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

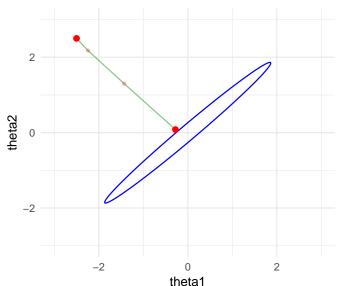
- Gelman, Lee, and Guo (2015) Stan: A probabilistic programming language for Bayesian inference and optimization. http://www.stat.columbia.edu/~gelman/ research/published/stan_jebs_2.pdf
- Carpenter et al (2017). Stan: A probabilistic programming language. Journal of Statistical Software 76(1). https://dox.doi.org/10.18637/jss.v076.i01
- 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

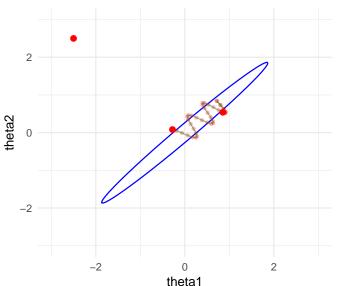
- demo12 1: HMC
- https://chi-feng.github.io/mcmc-demo/
- http://elevanth.org/blog/2017/11/28/ build-a-better-markov-chain/
- cmdstanr_demo, rstan_demo
- http://sumsar.net/blog/2017/01/ bayesian-computation-with-stan-and-farmer-jons/
- http://mc-stan.org/documentation/case-studies.html
- https://mc-stan.org/cmdstanr/
- https://mc-stan.org/rstan/

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

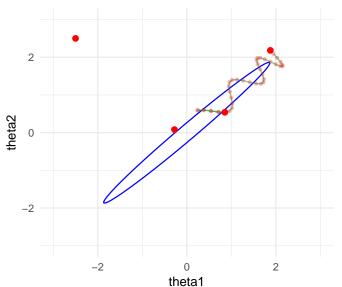
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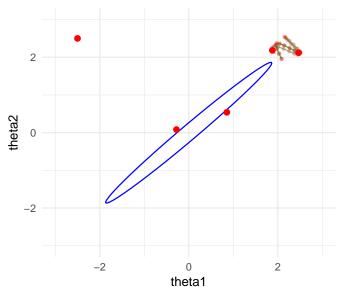
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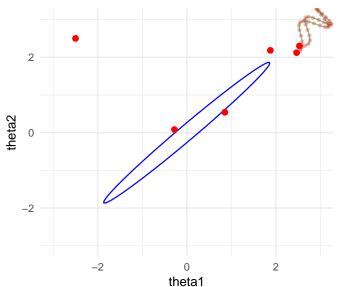
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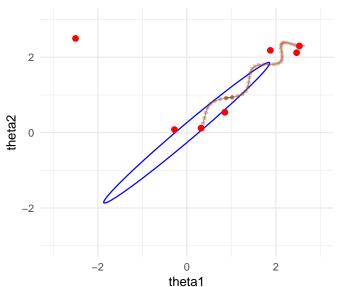
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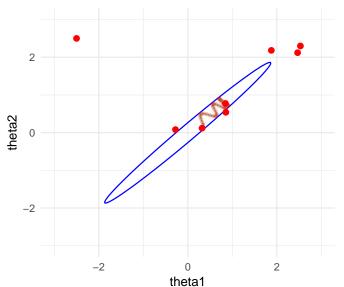
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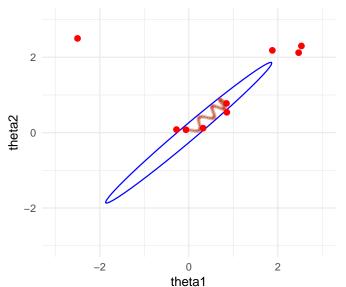
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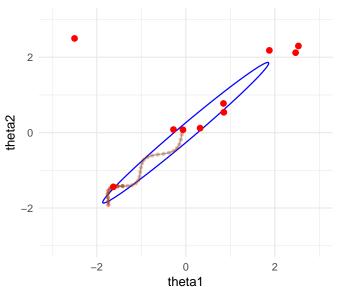
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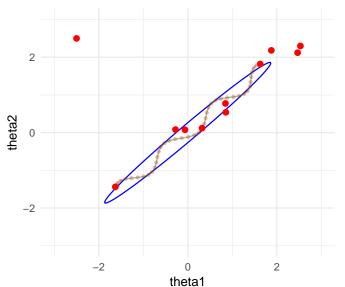
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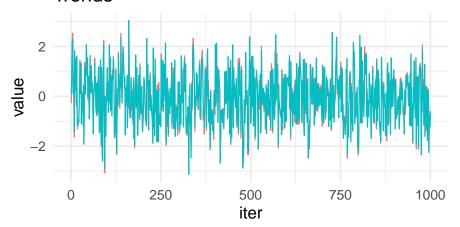


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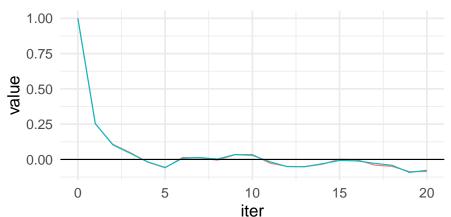
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Trends

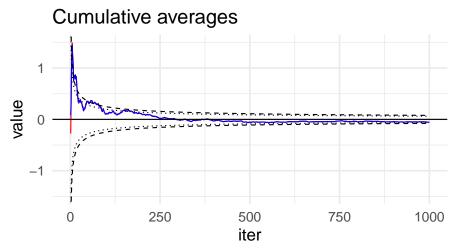


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Autocorrelation function



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-theta1 — theta2 - - 95% interval for MCMC error · · · · 95% interval for indepers

Hamiltonian Monte Carlo / No-U-Turn sampling

- 1. HMC basics (static HMC)
- 2. HMC + leapfrog discretization + Metropolis (static HMC)
- 3. NUTS + slice sampling + Metropolis (dynamic HMC)
- 4. NUTS + multinomial (dynamic HMC)

- Previously
 - · Factorizing: sample from

 - 1) $p(\sigma^2)$, 2) $p(\mu \mid \sigma^2)$

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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 $p(\theta, \phi) = p(\theta)p(\phi)$

- 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

$$p(\theta, \phi) = p(\theta)p(\phi)$$

$$= \frac{1}{Z} \exp(-(U(\theta) + K(\phi)))$$

$$= \frac{1}{Z} \exp(-H(\theta, \phi))$$

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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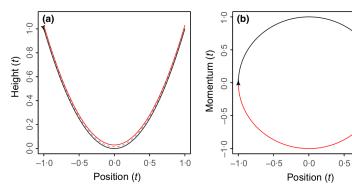
where

- U is potential energy function
- K is kinetic energy function
- H is Hamiltonian energy function
- 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

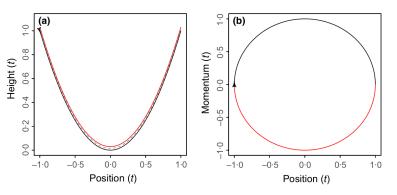
$$\frac{d\theta_i}{dt} = \frac{\partial H}{\partial \phi_i}$$
$$\frac{d\phi_i}{dt} = -\frac{\partial H}{\partial \theta_i}$$



From Monnahan et al (2017)

1.0

- 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 $p(\theta, \phi) \propto \exp(-H(\theta, \phi))$

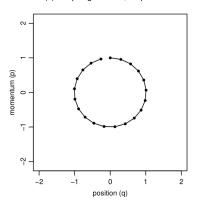


From Monnahan et al (2017)

Leapfrog discretization

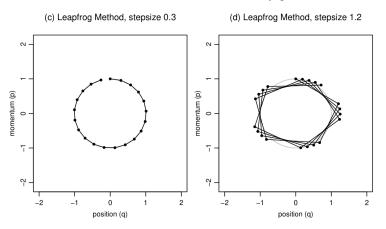
- Leapfrog discretization
 - preserves volume
 - reversible
 - discretization error does not usually grow in time

(c) Leapfrog Method, stepsize 0.3



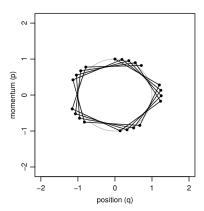
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Leapfrog discretization + Metropolis

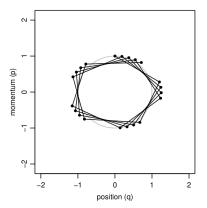
- Leapfrog discretization
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From Neal (2012)

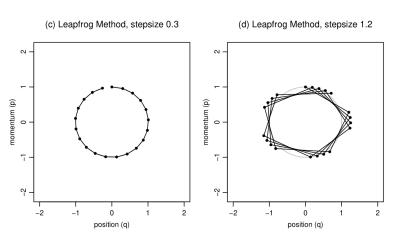
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- Metropolis step with $r = \exp\left(H(\theta^*, \phi^*) H(\theta^{(t-1)}, \phi^{(t-1)})\right)$
 - · accept if the Hamiltonian energy in the end is higher
 - accept with some probability if the Hamiltonian energy in the end is lower



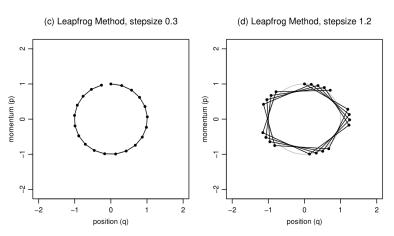
Two steps of Hamiltonian Monte Carlo

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



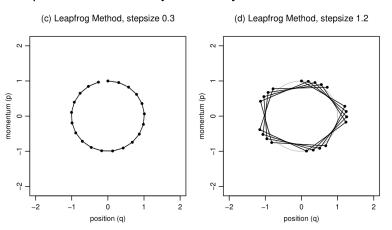
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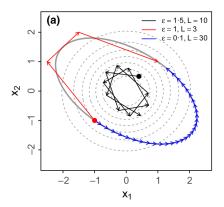
Two steps of Hamiltonian Monte Carlo

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



Leapfrog discretization, step size

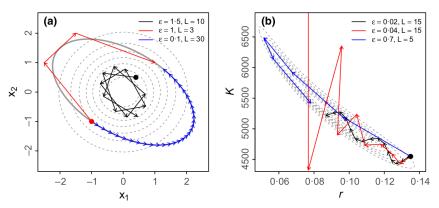
- Small step size → high acceptance rate, but many log density and gradient evaluations
- \bullet Big step size \to less log density and gradient evaluations, but lower acceptance rate



From Monnahan et al (2017)

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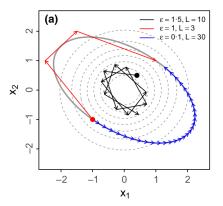
- Small step size → high acceptance rate, but many log density and gradient evaluations
- Big step size → less log density and gradient evaluations, but lower acceptance rate and the simulation may diverge



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



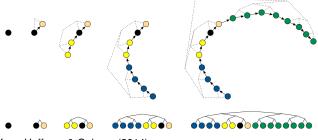
From Monnahan et al (2017)

Static Hamiltonian Monte Carlo

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

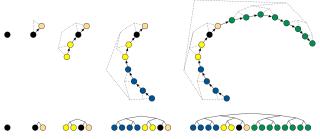
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No-U-Turn sampler with multinomial sampling

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Mass matrix and the step size adaptation

- Mass matrix refers to having different scaling for different parameters and optionally also rotation to reduce correlations
 - mass matrix is estimated during the adaptation phase of the warm-up
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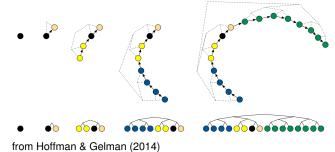
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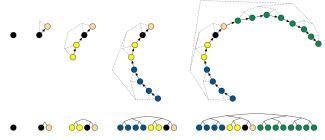
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- After adaptation the algorithm parameters are fixed and some more iterations run to finish the warmup

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



• NUTS specific diagnostic

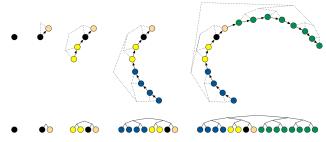
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from Hoffman & Gelman (2014)

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

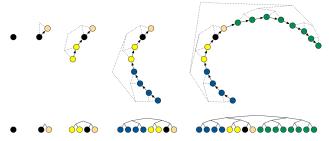
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 - very low inefficiency can indicate problems that need to be inverse-distance
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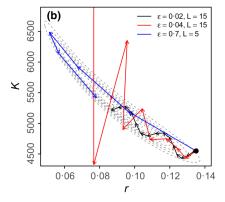
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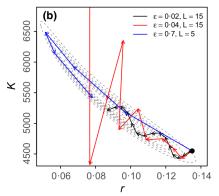
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- Different parameterizations matter

- 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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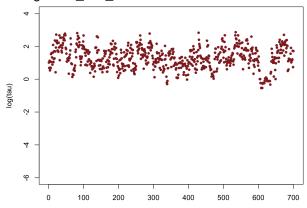


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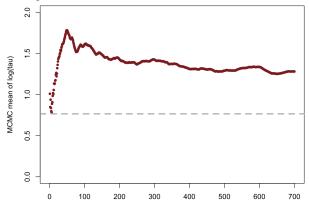
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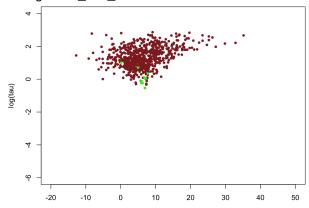
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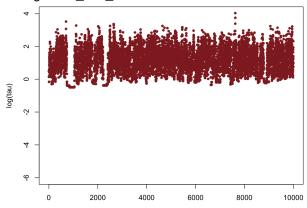
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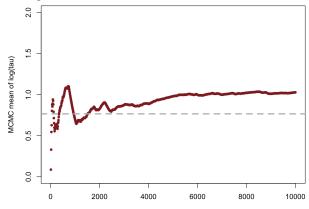


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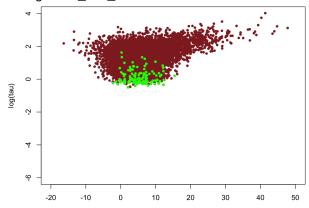
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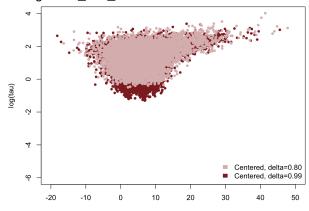


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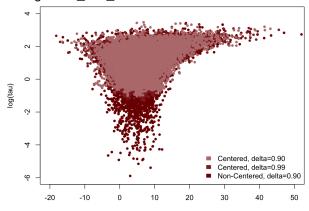
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 - difficult to move from one mode to another
- Long-tailed with non-finite variance and mean
 - efficiency of exploration is reduced
 - central limit theorem doesn't hold for mean and variance

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, ...

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



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 - autodiff to compute gradients of the log density
- More than 100K users in social, biological, and physical sciences, medicine, engineering, and business



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- Several full time developers, 40+ developers, more than 100 contributors
- R, Python, Julia, Scala, Stata, Matlab, command line interfaces
- More than 140 R packages using Stan



Stan

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

```
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 binor
model
  theta \sim 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

- 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

```
parameters {
    real < lower = 0, upper = 1 > theta;
}
```

- 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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    real < lower = 0, upper = 1 > theta;
}
```

- 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)

```
model {
  theta ~ beta(1,1); // prior
  y ~ binomial(N,theta); // likelihood
}
```

```
model {
  theta \sim beta(1,1); // prior
  y ~ binomial(N, theta); // likelihood
    \sim is syntactic sugar and this is equivalent to
model {
  target += beta lpdf(theta | 1, 1);
  target += binomial lpmf(y | N, theta);

    target is the log posterior density
```

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  theta \sim beta(1,1); // prior
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    target is the log posterior density

    lpdf for continuous, lpmf for discrete distributions

    (discrete for the left hand side of |)
```

- target is the log posterior density
- _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

- target is the log posterior density
- _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

CmdStanB

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)</pre>
```

CmdStanB

RStan library (cmdstanr) options (mc. cores = 1) d_bin <- list (N = 10, y = 7)

mod bin <- cmdstan model(stan file = 'binom.stan')</pre>

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, $n_{\rm eff}$, \hat{R}

- 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

```
data {
  int < lower = 0 > N1;
  int <lower = 0 > y1;
  int < lower = 0 > N2;
  int < lower = 0 > v2;
parameters {
  real<lower=0,upper=1> theta1;
  real < lower = 0, upper = 1 > theta2;
model {
  theta1 \sim beta(1,1);
  theta2 \sim beta(1,1);
  y1 ~ binomial(N1, theta1);
  y2 ~ binomial(N2, theta2);
generated quantities {
  real oddsratio:
  oddsratio = (theta2/(1-theta2))/(theta1/(1-theta1));
```

```
data
  int < lower = 0 > N1:
  int <lower = 0 > v1;
  int < lower = 0 > N2;
  int < lower = 0 > v2;
parameters
  real < lower = 0, upper = 1 > theta1;
  real < lower = 0, upper = 1 > theta2;
model
  theta1 \sim beta(1,1);
  theta2 \sim beta(1,1);
  y1 ~ binomial(N1, theta1);
  y2 ~ binomial(N2, theta2);
generated quantities {
  real oddsratio:
```

oddsratio = (theta2/(1-theta2))/(theta1/(1-theta1));

39/63

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

generated quantities is run after the sampling

```
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)
```

...
All 4 chains finished successfully.
Mean chain execution time: 0.0 seconds.
Total execution time: 0.2 seconds.

Chain 1 Iteration: 1001 / 2000 [50%] (Sampling)
Chain 1 Iteration: 2000 / 2000 [100%] (Sampling)

fit_bin2\$summary()

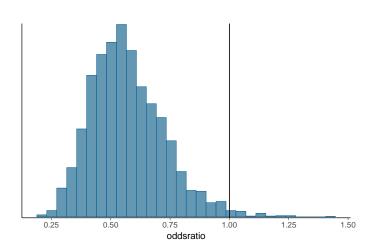
| | variable | mean | median | sd | mad | q5 | q95 | rhat | ess_bulk | ess_tail |
|---|-----------|-------|--------|--------|--------|---------------|---------------|------|----------|----------|
| 1 | lp | -253. | -253. | 1.0 | 0.74 | -255 . | −253 . | 1.0 | 1751. | 2231. |
| 2 | theta1 | 0.059 | 0.059 | 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. |

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. |

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

```
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)))</pre>
```

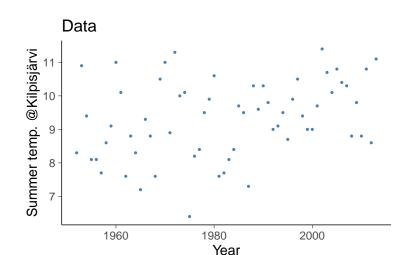


Shinystan

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;
}</pre>
```

 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] v: //
    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

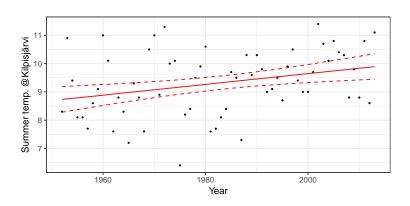
```
parameters {
  real alpha;
  real beta;
  real < lower = 0 > sigma;
  real < lower = 1, upper = 80 > nu;
transformed parameters {
  vector[N] mu;
  mu <- alpha + beta *x;
model {
  nu ~ gamma(2, 0.1);
  y ~ student_t(nu, mu, sigma);
```

Priors

• Prior for temperature increase?

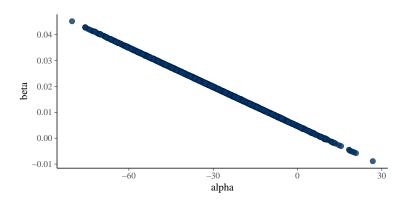
Kilpisjärvi summer temperature

Posterior fit



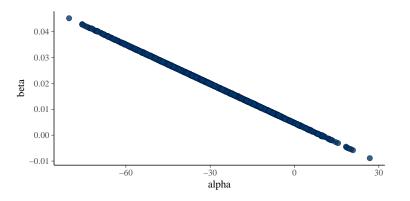
Kilpisjärvi summer temperature

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 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:

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:

Gaussian linear model

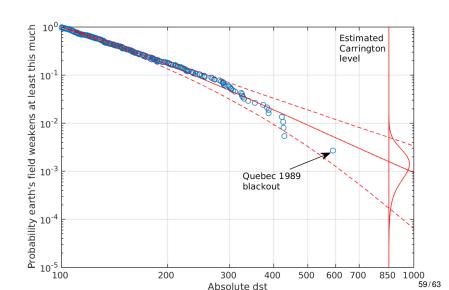
```
fit_lin <- stan_glm(temp ~ year, data = d_lin)</pre>
```

BRMS

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

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 \leftarrow 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);</pre>
```

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 \leftarrow 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/\text{sigma}); // limit k \rightarrow 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