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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 - 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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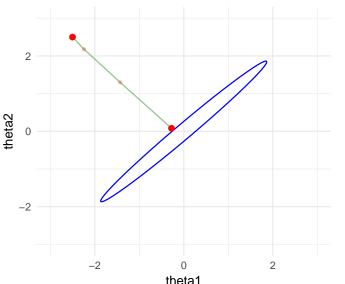
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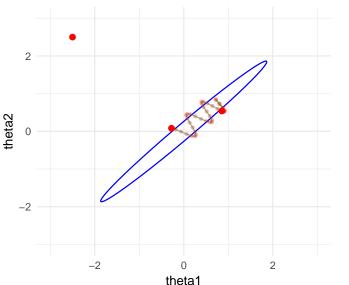
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- Also used as the a high-fidelity reference in Approximate Inference in Bayesian Deep Learning competition https://izmailovpavel.github.io/neurips_bdl_competition/

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

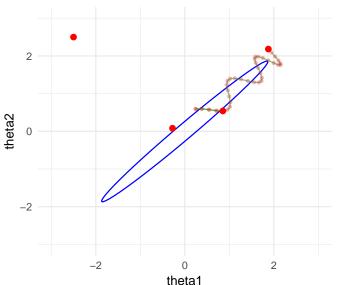
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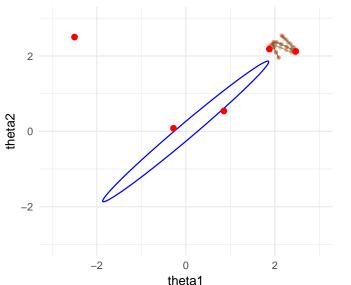
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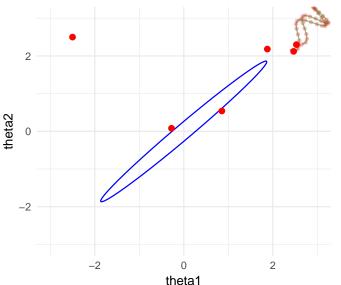
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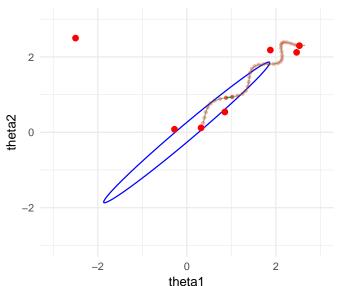
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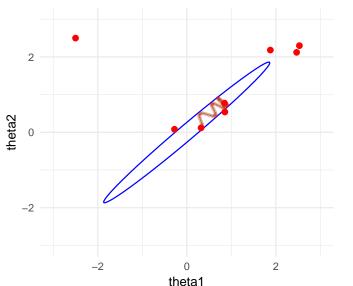
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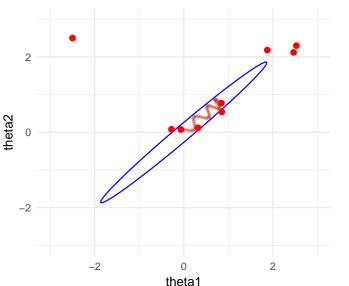
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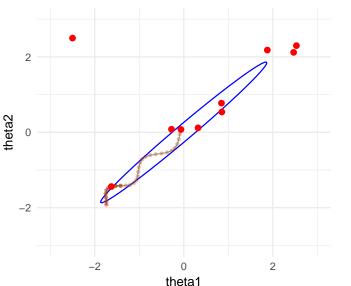
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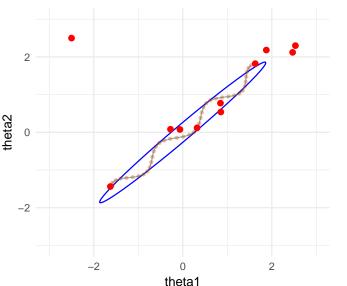
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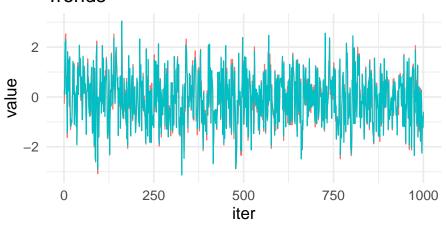


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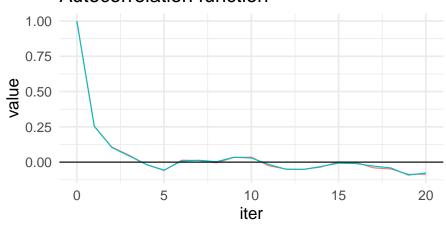
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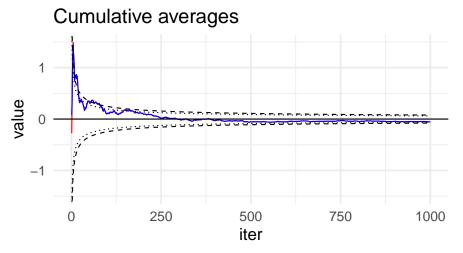


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-theta1 — theta2 - - 95% interval for MCMC error ··· · 95% interval for indeper

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

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

- Related methods
 - Factorizing p(θ₁, θ₂) = p(θ₁ | θ₂)p(θ₂): sample from 1) p(θ₂),
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 - Metropolis: jointly $p(\theta_1, \theta_2)$ jump distribution is a combination of proposal distribution and point mass at the previous value
- HMC
 - Augment with ϕ (the same dimensionality as θ)
 - 1) sample directly from $p(\phi)$,
 - 2) make a special joint Metropolis step for $p(\theta, \phi) = p(\theta)p(\phi)$

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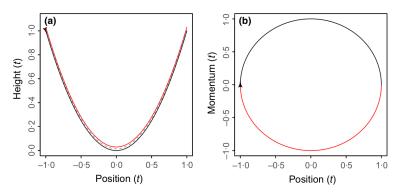
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- ϕ is called a momentum variable
- The potential energy is the negative log density $U(\theta) = -\log(p(\theta)) + C$

Hamiltonian dynamic simulation

Equations of motion, use also the gradient

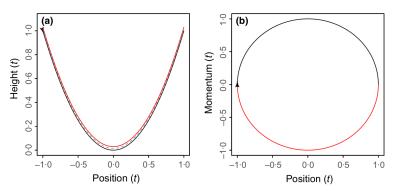
$$\frac{d\theta_i}{dt} = \frac{\partial H}{\partial \phi_i}$$
$$\frac{d\phi_i}{dt} = -\frac{\partial H}{\partial \theta_i}$$



From Monnahan et al (2017)

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

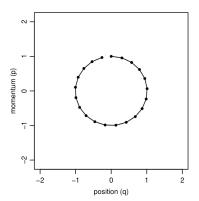


From Monnahan et al (2017)

Leapfrog discretization

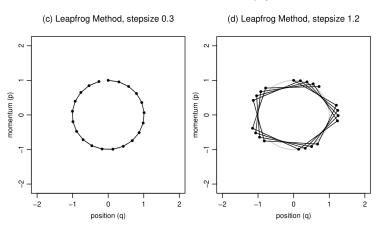
- Leapfrog discretization
 - preserves volume
 - reversible
 - discretization error does not usually grow in time

(c) Leapfrog Method, stepsize 0.3



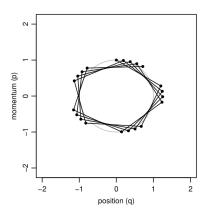
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Leapfrog discretization + Metropolis

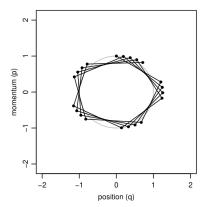
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From Neal (2012)

Leapfrog discretization + Metropolis

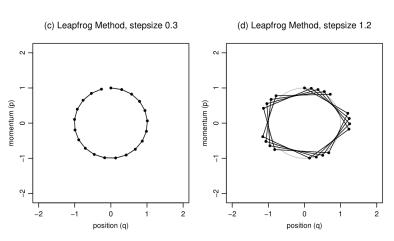
- Leapfrog discretization
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- Metropolis step with $r = \exp(-H(\theta^*, \phi^*) + H(\theta^{(t-1)}, \phi^{(t-1)}))$
 - accept if the Hamiltonian energy in the end is higher
 - accept with some probability if the Hamiltonian energy in the end is lower



From Neal (2012)

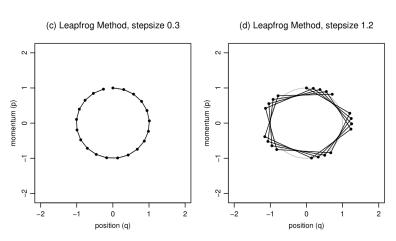
Two steps of Hamiltonian Monte Carlo

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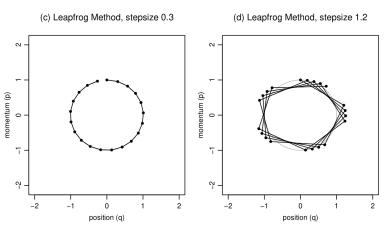
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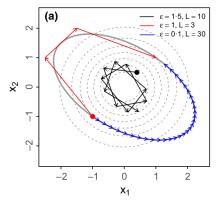
Two steps of Hamiltonian Monte Carlo

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



Leapfrog discretization, step size

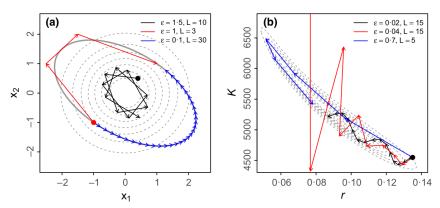
- Small step size → high acceptance rate, but many log density and gradient evaluations
- Big step size → less log density and gradient evaluations, but lower acceptance rate



From Monnahan et al (2017)

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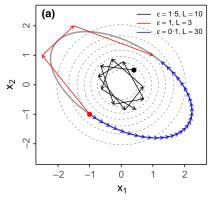
- Small step size → high acceptance rate, but many log density and gradient evaluations
- Big step size → less log density and gradient evaluations, but lower acceptance rate and the simulation may diverge



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



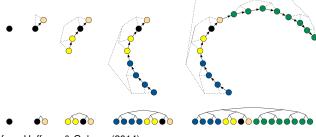
From Monnahan et al (2017)

Static Hamiltonian Monte Carlo

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

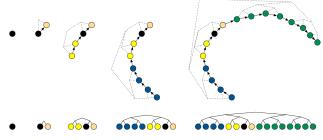
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Mass matrix and the step size adaptation

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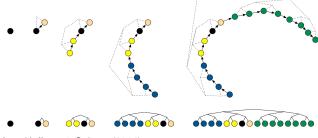
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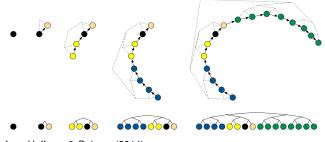
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- After adaptation the algorithm parameters are fixed and some more iterations run to finish the warmup

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



from Hoffman & Gelman (2014)

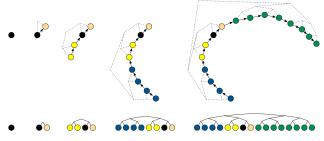
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from Hoffman & Gelman (2014)

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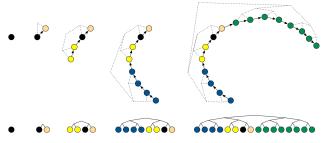
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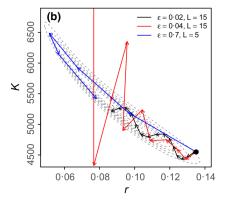
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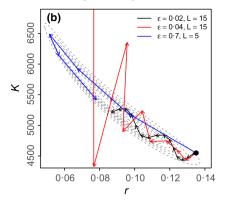
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- Different parameterizations matter

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 - indicates possibility of biased estimates



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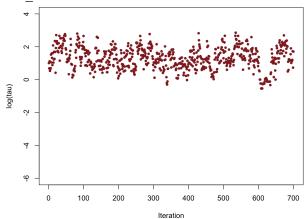


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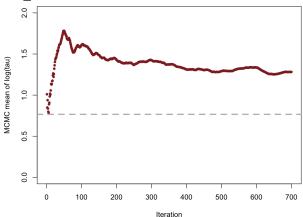
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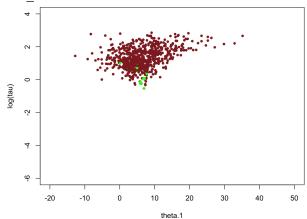
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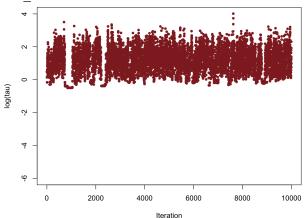
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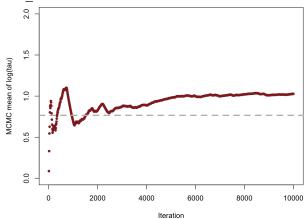
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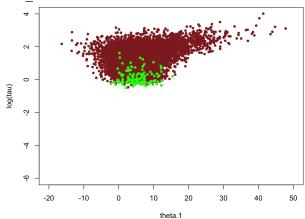


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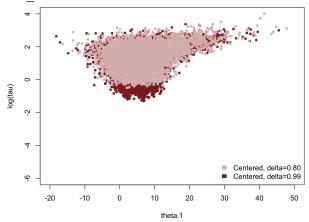
Divergences

- HMC specific: indicates that Hamiltonian dynamic simulation has problems with unexpected fast changes in log-density
 - indicates possibility of biased estimates
- http://mc-stan.org/users/documentation/case-studies/divergences_ and bias.html



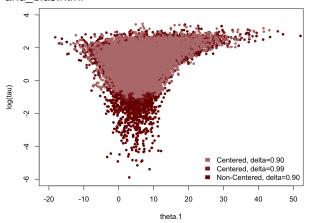
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- Multimodal
 - difficult to move from one mode to another
- Long-tailed with non-finite variance and mean
 - efficiency of exploration is reduced
 - central limit theorem doesn't hold for mean and variance

Some other recent HMC and gradient based variants

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

Probabilistic programming language

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

Probabilistic programming language

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

Probabilistic programming

- Enables agile workflow for developing probabilistic models
 - language
 - automated inference
 - diagnostics
- Many frameworks Stan, PyMC, Pyro (Uber), TFP (Google), Turing.jl, JAGS, ELFI, ...

- 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 200K users in social, biological, and physical sciences, medicine, engineering, and business
- Several full time developers, 40+ developers, more than 100 contributors
- R, Python, Julia, Scala, Stata, command line interfaces
- More than 200 R packages using Stan



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 binomial
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

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- 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;
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```

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

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

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

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target is the log posterior density (Lecture 4 discussed log)

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- target is the log posterior density (Lecture 4 discussed log)
- _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)</pre>
```

CmdStanR

```
RStan

library (cmdstanr)

options (mc.cores = 1)

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

mod_bin <- cmdstan_model(stan_file = 'binom.stan')

fit_bin <- mod_bin$sample(data = d_bin)
```

PyStan

PyStan

```
import pystan import stan_utility
```

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

PyStan

```
PyStan
import pystan
import stan_utility

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

Stan

- Compilation (unless previously compiled model available)
- Warm-up including adaptation
- Sampling
- Generated quantities
- Save posterior draws
- Report divergences, n_{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

```
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));
```

```
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));
```

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

generated quantities is run after the sampling

```
d bin2 \leftarrow 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 MOMC 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.

fit_bin2\$summary()

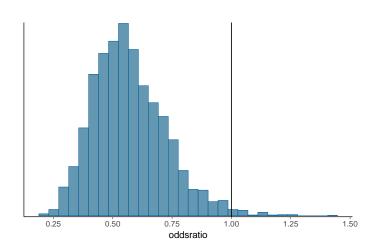
	variable	mean	median	sd	mad	q5	q95	rhat	ess_bulk	ess_tail
1	lp	-253.	-253.	1.0	0.74	-255.	-253.	1.0	1751.	2231.
2	theta1	0.059	0.059	0.0093	0.0093	0.045	0.075	1.0	3189.	2657.
3	theta2	0.034	0.033	0.0069	0.0067	0.023	0.046	1.0	3229.	2163.
4	oddsratio	0.57	0.55	0.16	0.15	0.35	0.87	1.0	2998.	2685.

fit_bin2\$summary()

```
variable
              mean
                     median
                                    mad
                                              a5
                                                     q95
                                                          rhat ess bulk ess tail
1 lp___
           -253.
                   -253.
                            1.0
                                  0.74
                                                           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

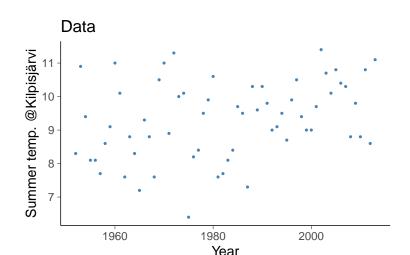
```
draws <- fit_bin2$draws()
mcmc_hist(draws, pars = 'oddsratio') +
  geom_vline(xintercept = 1) +
  scale_x_continuous(breaks = c(seq(0.25,1.5,by=0.25)))</pre>
```



Shinystan

Graphical user interface for analysing MCMC results

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



```
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);
```

```
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

```
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
- only integer arrays: array[N] int x

```
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);
```

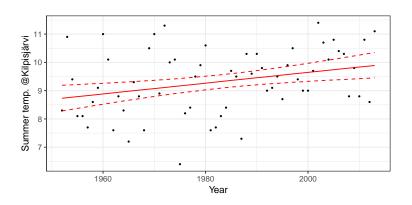
Student-t linear model

```
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 \sim gamma(2,0.1);
  y ~ student_t(nu, mu, sigma);
```

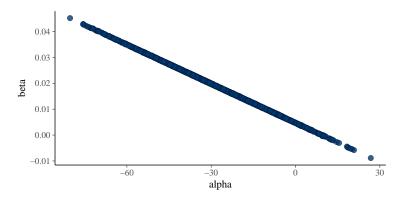
Priors

• Prior for temperature increase?

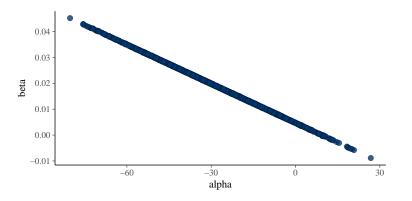
Posterior fit



Posterior draws of alpha and beta



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.

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);
   x_pred_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

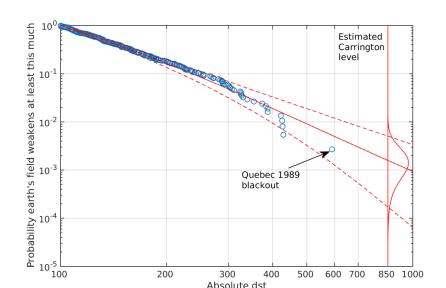
```
fit_lin \leftarrow stan_glm(temp \sim year, data = d_lin)
```

brms

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

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);</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 (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) \cdot \log 1 \operatorname{pv}(y/\operatorname{sigma} \cdot k));
    else
      return \exp(-y/\text{sigma}); // limit k \rightarrow 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 (Lecture 5)
- shinystan interactive diagnostics
- bayesplot visualization and model checking (Lectures 5 and 8)
- tidybayes and ggdist more posterior and prediction visualization
- loo cross-validation model assessment and comparison (Lecture 9)
- projpred projection predictive variable selection (Lecture 12)
- priorsense prior and likelihood sensitivity diagnostics (can be useful in project)
- Python
 - ArviZ visualization, and model checking and assessment