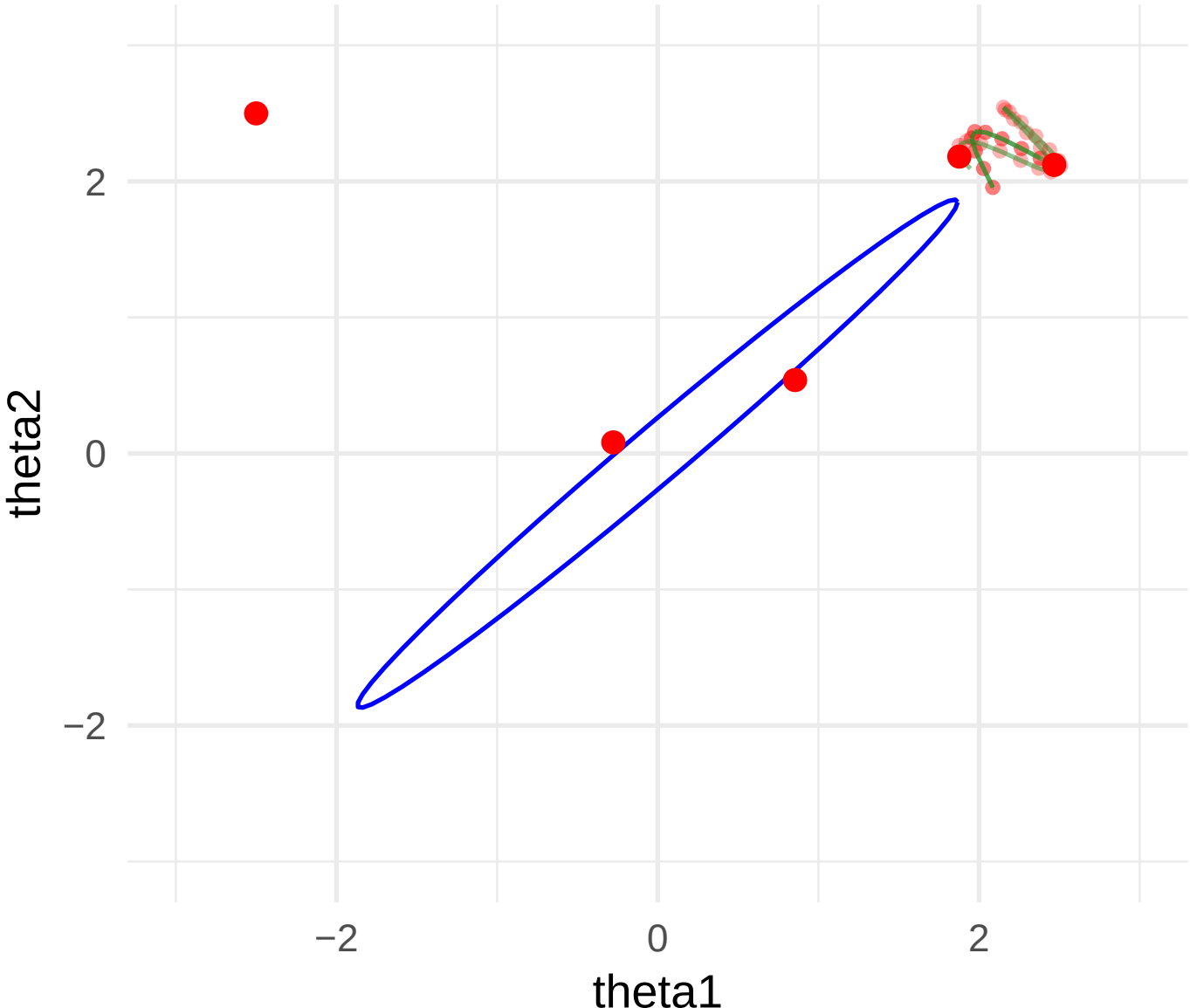

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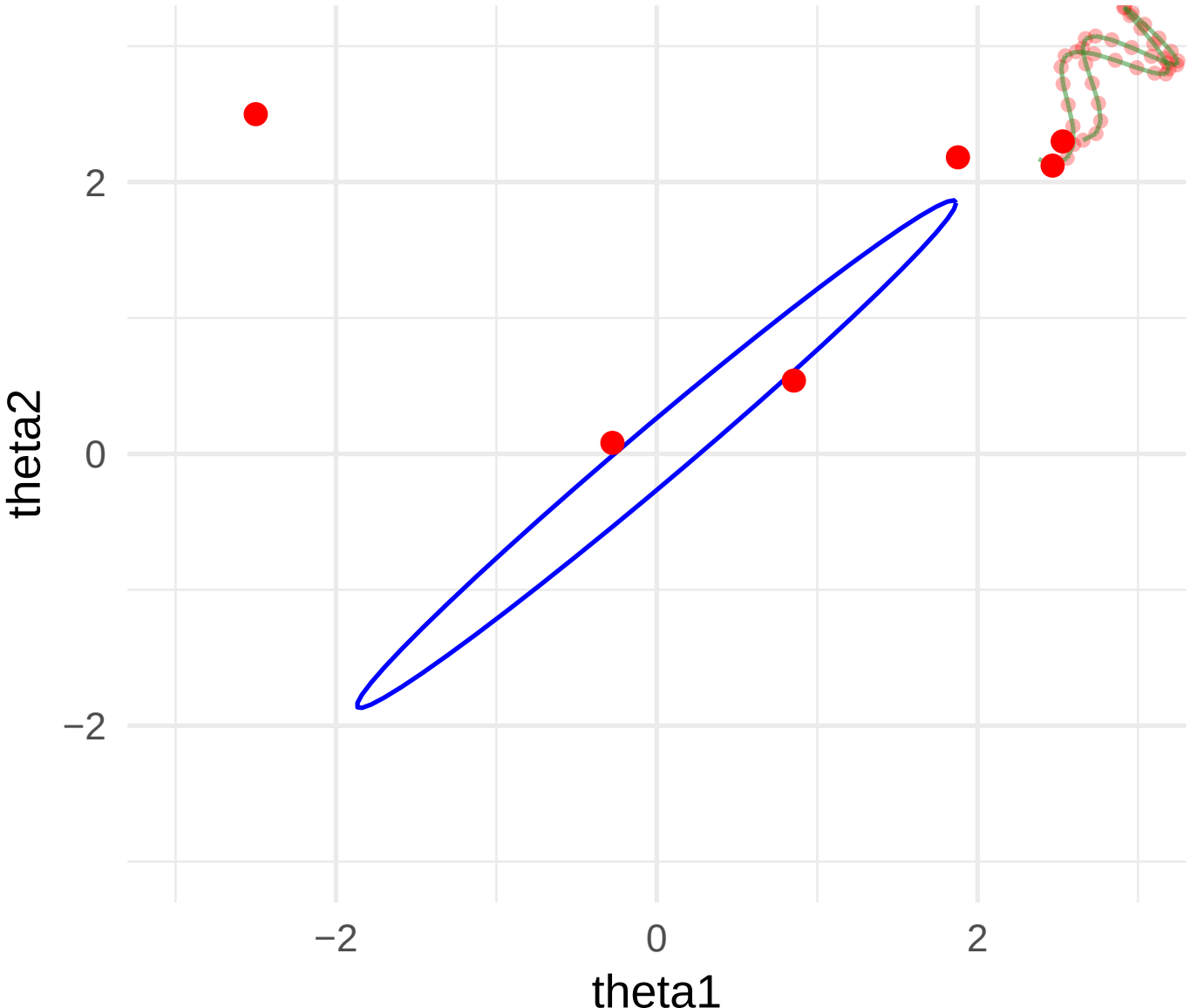

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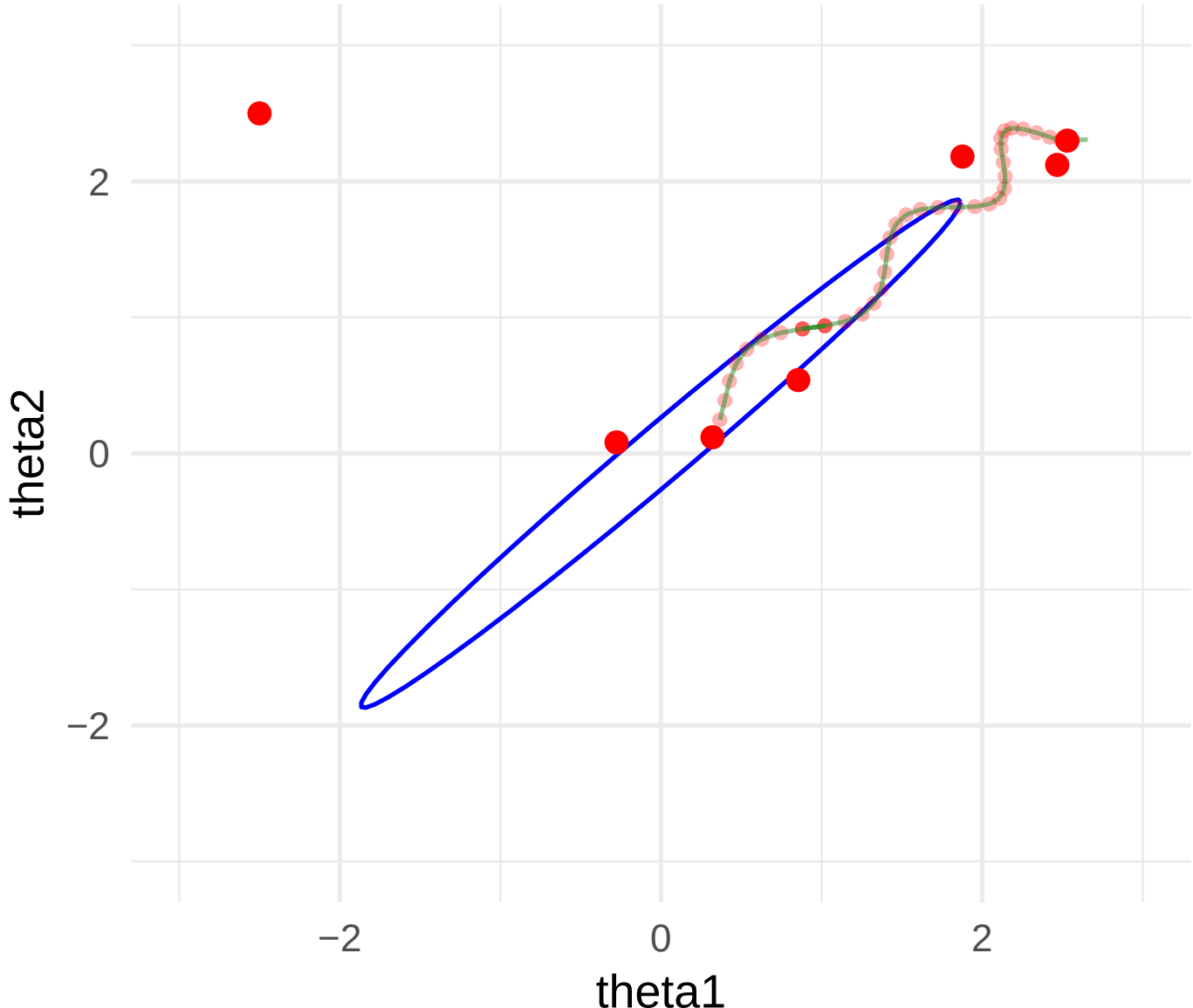

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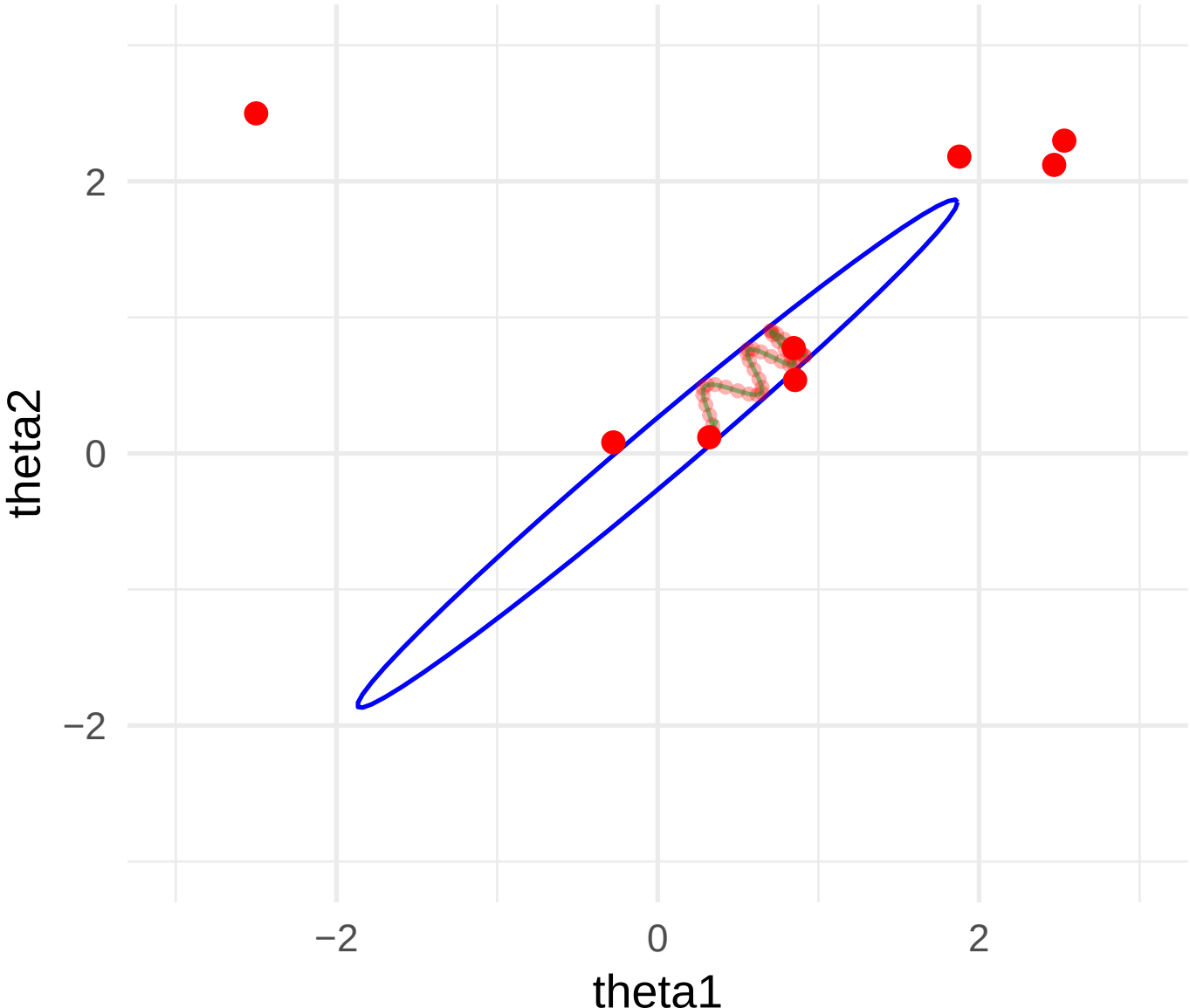

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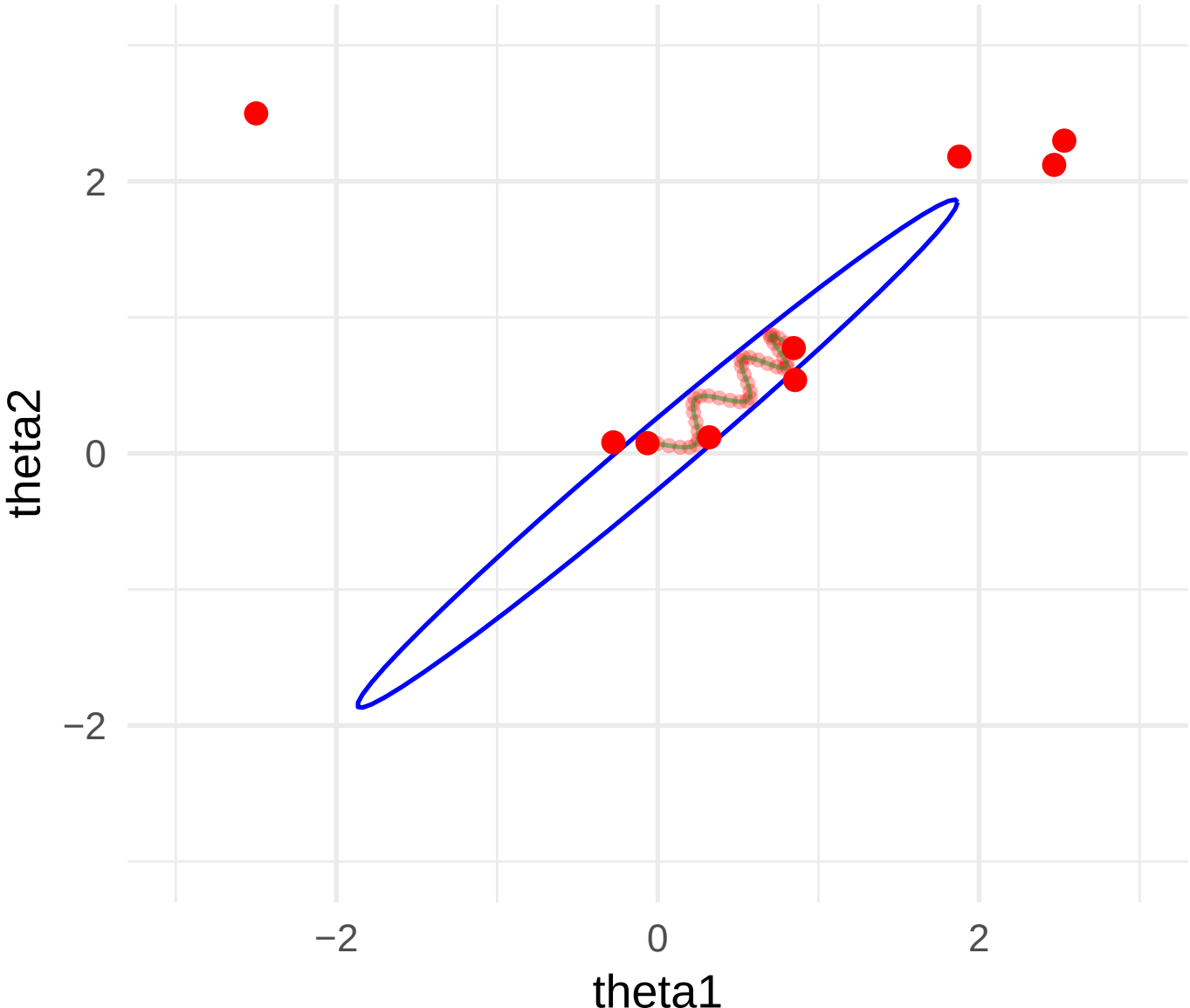

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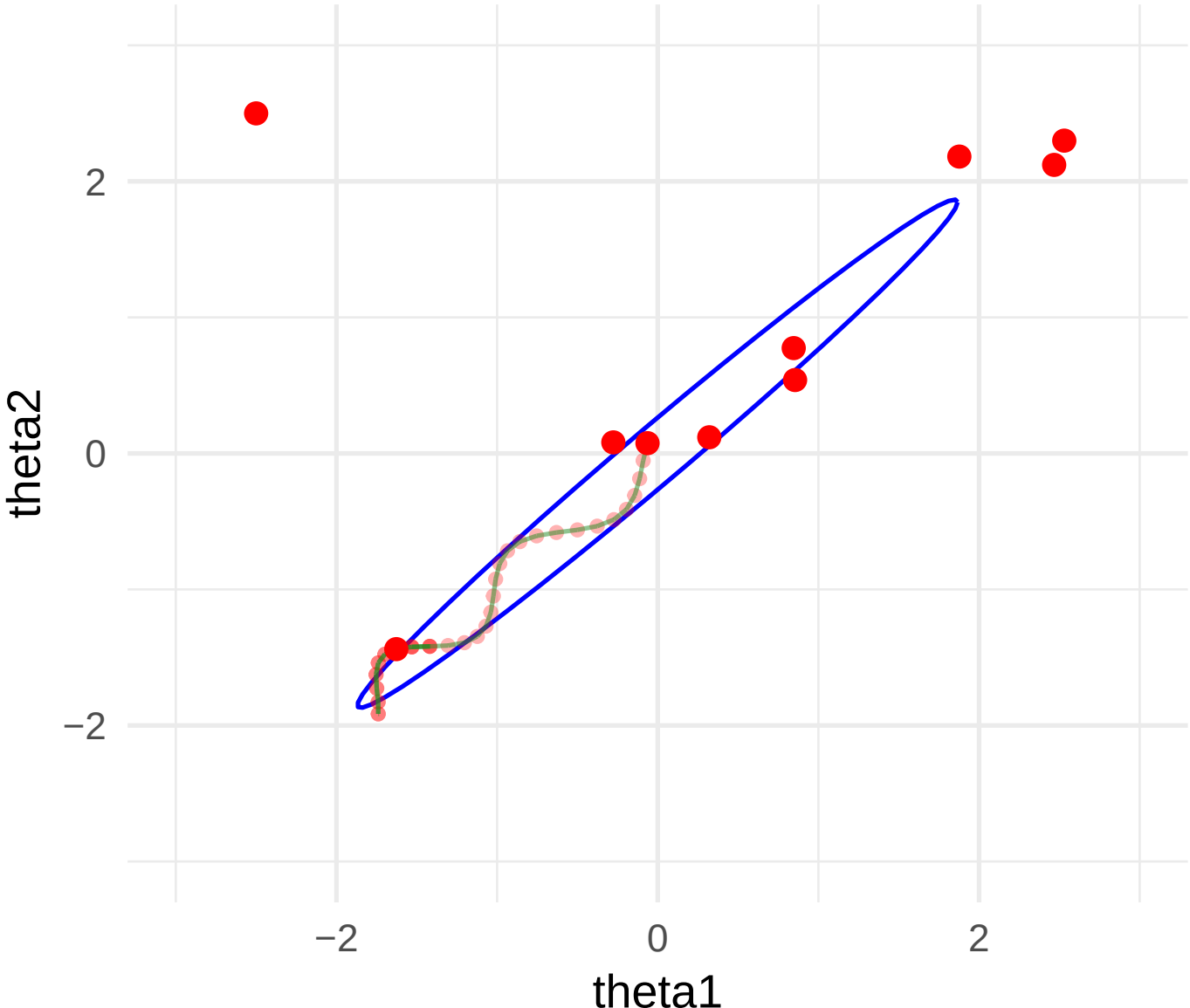

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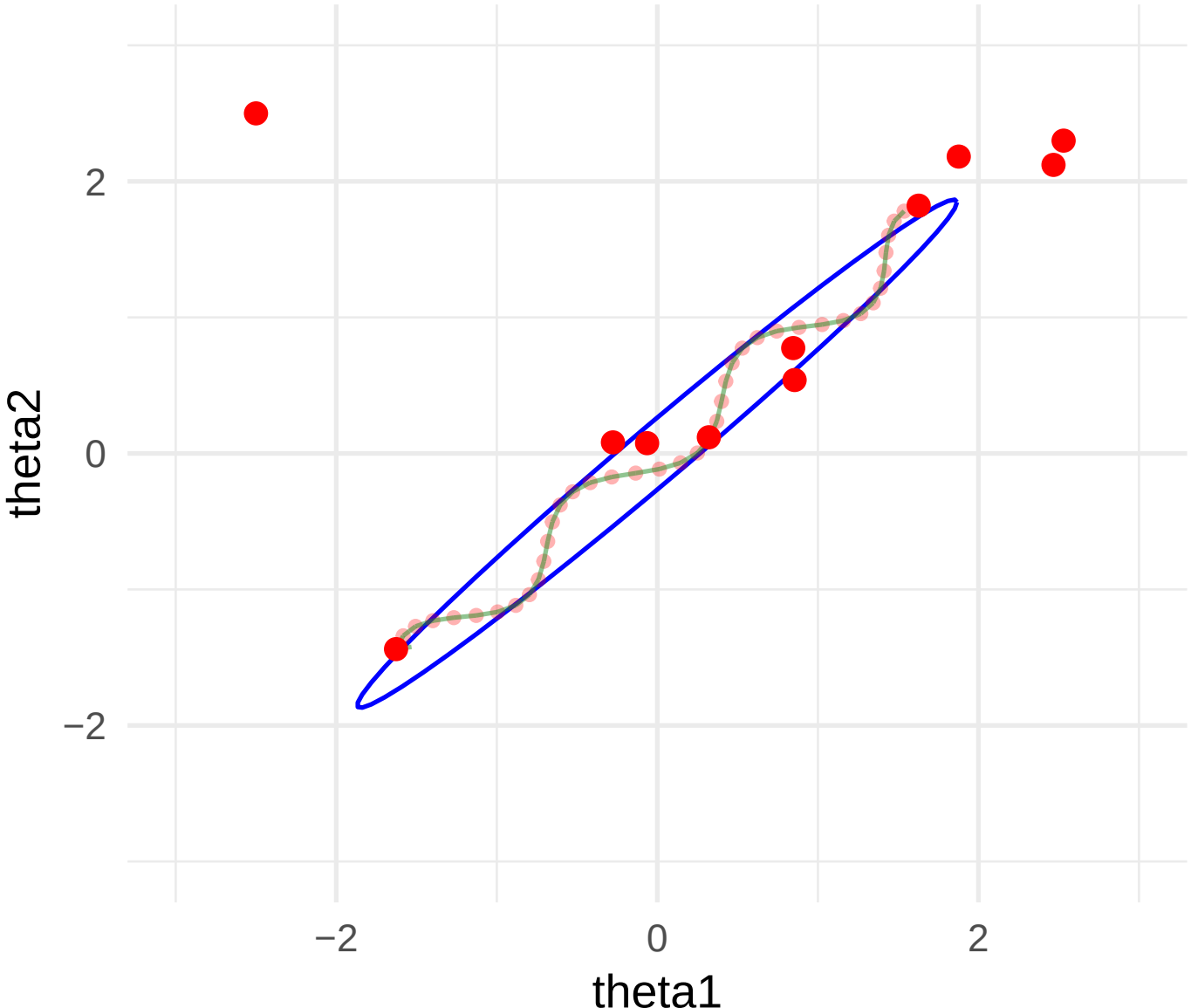

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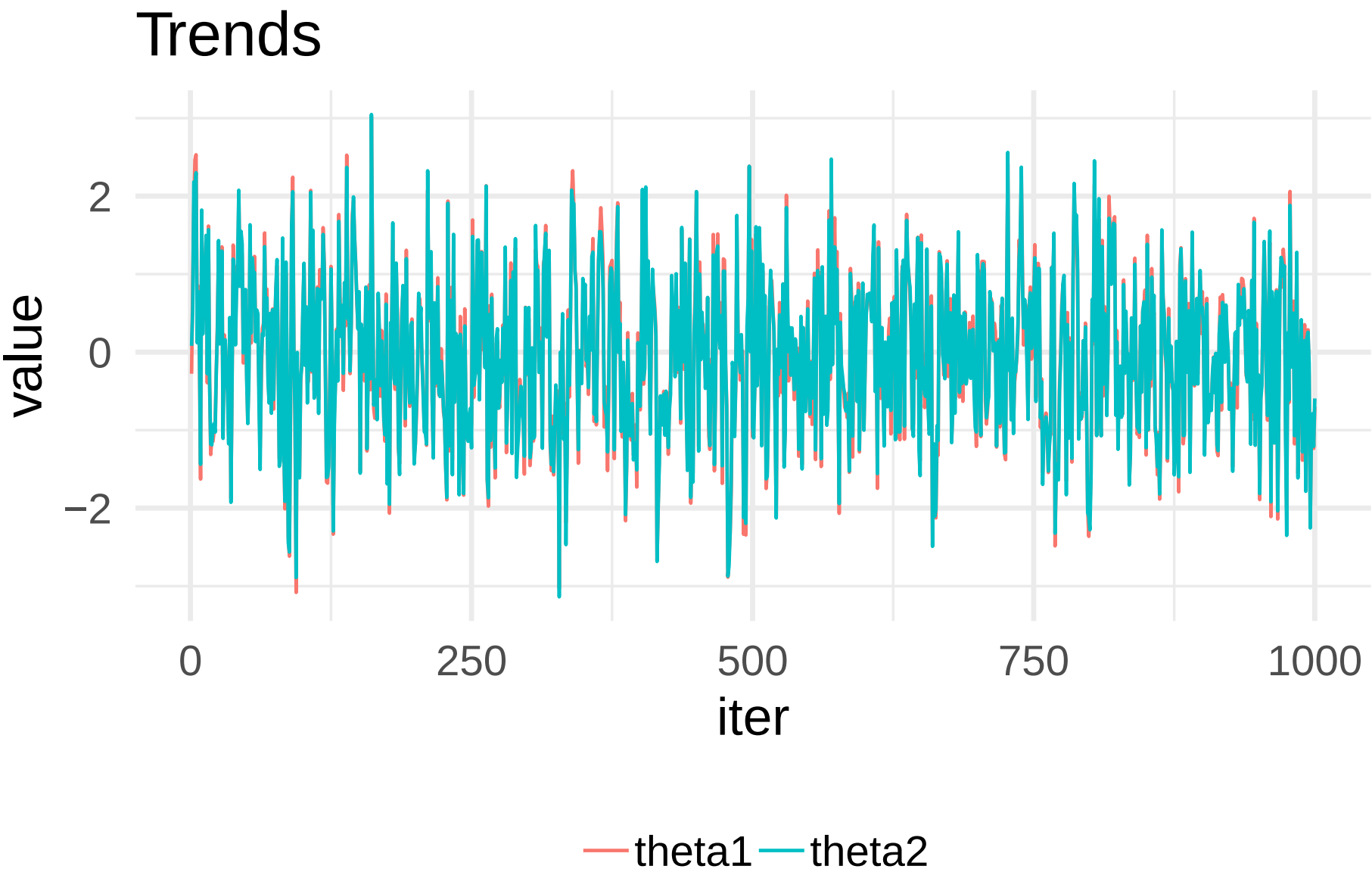

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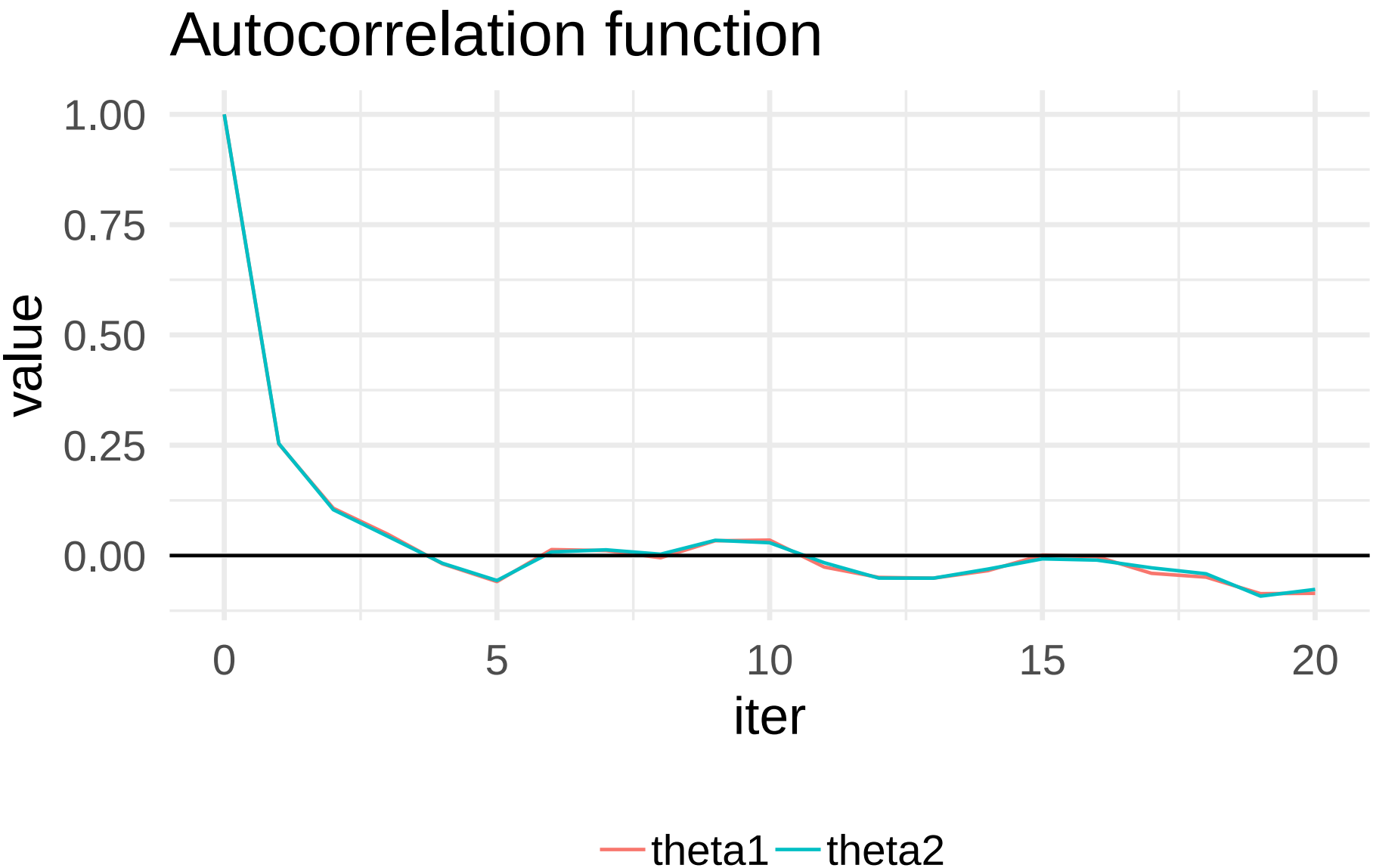

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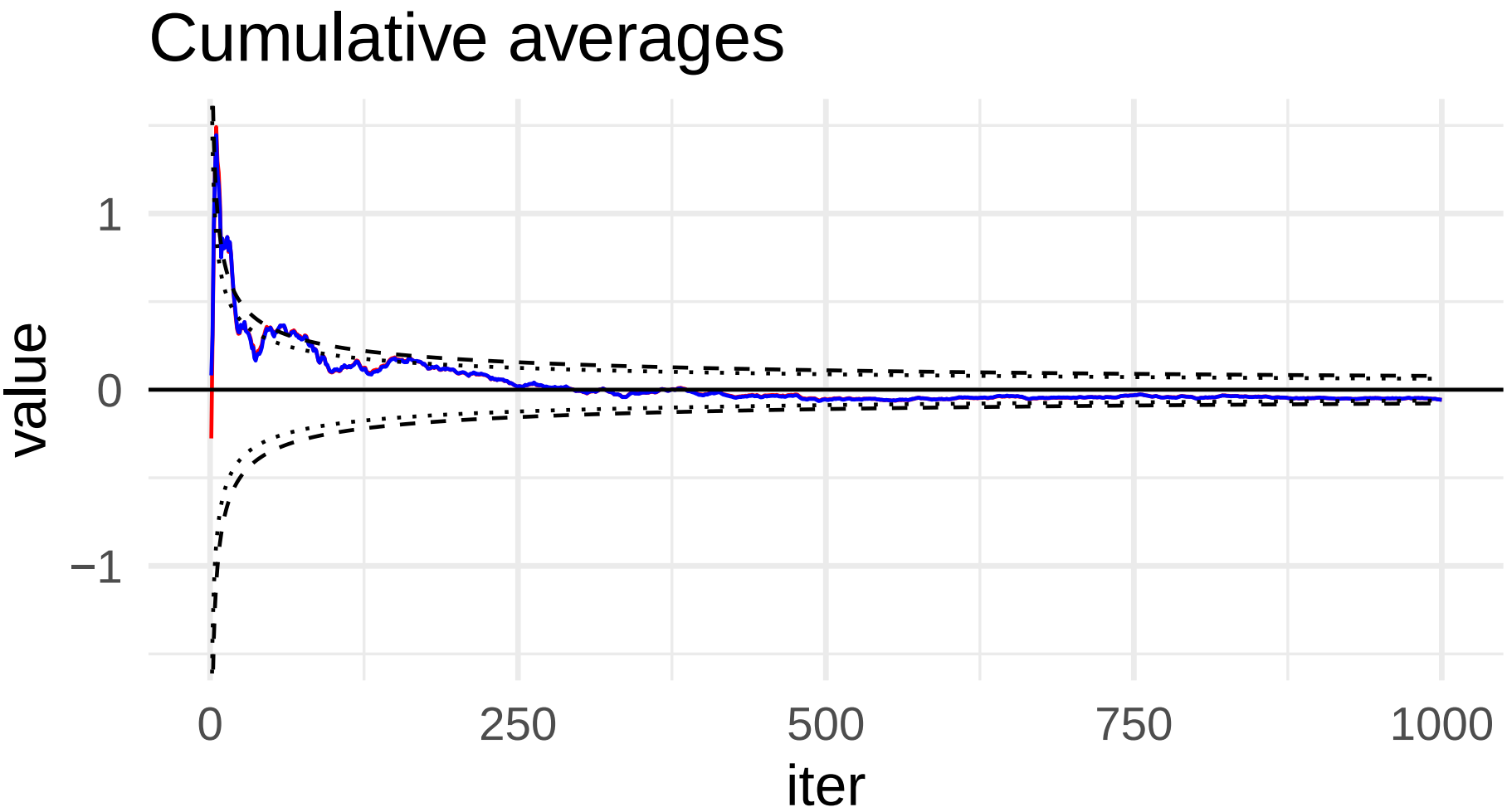

# Hamiltonian Monte Carlo / No-U-Turn sampling

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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 $\phi$ (the same dimensionality as $\theta$)
  - 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}
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where

- $U$ is potential energy function
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- $H$ is Hamiltonian energy function
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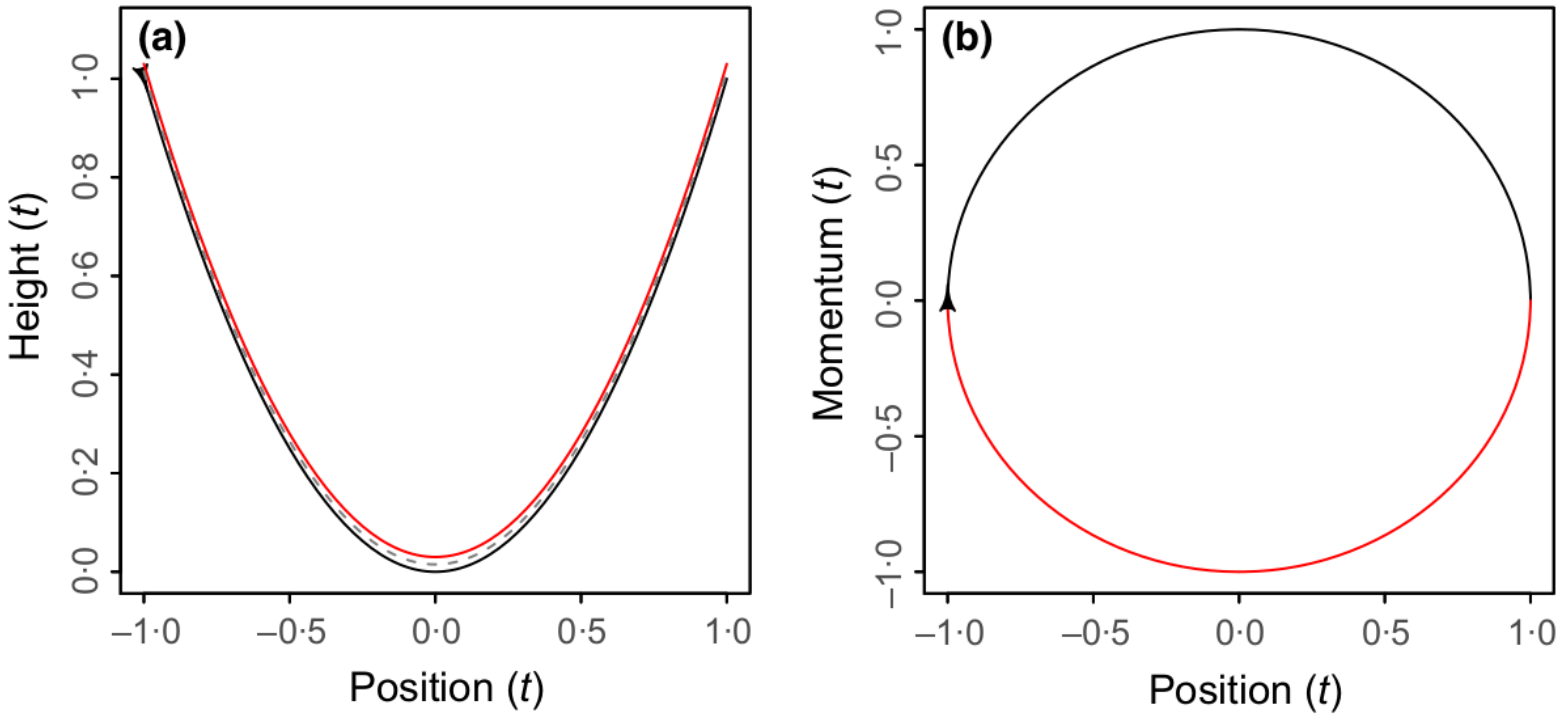
  - $\phi$ is called a momentum variable
- The potential energy is the negative log density $U(\theta) = -\log(p(\theta)) + C$

# 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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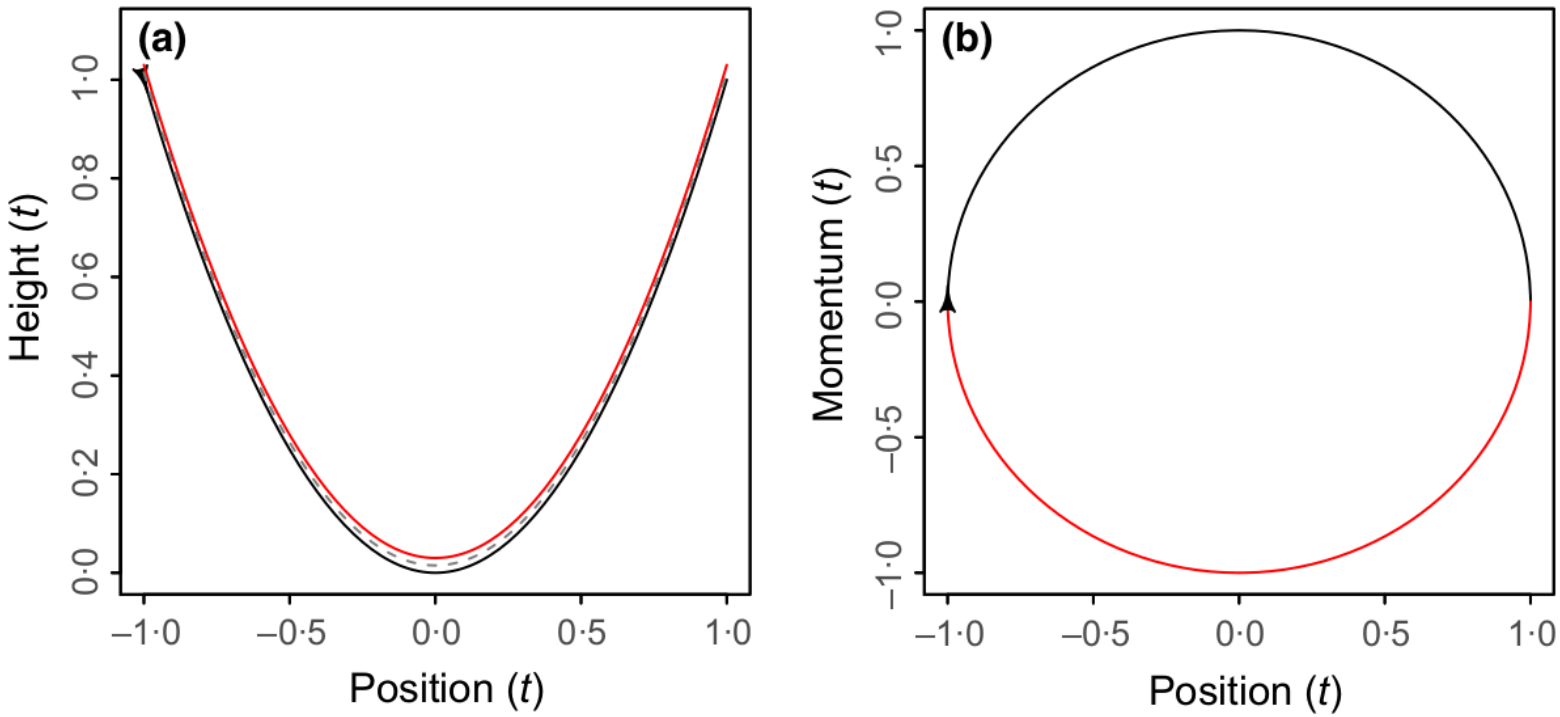


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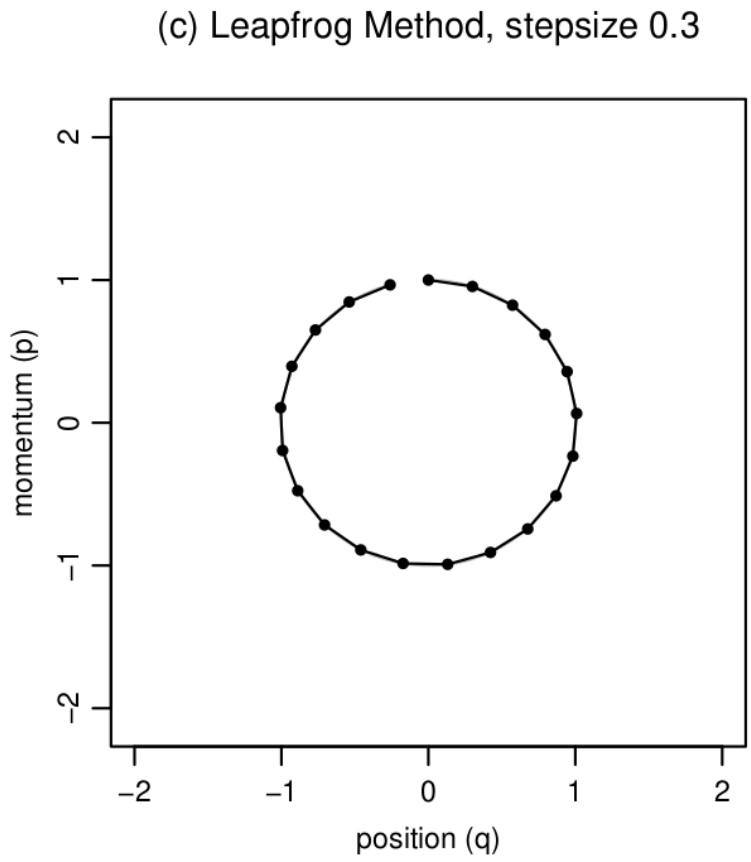
# Leapfrog discretization

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

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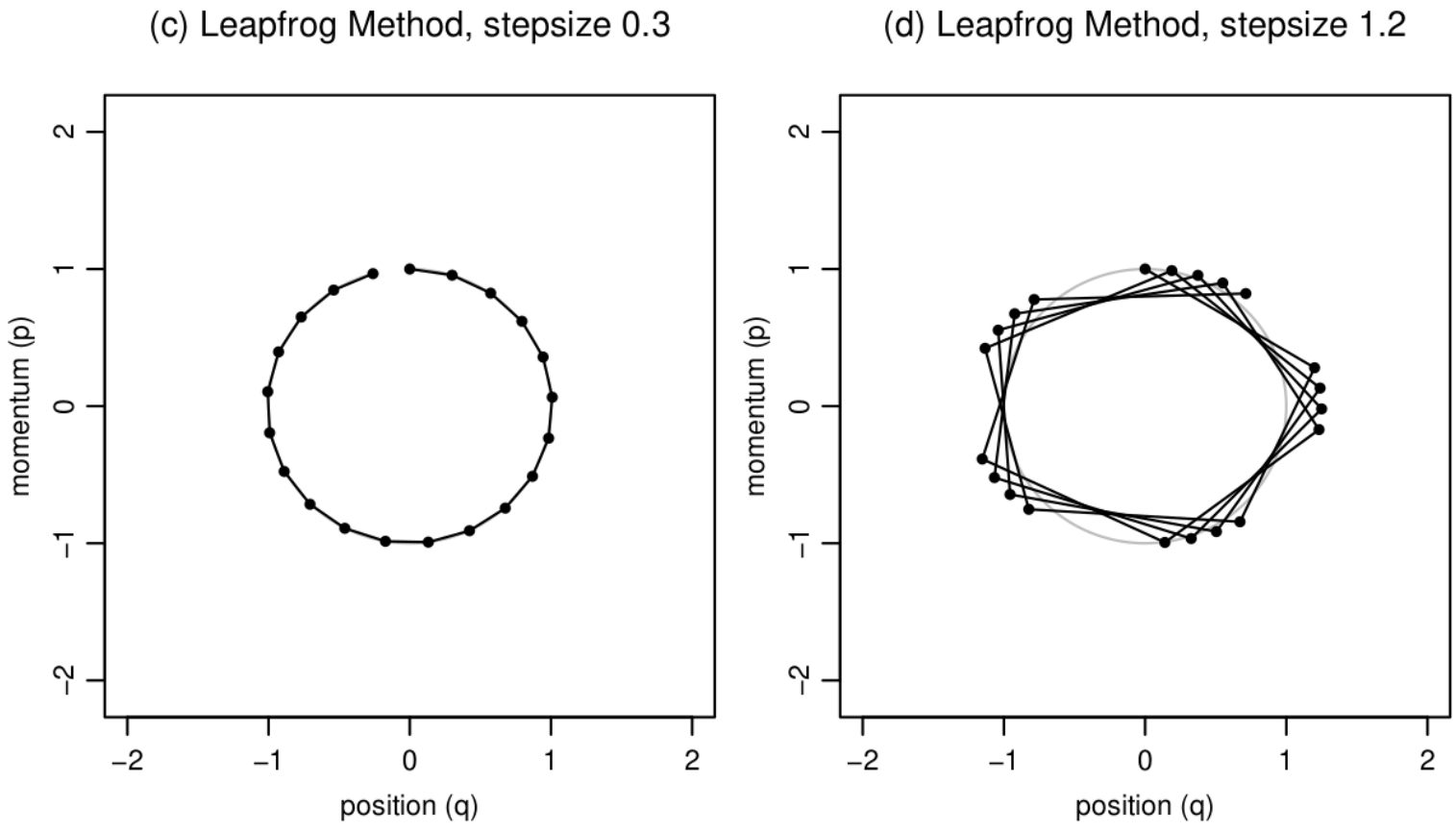


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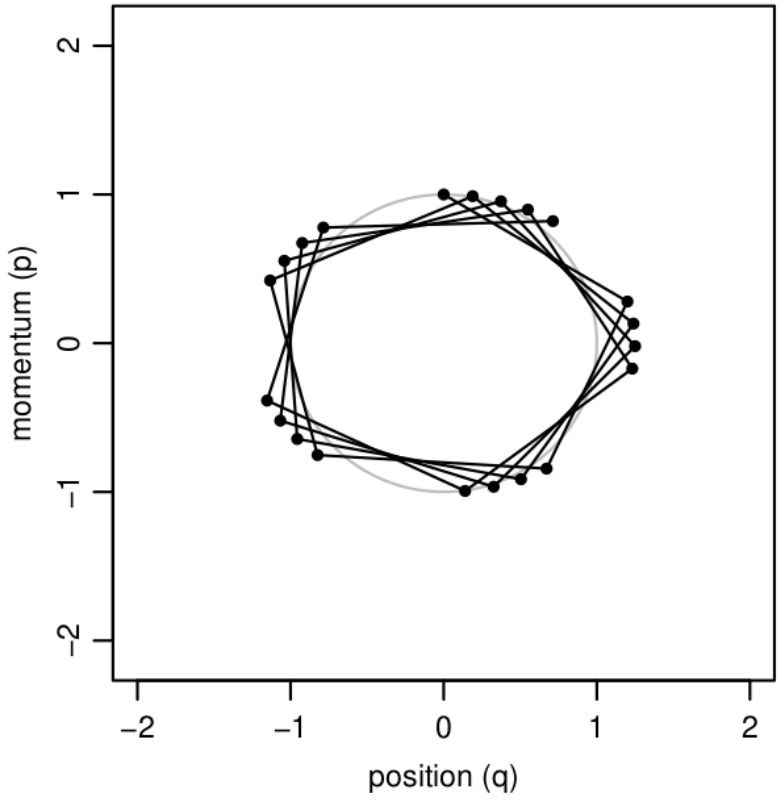


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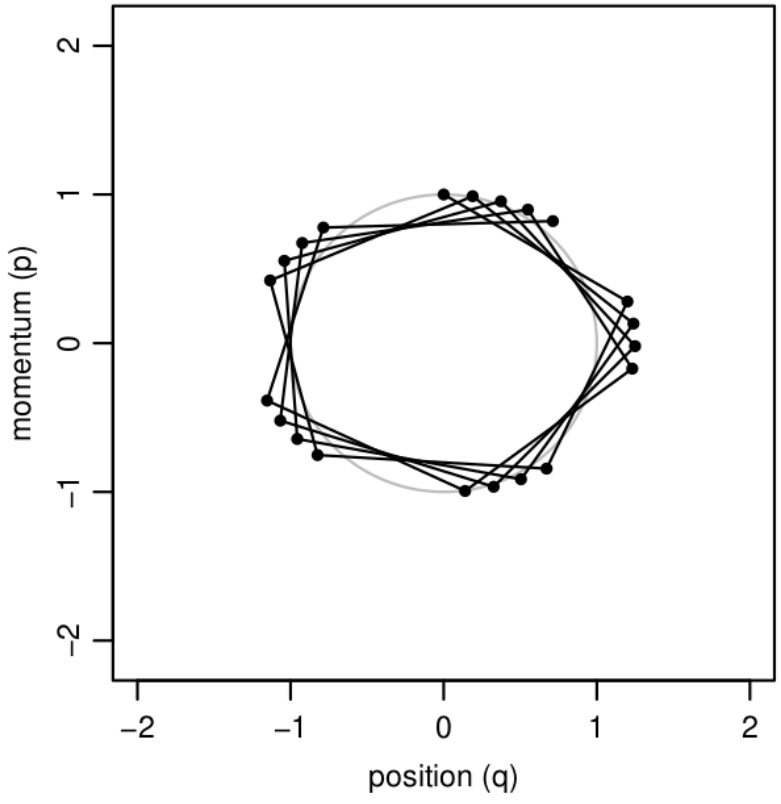
- Metropolis step with $r = \exp\left(-H(\theta^*, \phi^*) + H(\theta^{(t-1)}, \phi^{(t-1)})\right)$
  - accept if the Hamiltonian energy in the end is higher
  - accept with some probability if the Hamiltonian energy in the end is lower

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# Two steps of Hamiltonian Monte Carlo

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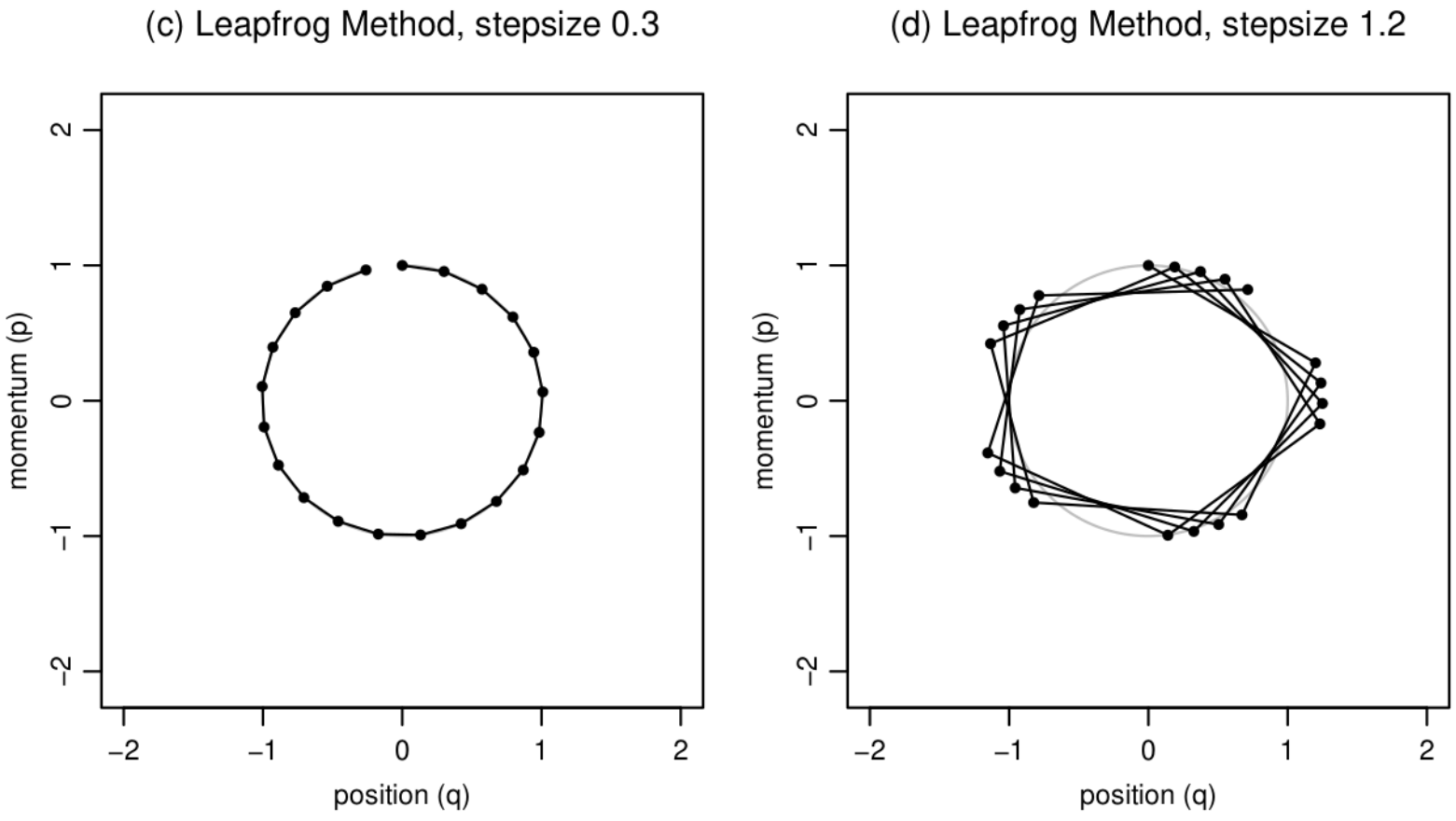


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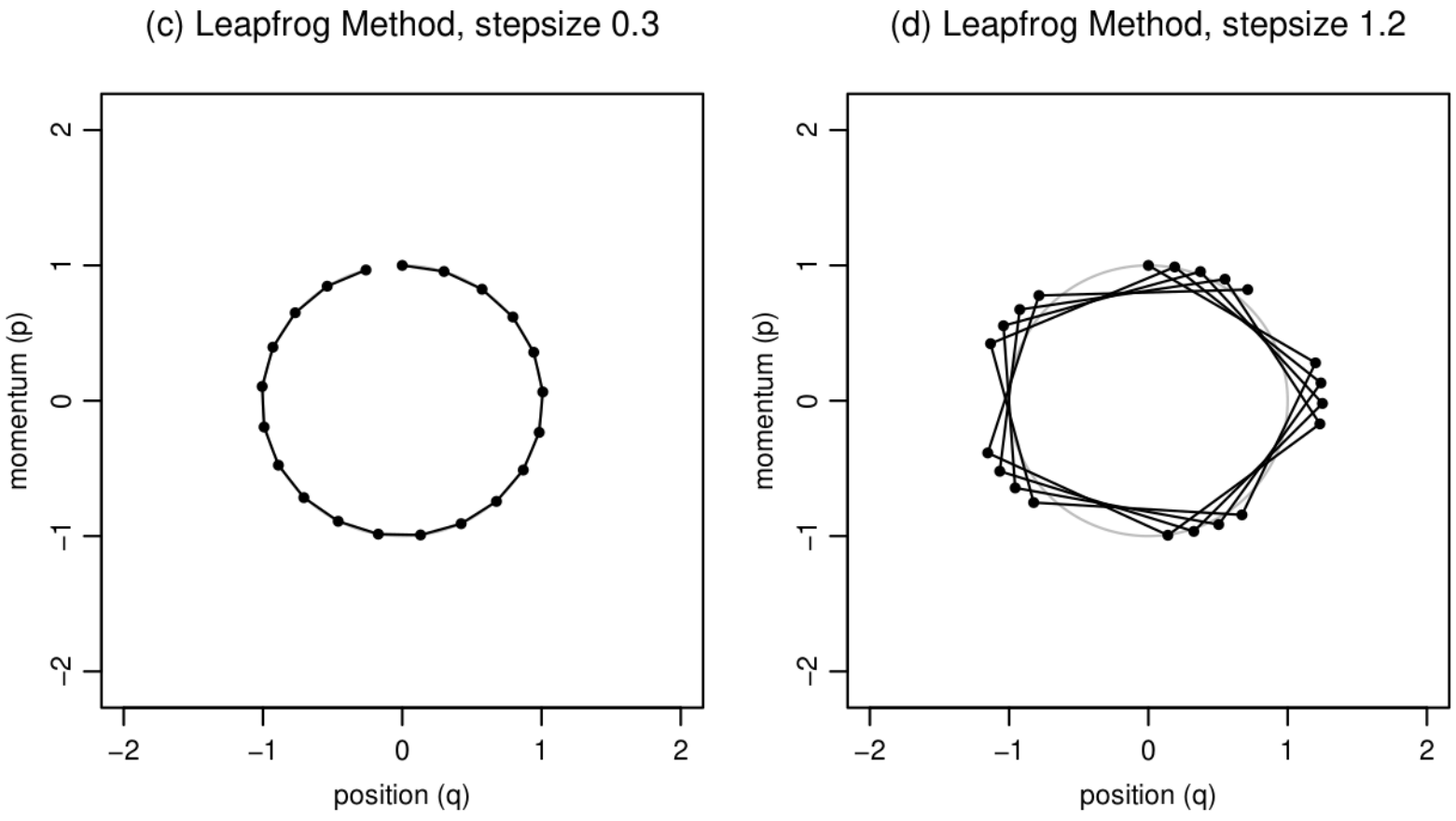


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# Two steps of Hamiltonian Monte Carlo

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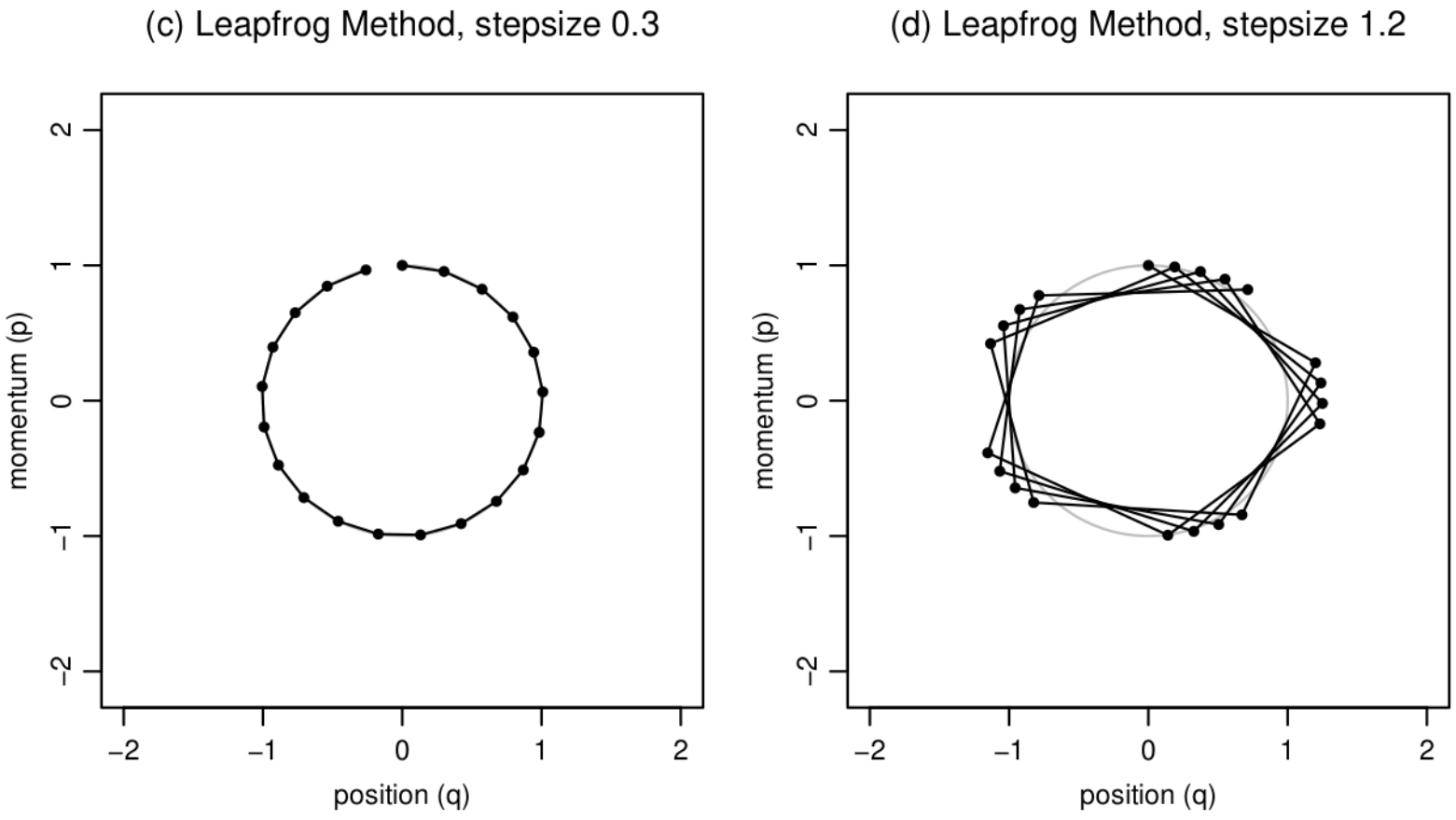
- Alternating sampling from $p(\phi)$ is crucial for moving to $(\theta, \phi)$ points with different joint density

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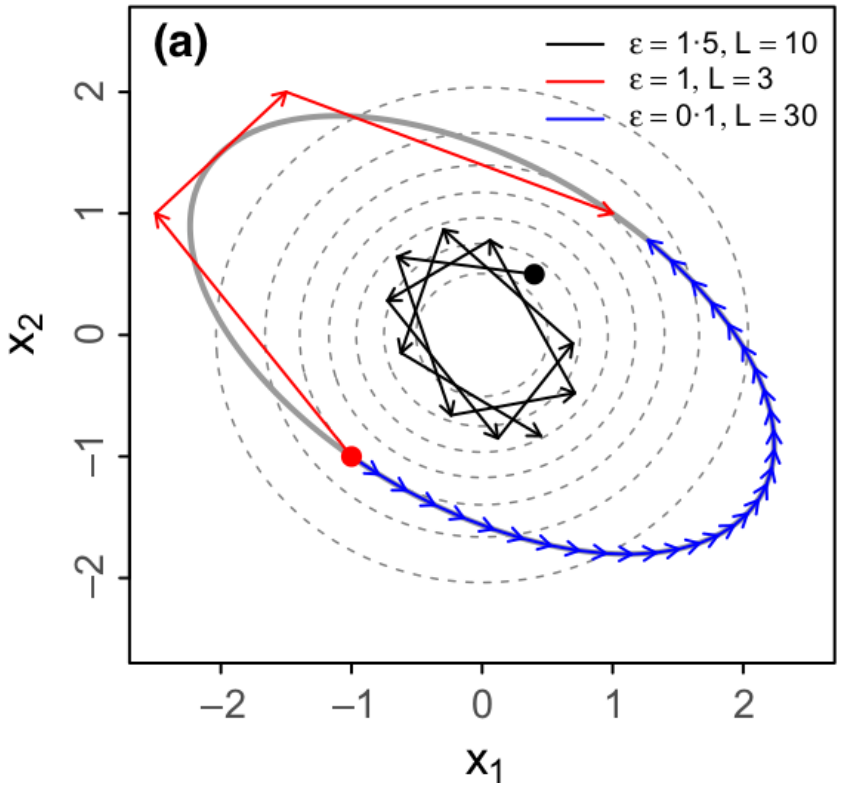


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# Leapfrog discretization, step size

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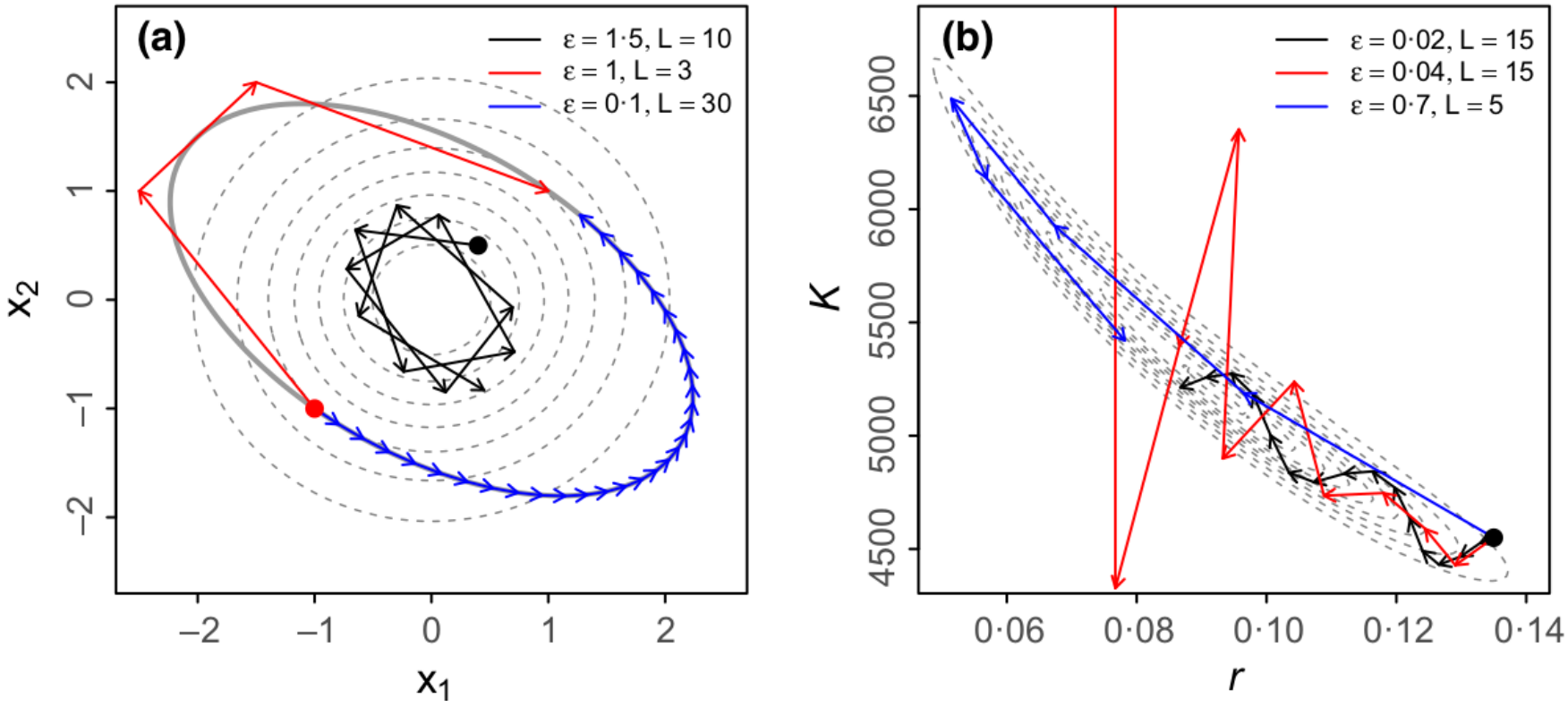
- Big step size → less log density and gradient evaluations, but lower acceptance rate and the simulation may diverge

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# Leapfrog discretization, the number of steps

- Many steps can reduce random walk
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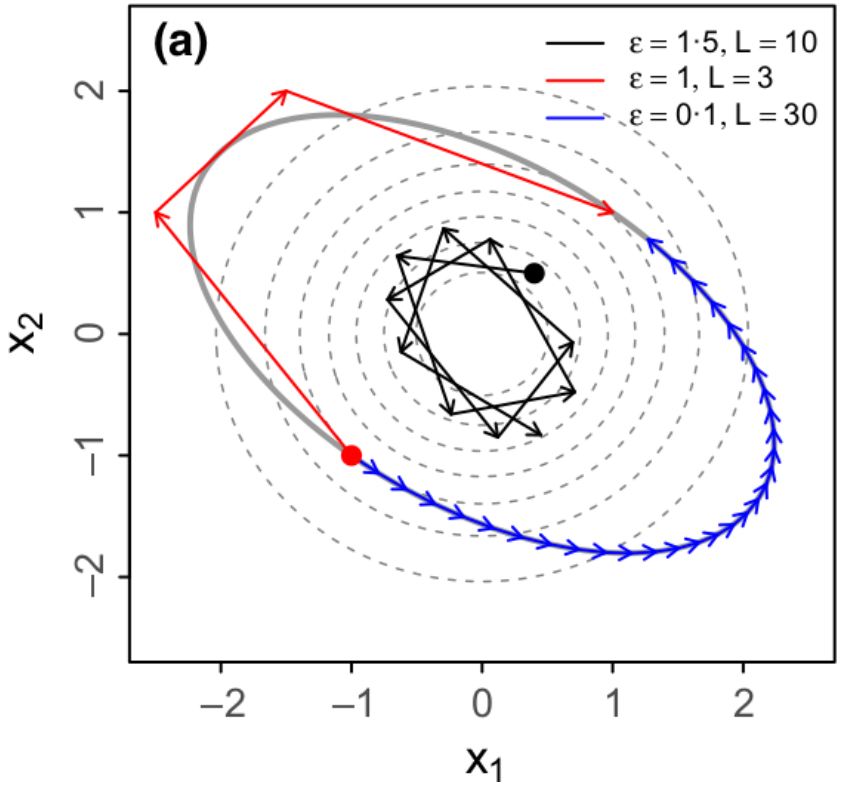


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# Static Hamiltonian Monte Carlo

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

# No-U-Turn sampler

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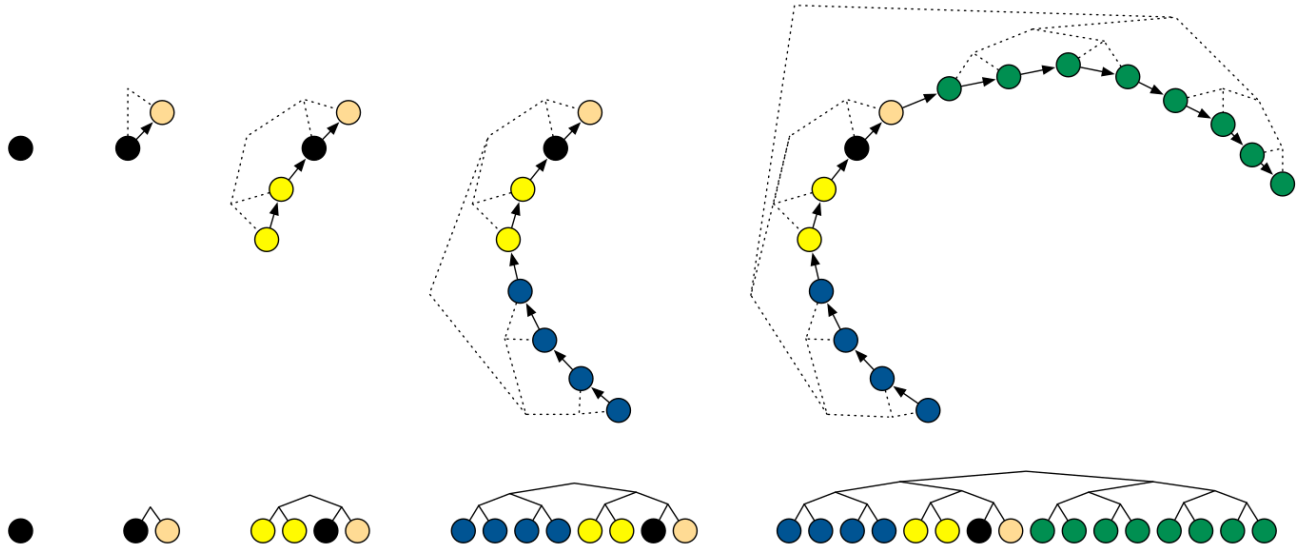

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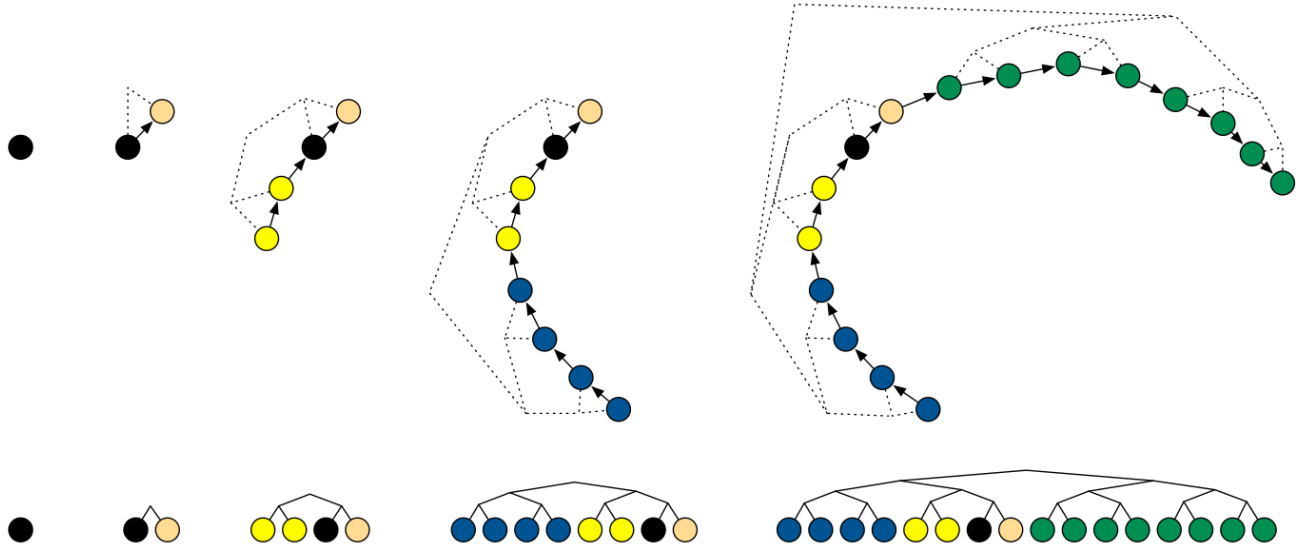

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- NUTS with multinomial sampling
  - compute the probability of selecting a point and accepting it for all points
  - select the point with multinomial sampling
  - more likely to accept a point that is not the previous one

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  - if the proposal is rejected the previous state is also the new state
- NUTS with multinomial sampling
  - compute the probability of selecting a point and accepting it for all points
  - select the point with multinomial sampling
  - more likely to accept a point that is not the previous one
- Demo https://chi-feng.github.io/mcmc-demo/

# Mass matrix and the step size adaptation

- Mass matrix refers to having different scaling for different parameters and optionally also rotation to reduce correlations
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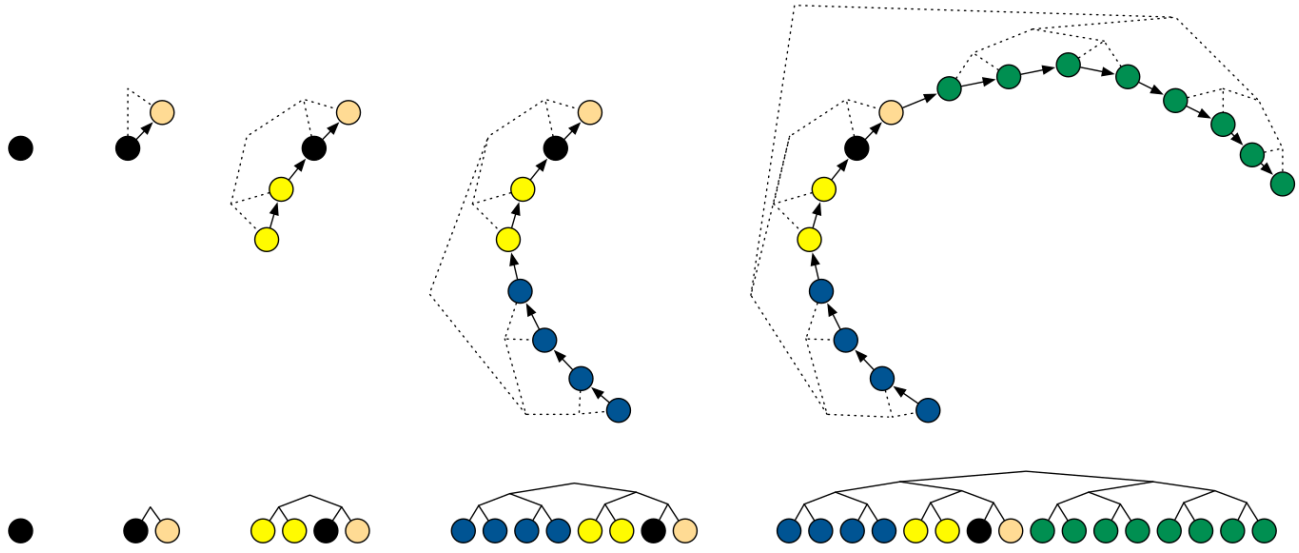
  - adjusted to be as big as possible while keeping discretization error in control (adapt_delta)
  - “Dual averaging” demo https://chi-feng.github.io/mcmc-demo/
- After adaptation the algorithm parameters are fixed and some more iterations run to finish the warmup

# Max tree depth diagnostic

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



from Hoffman & Gelman (2014)

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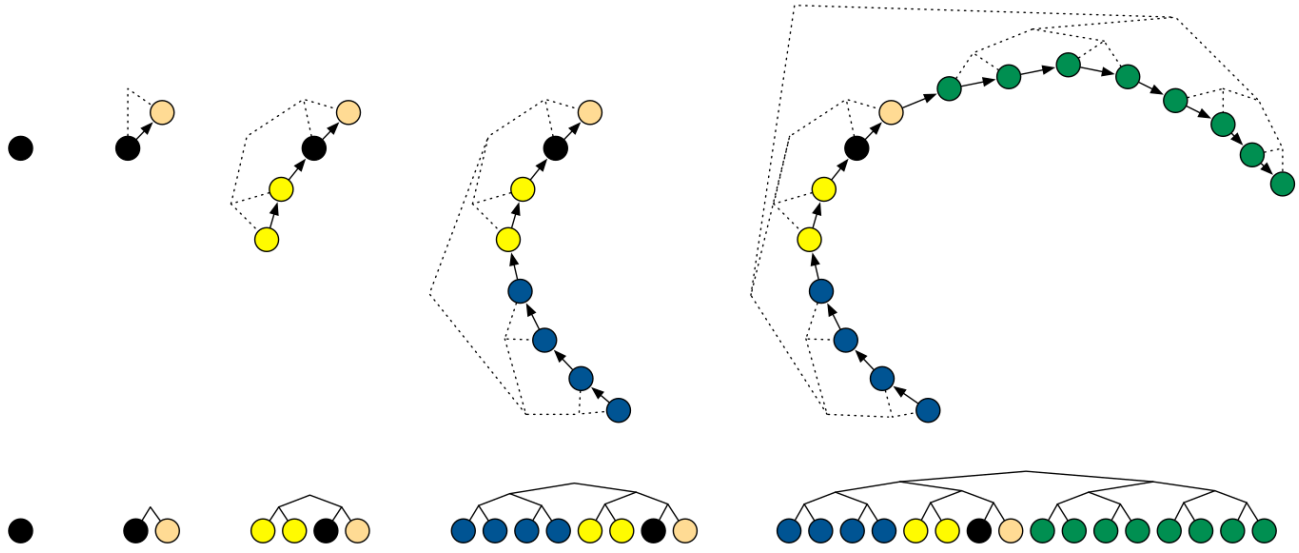

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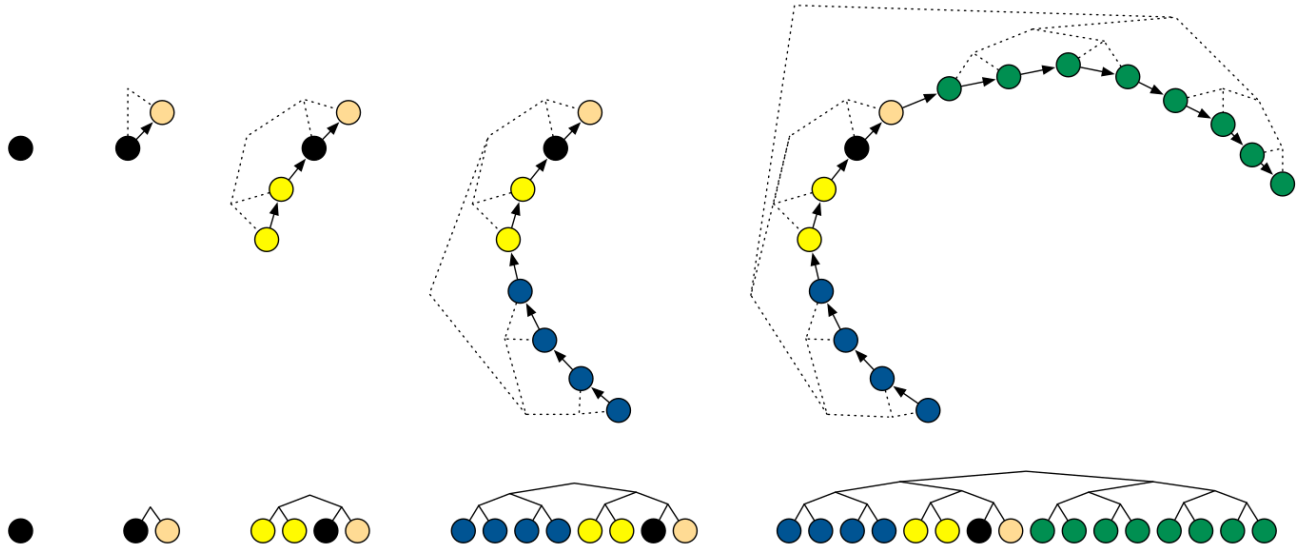

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  - maximum simulation length is capped to avoid very long waiting times in case of bad behavior
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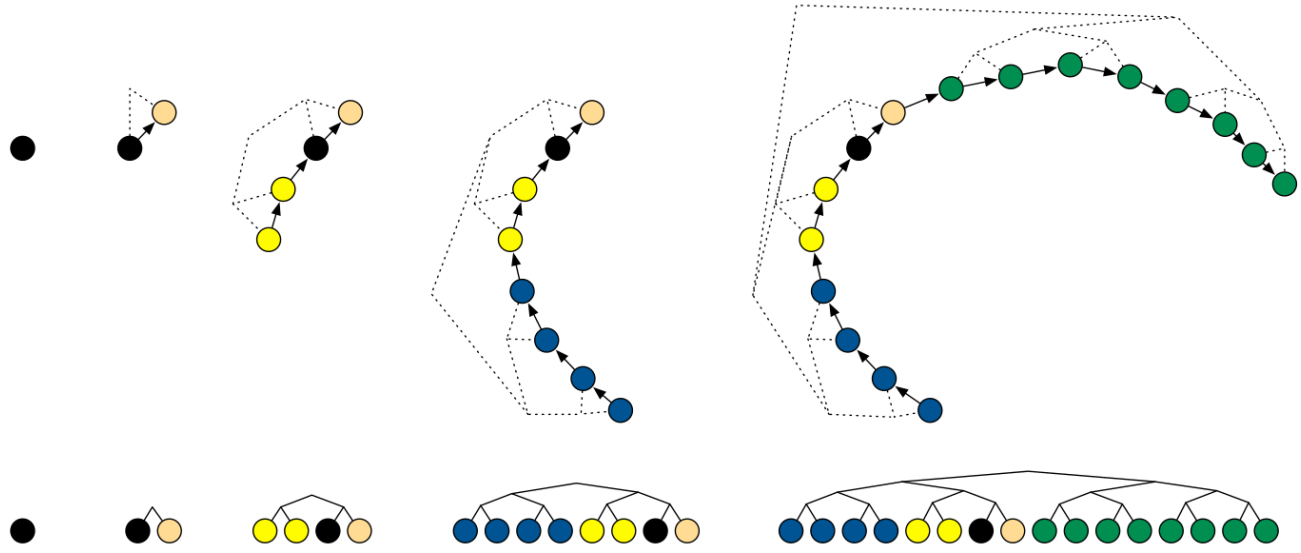

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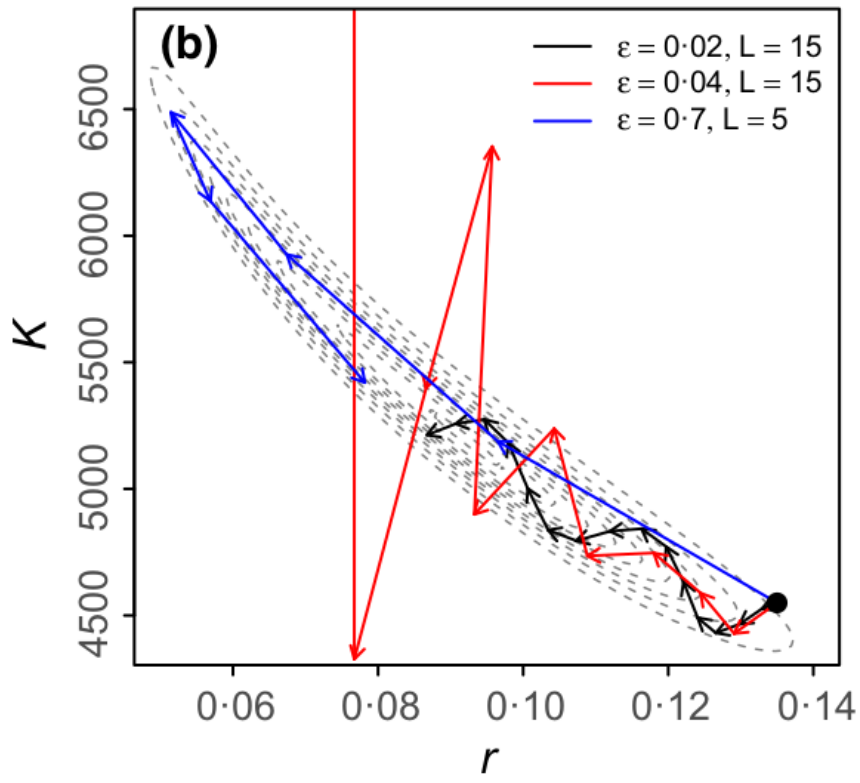
  - moderate inefficiency doesn't invalidate the result
- Different parameterizations matter

# 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

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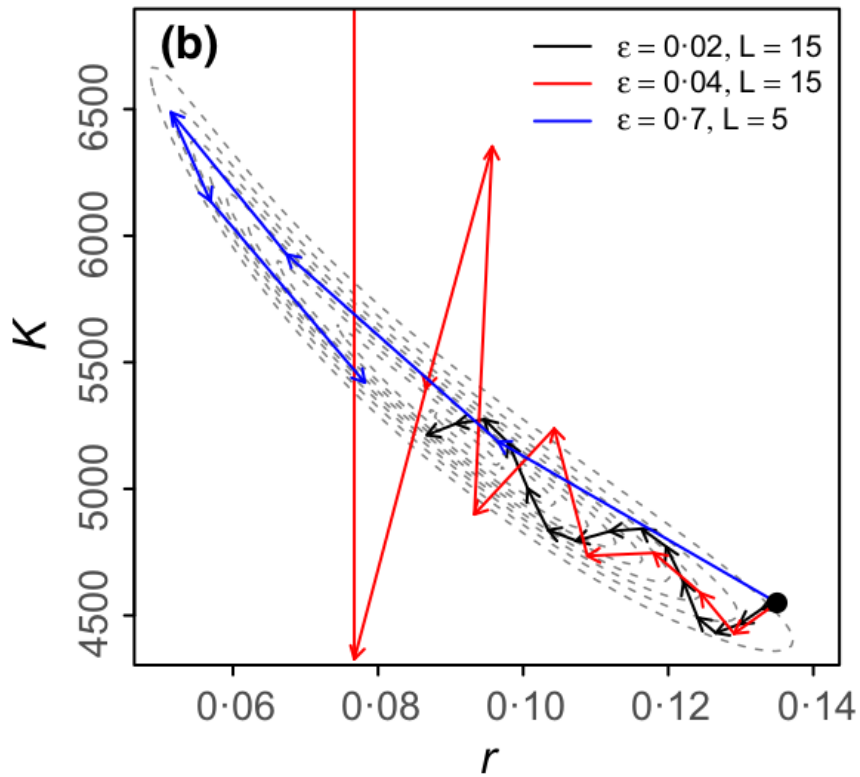


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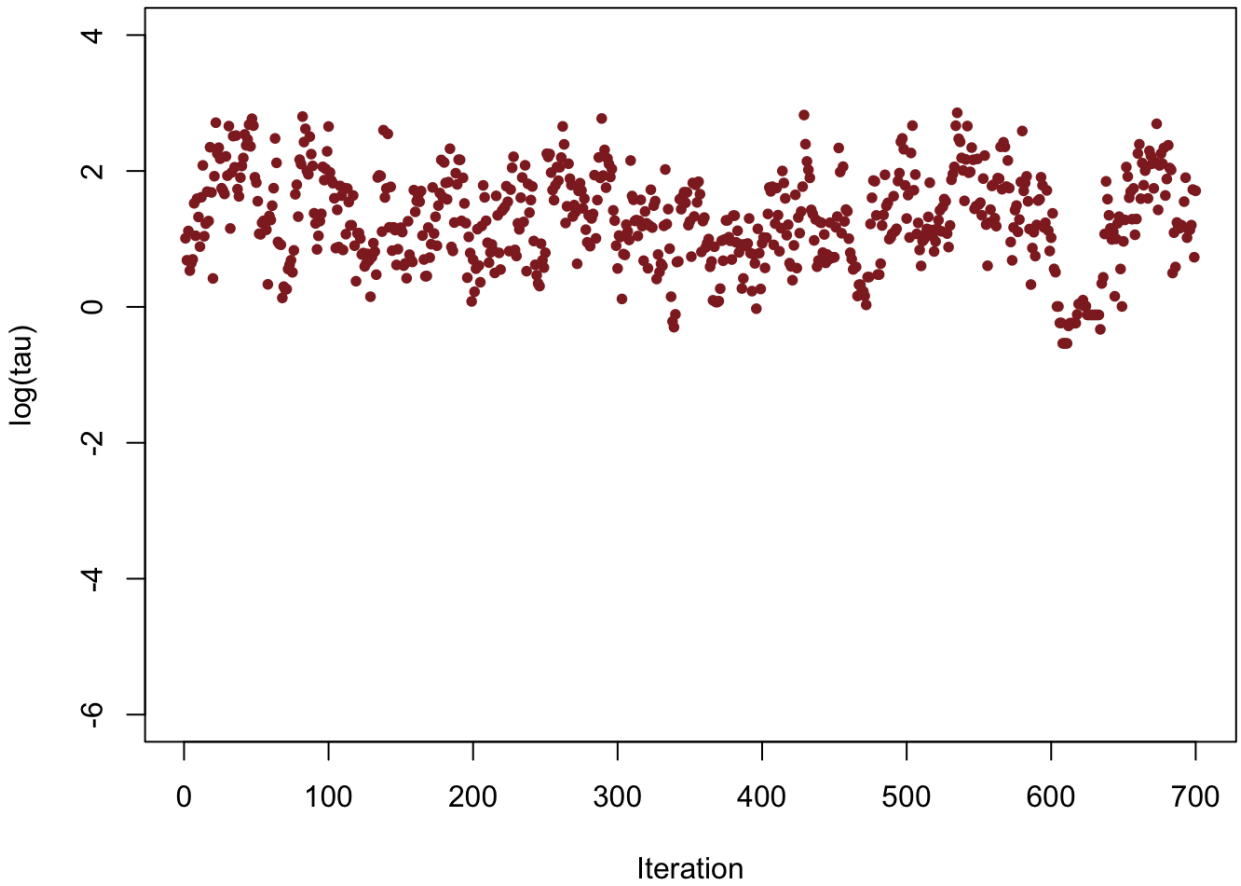

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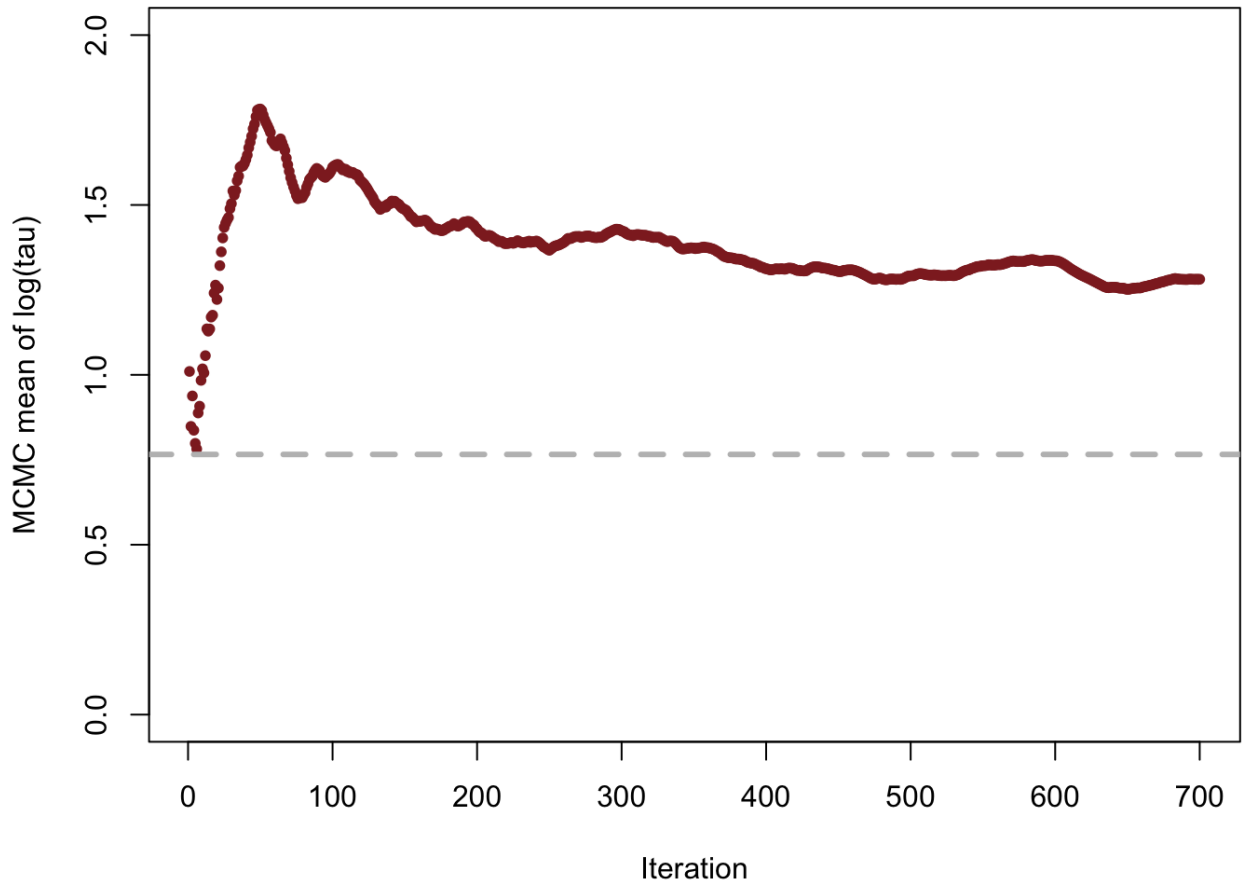

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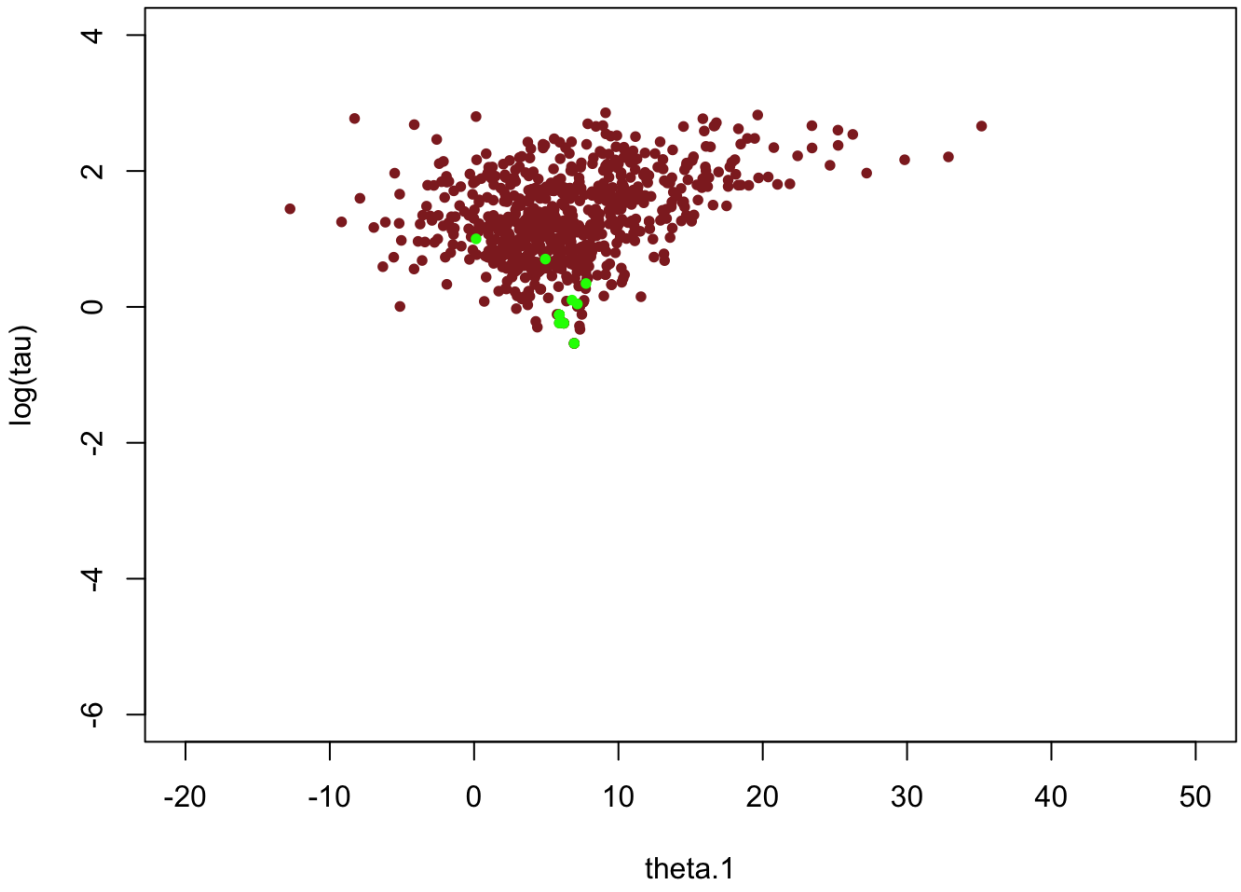

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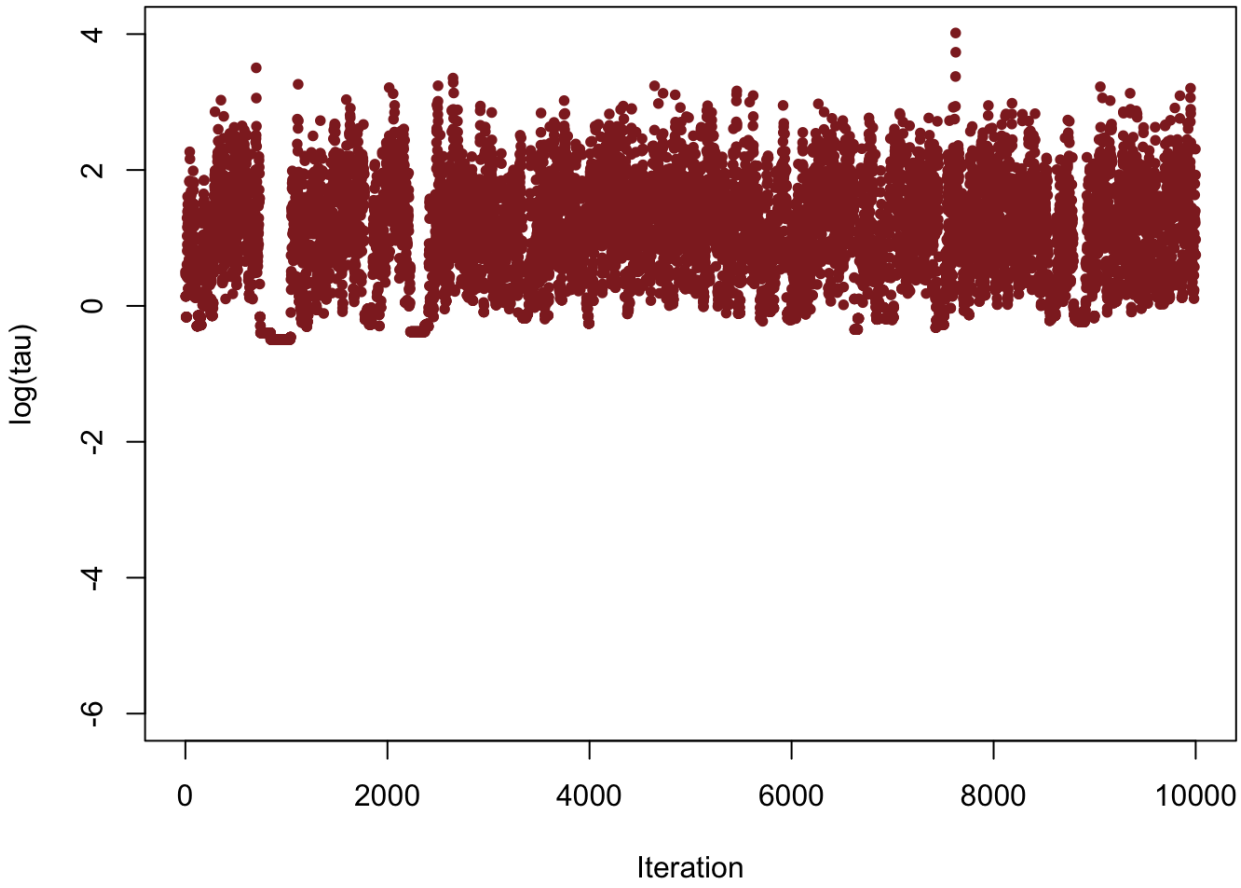

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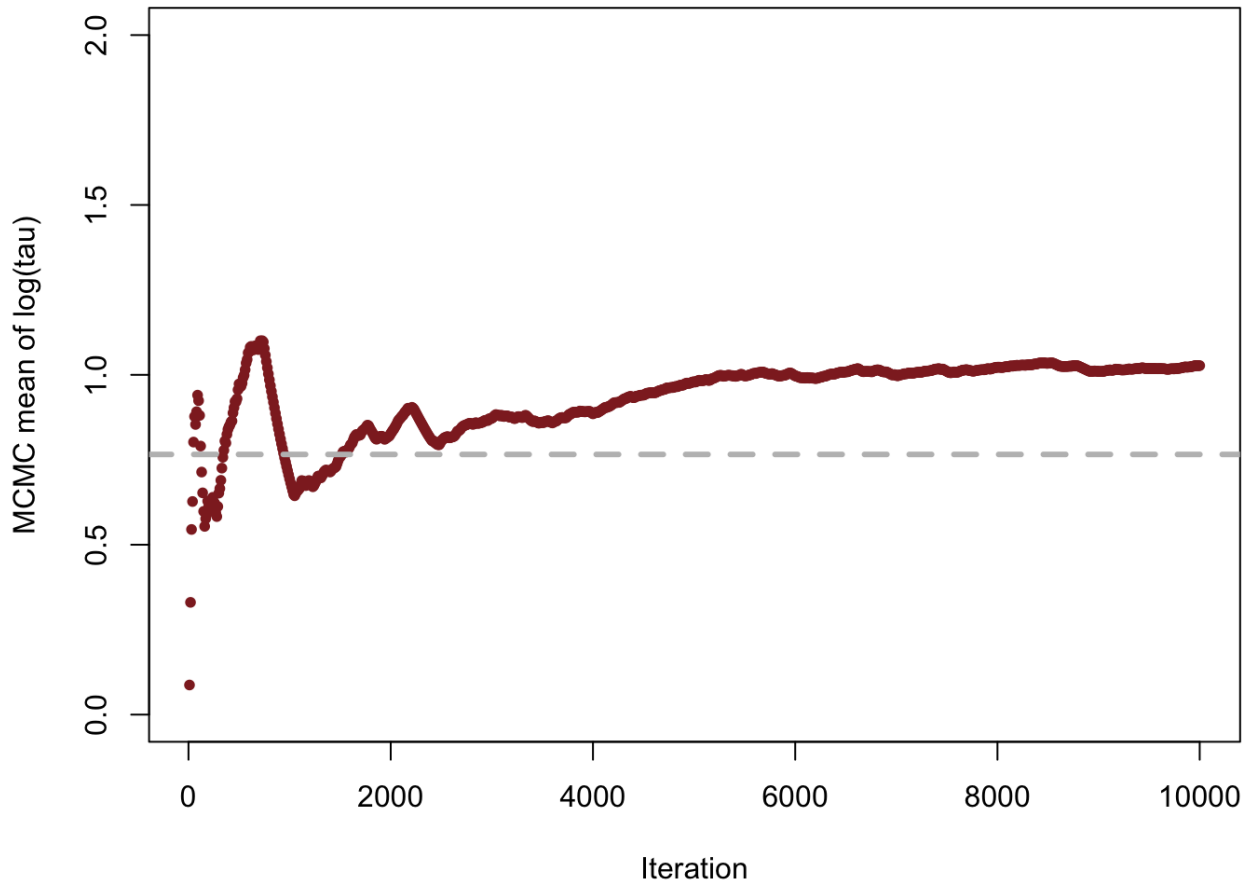

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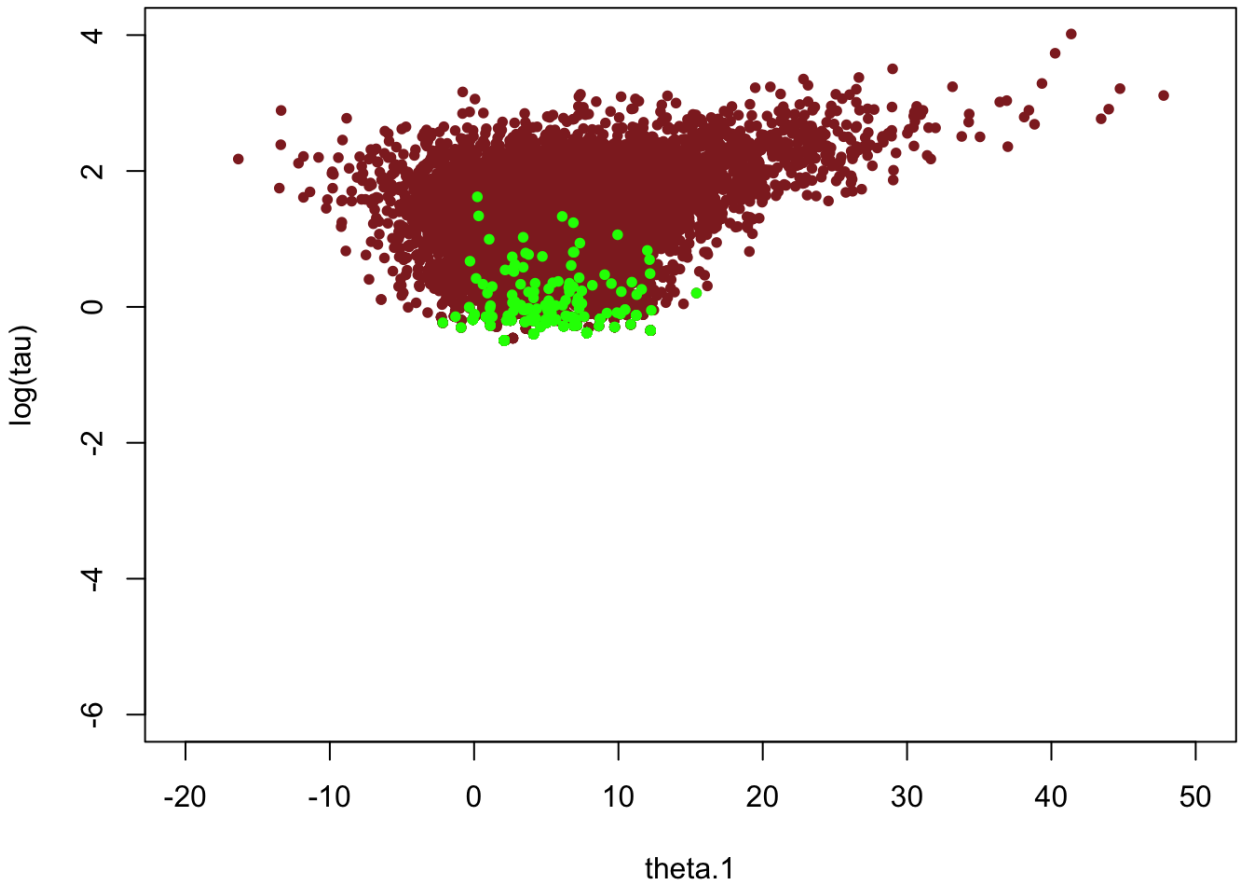

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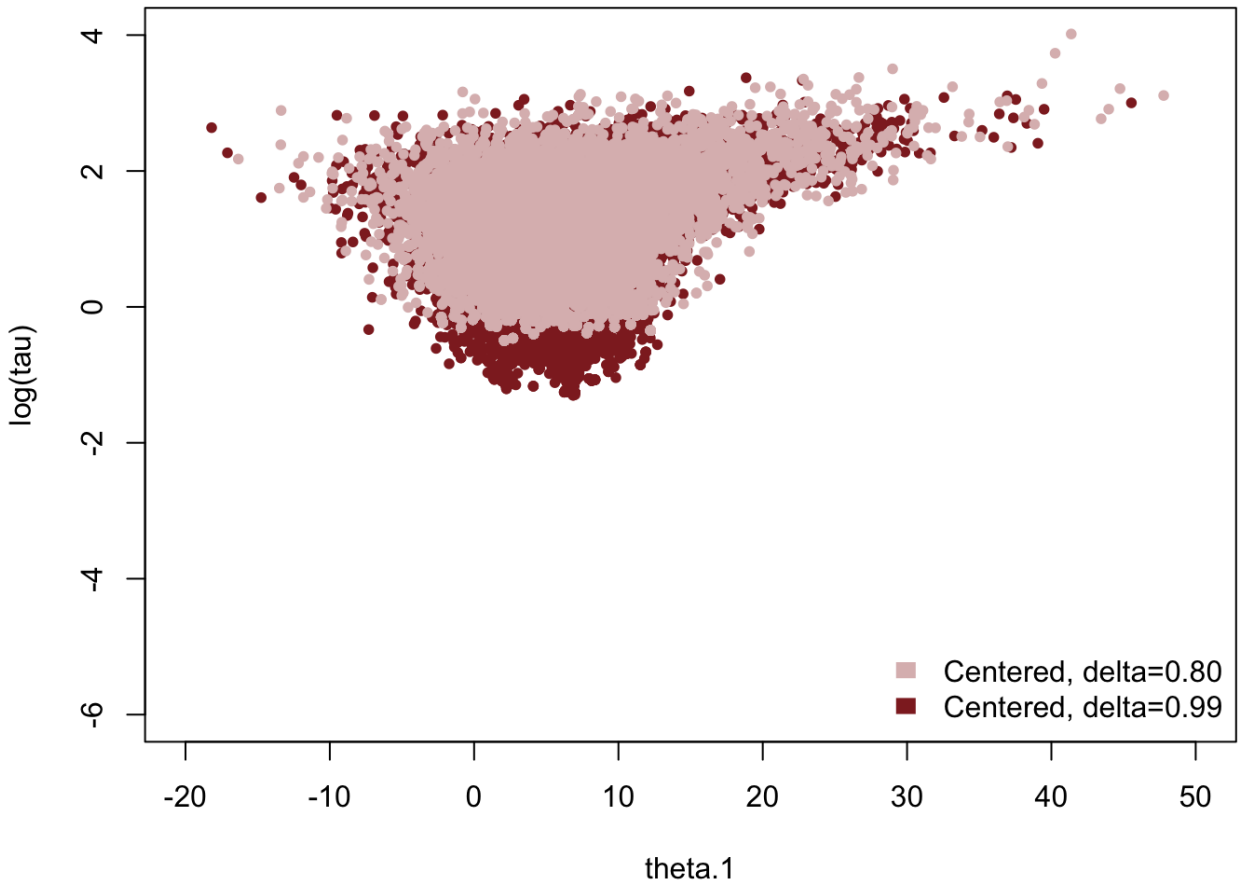

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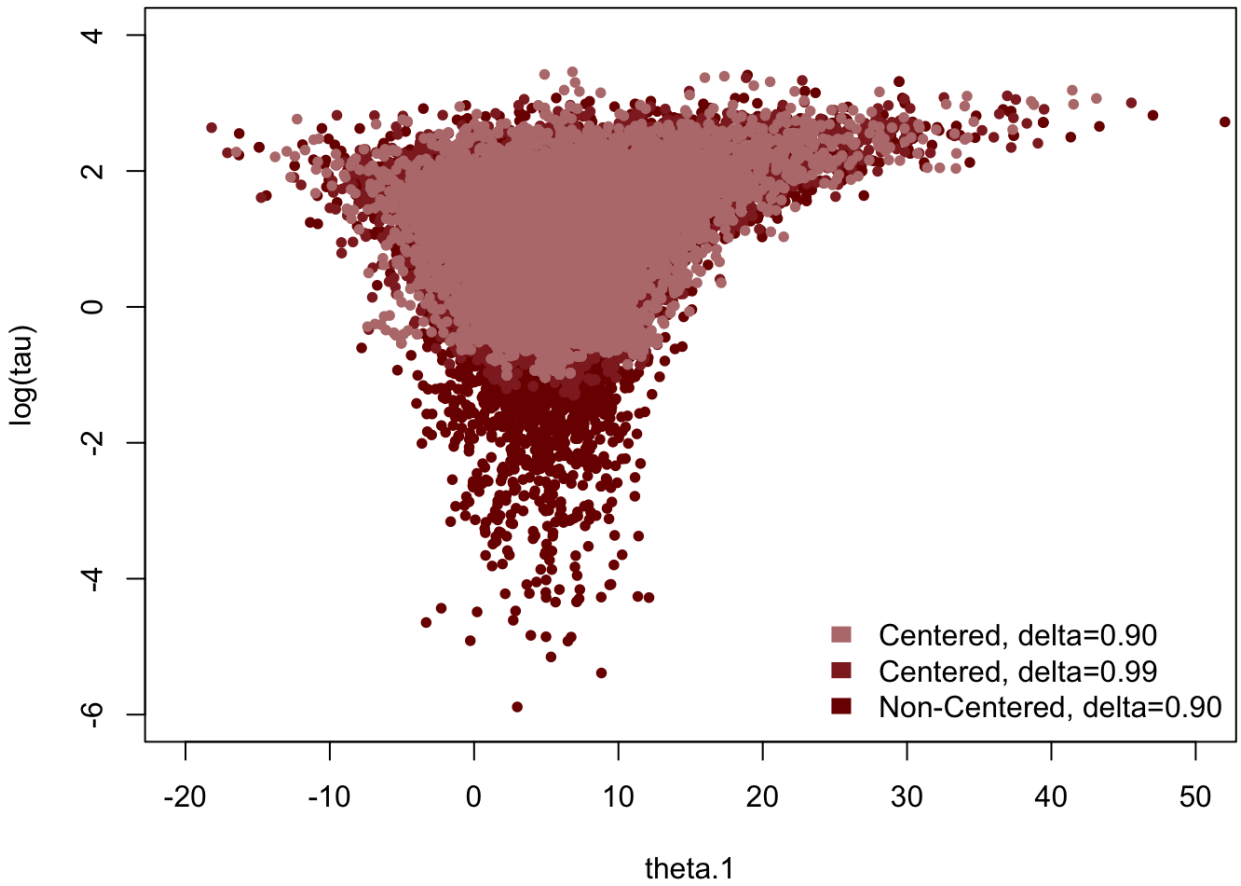

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  - difficult to move from one mode to another
- Long-tailed with non-finite variance and mean
  - efficiency of exploration is reduced
  - central limit theorem doesn't hold for mean and variance

# Some other 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 realted to GHMC
  - but avoids momentum flips after rejection

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- 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, ...

# Stan - probabilistic programming framework

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

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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

```
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 model
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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

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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>

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  - e.g. log transformation for <lower=a>
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- For these declared transformation Stan automatically takes into account the Jacobian of the transformation (see BDA3 p. 21)

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```
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}
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- `_lpdf` for continuous, `_lpmf` for discrete distributions (discrete for the left hand side of `|`)
- for Stan sampler there is no difference between prior and likelihood, all that matters is the final `target`
- you can write in Stan language any program to compute the log density (Stan language is Turing complete)

# Stan

- 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

# 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

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library(cmdstanr)
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d_bin <- list(N = 10, y = 7)
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```

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

# Stan

- Compilation (unless previously compiled model available)
- Warm-up including adaptation
- Sampling
- Generated quantities
- Save posterior draws
- Report divergences, $n_{\text{eff}}$, $\widehat{R}$

# 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

```
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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

```
fit_bin2$summary()
```

| | variable | mean | median | sd | mad | q5 | q95 | rhat | ess_bulk | ess_tail |
|---|---|---|---|---|---|---|---|---|---|---|
| 1 | lp__ | −253. | −253. | 1.0 | 0.74 | −255. | −253. | 1.0 | 1751. | 2231. |
| 2 | theta1 | 0.059 | 0.059 | 0.0093 | 0.0093 | 0.045 | 0.075 | 1.0 | 3189. | 2657. |
| 3 | theta2 | 0.034 | 0.033 | 0.0069 | 0.0067 | 0.023 | 0.046 | 1.0 | 3229. | 2163. |
| 4 | oddsratio | 0.57 | 0.55 | 0.16 | 0.15 | 0.35 | 0.87 | 1.0 | 2998. | 2685. |

# Difference between proportions

```
fit_bin2$summary()
```

| | variable | mean | median | sd | mad | q5 | q95 | rhat | ess_bulk | ess_tail |
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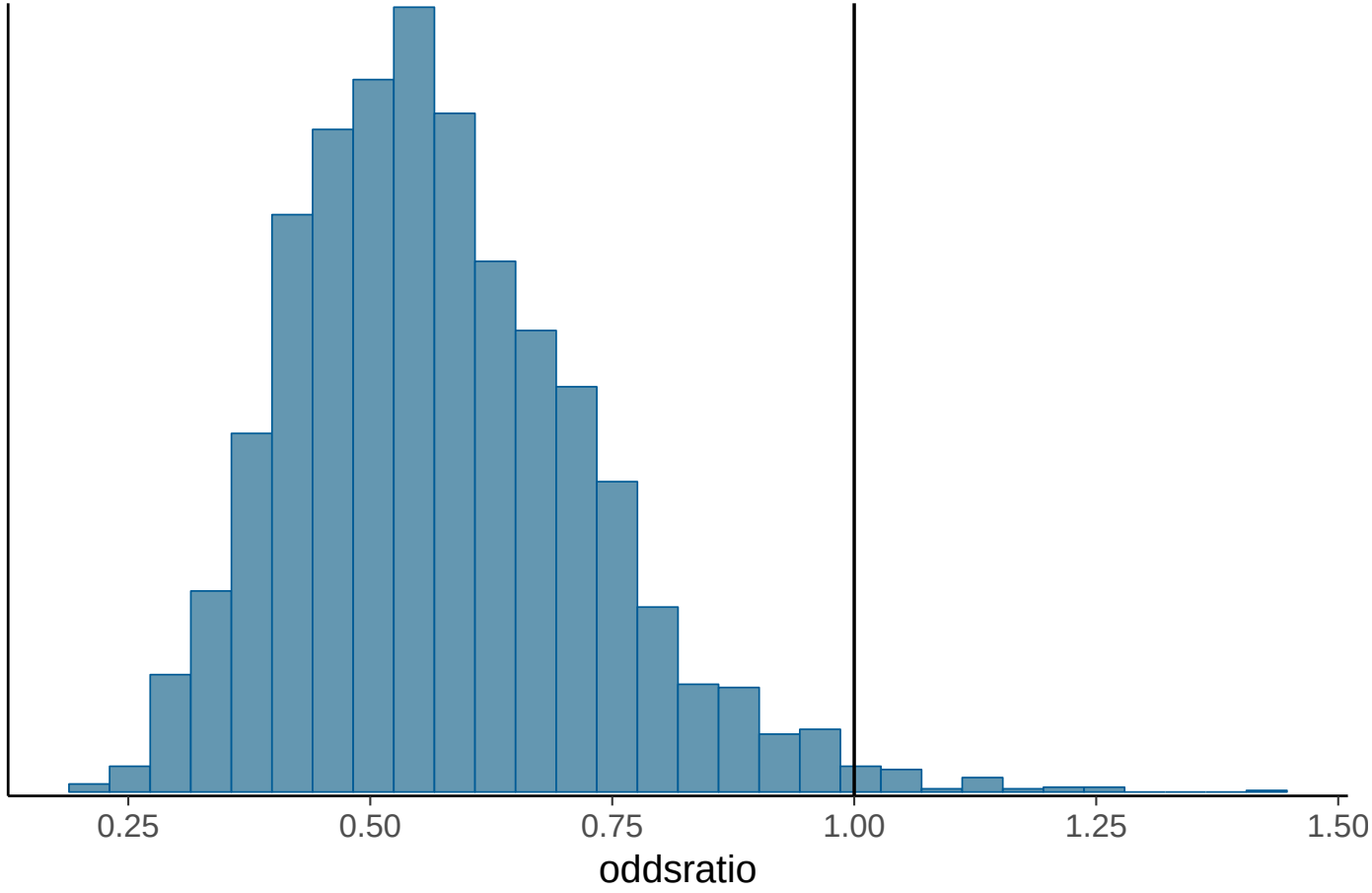
| 4 | oddsratio | 0.57 | 0.55 | 0.16 | 0.15 | 0.35 | 0.87 | 1.0 | 2998. | 2685. |

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

# Difference between proportions

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

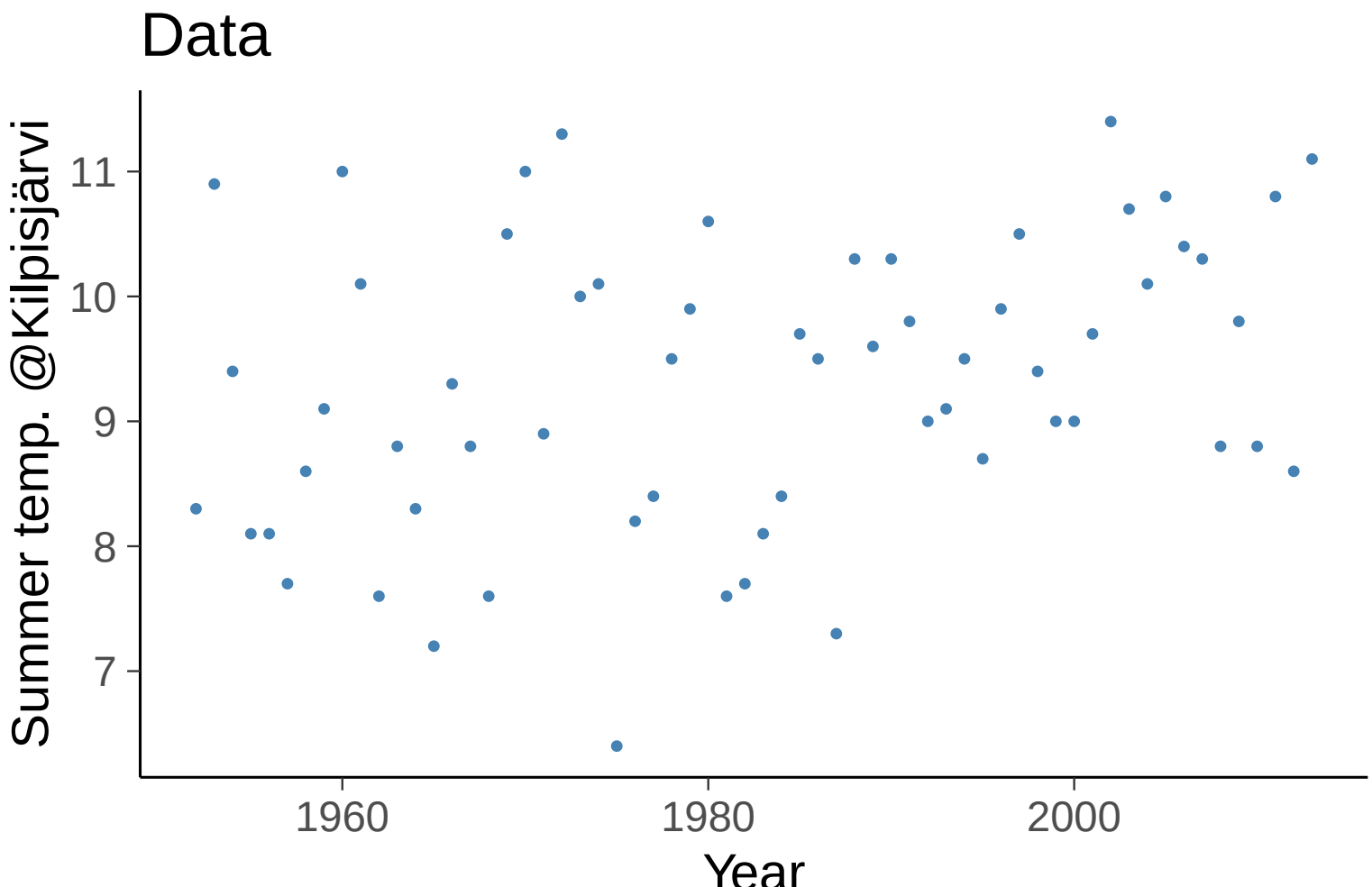


# Shinystan

- Graphical user interface for analysing MCMC results

# Kilpisjärvi summer temperature

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



# Gaussian linear model

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

# Gaussian linear model

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

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

# Gaussian linear model

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

- difference between `vector[N] x` and `array[N] real x`
- no integer vectors: `array[N] int x`

# Gaussian linear model

```
parameters {
      real alpha;
      real beta;
      real<lower=0> sigma;
}
transformed parameters {
      vector[N] mu;
      mu <- alpha + beta*x;
}
```

- transformed parameters are deterministic transformations of parameters and data

# Priors for Gaussian linear model

```
data {
    int<lower=0> N; // number of data points
    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);
    beta ~ normal(pmubeta,psbeta);
    y ~ normal(mu, sigma);
}
```

# Student-$t$ linear model

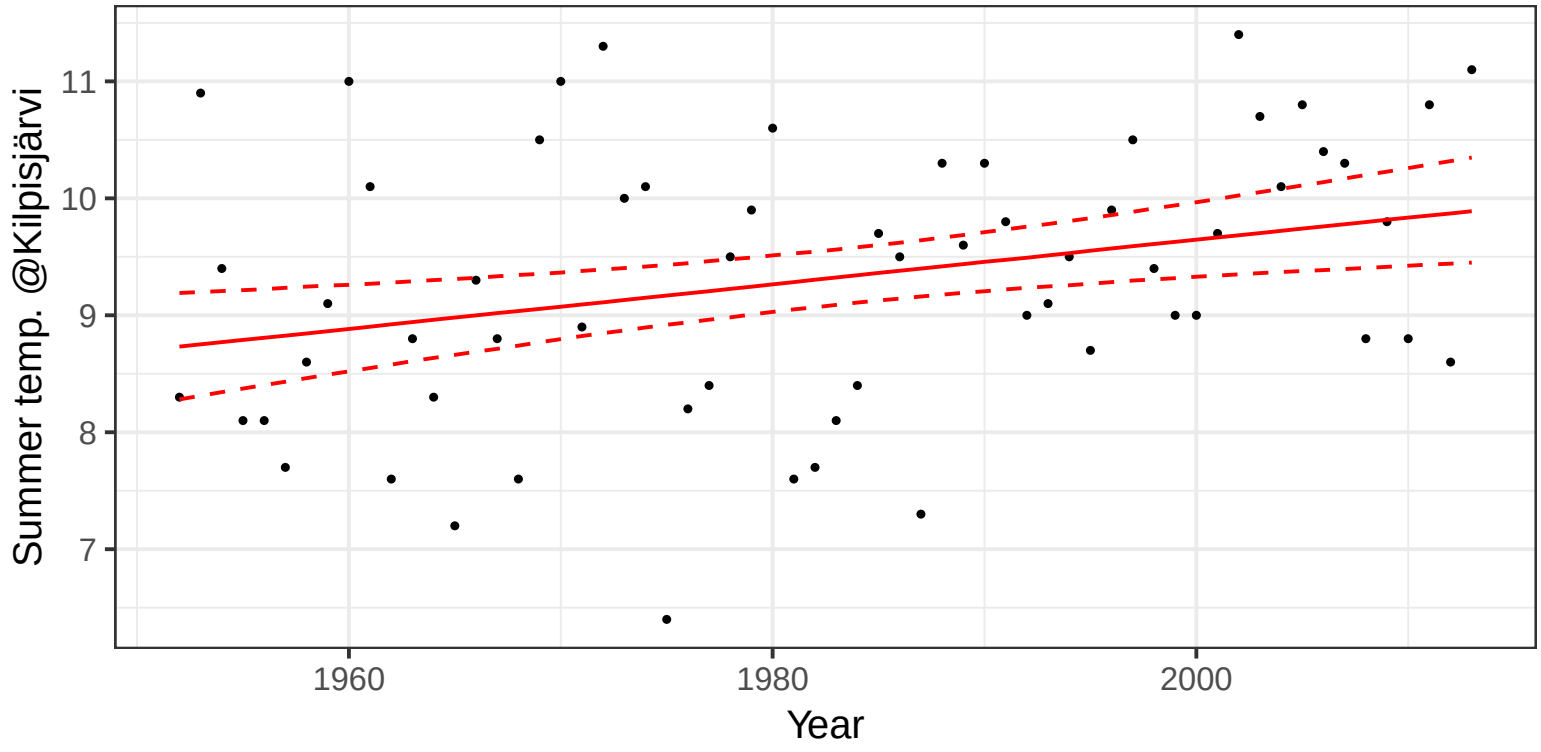
```
...
parameters {
  real alpha;
  real beta;
  real<lower=0> sigma;
  real<lower=1,upper=80> nu;
}
transformed parameters {
  vector[N] mu;
  mu <- alpha + beta*x;
}
model {
  nu ~ gamma(2,0.1);
  y ~ student_t(nu, mu, sigma);
}
```

# Priors

- Prior for temperature increase?

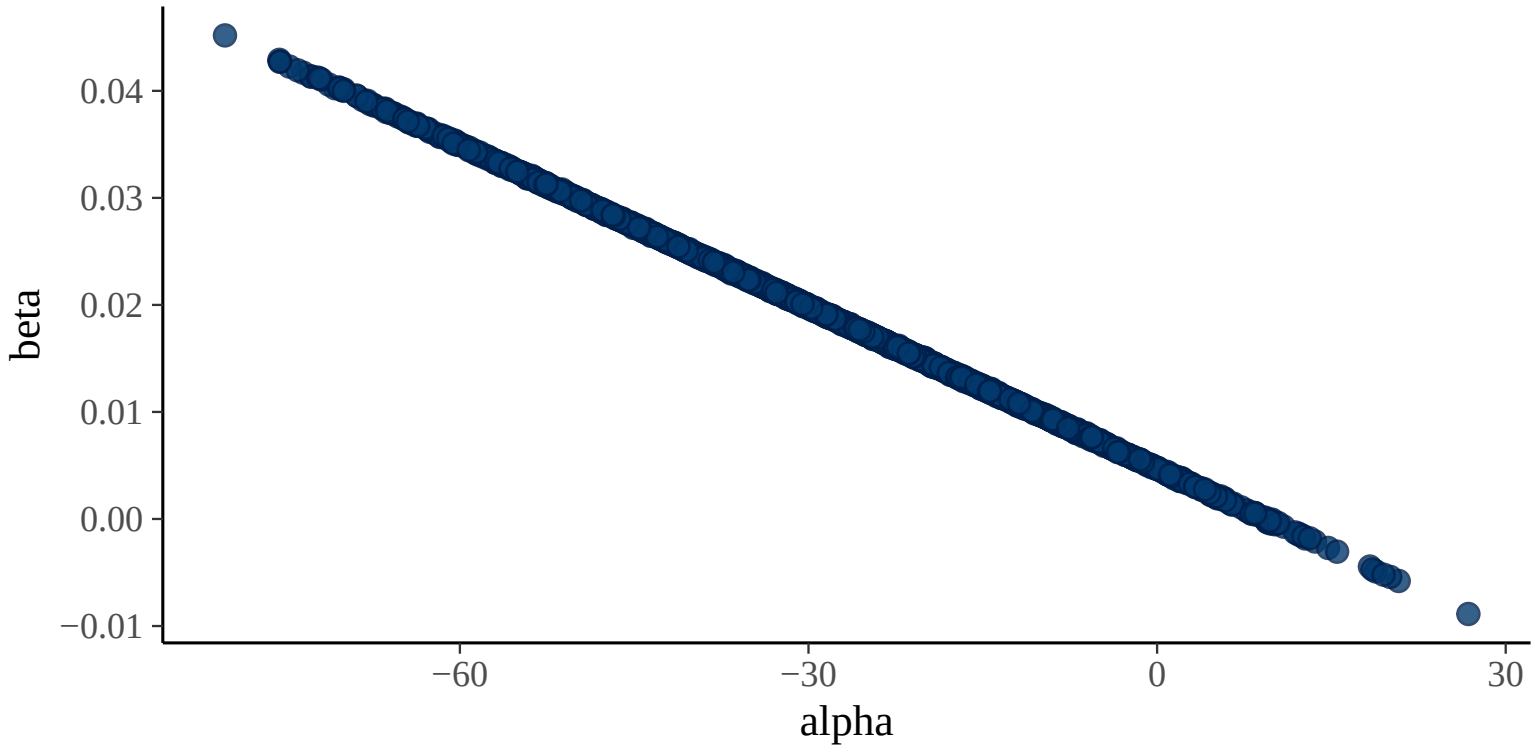
# Kilpisjärvi summer temperature

Posterior fit



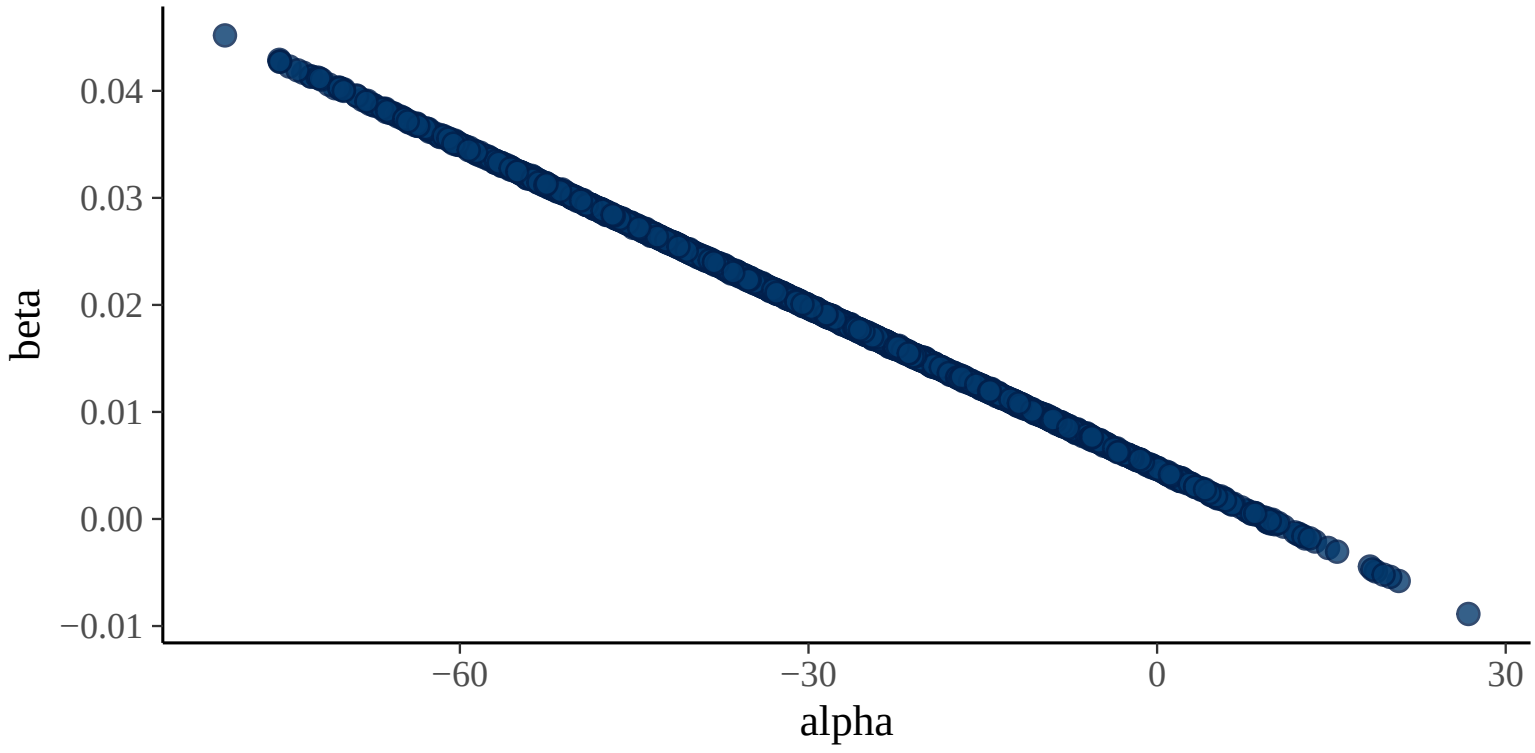
# Kilpisjärvi summer temperature

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 1
See https://mc-stan.org/misc/warnings for details.
```

# Linear regression model in Stan

```
data {
  int<lower=0> N; // number of data points
  vector[N] x; //
  vector[N] y; //
  real xpred; // input location 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);
}
```

# 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)
```

Gaussian linear model

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

# BRMS

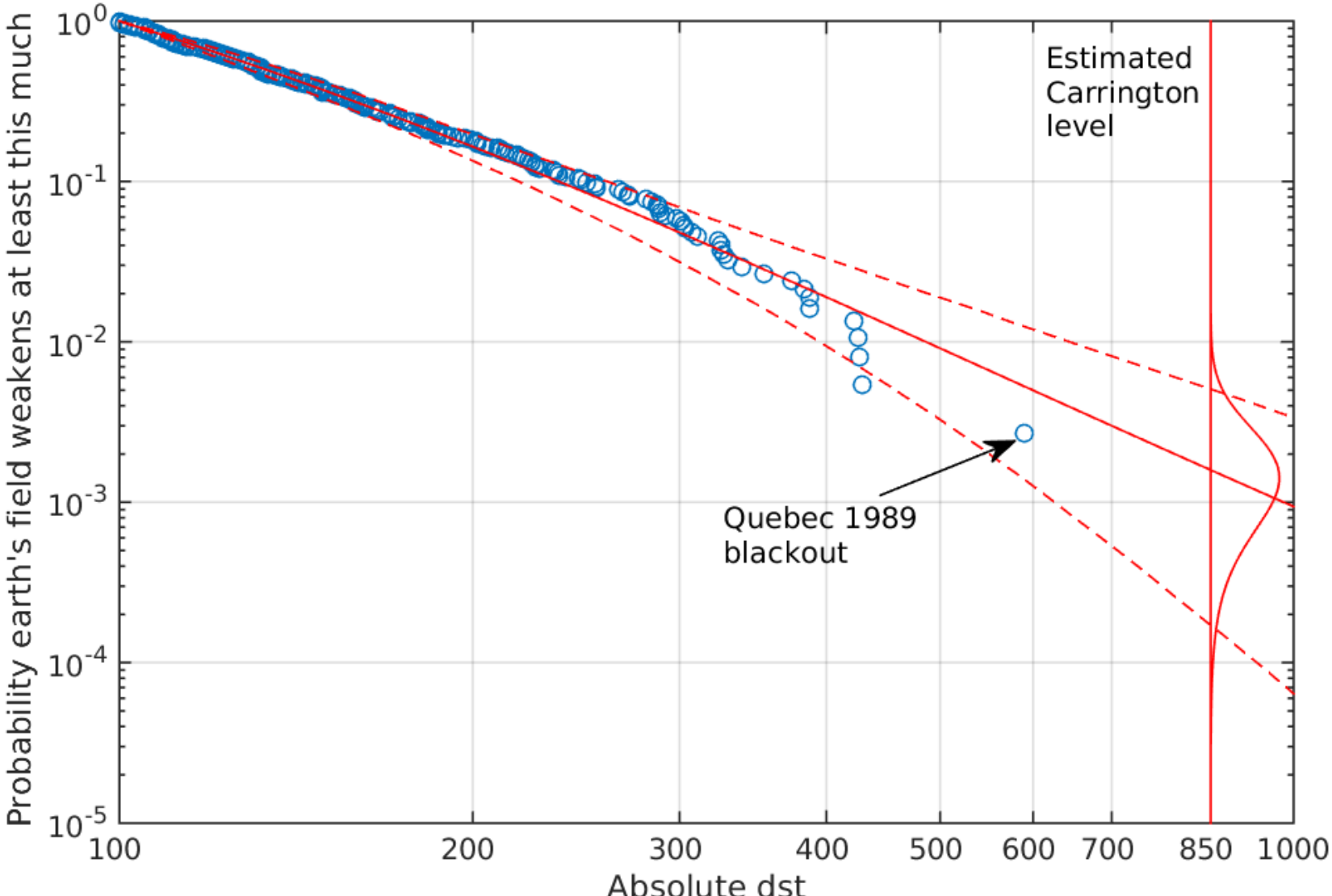
- BRMS provides simplified model description
  - a larger set of models than RStanARM, but still restricted
  - need to wait for the compilation

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

```
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;
  ymax <- max(y);
}
parameters {
  real<lower=0> sigma;
  real<lower=-sigma/ymax> k;
}
model {
  y ~ gpareto(k, sigma);
}
generated quantities {
  vector[Nt] predccdf;
  predccdf<-gpareto_ccdf(yt,k,sigma);
}
```

# 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 (fabs(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 (fabs(k) > 1e-15)
      return exp((-1/k)*log1pv(y/sigma*k));
    else
      return exp(-y/sigma); // limit k->0
  }
}
```

# Other packages

- R
  - posterior — posterior handling and diagnostics
  - shinystan — interactive diagnostics
  - bayesplot — visualization and model checking (see model checking in Ch 6)
  - tideybayes and ggdist – more visualization
  - loo — cross-validation model assessment and comparison (see Ch 7)
  - projpred — projection predictive variable selection
  - priorsense — prior and likelihood sensitivity diagnostics

- Python
  - ArviZ — visualization, and model checking and assessment (see Ch 6 and 7)

# Different interfaces

- CmdStanR / CmdStanPy
  - Lightweight interface on top of commandline program CmdStan
  - Lacks some features that are not needed in this course, but is usually easier to install
- 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
- More recent useful R packages
  - posterior: for handling posterior draws, convergence diagnostics, and summaries
  - tidybayes + ggdist: pretty plots