Bayesian Statistics and Data Analysis
Lecture 6

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Section 1

Introduction

Extra material for dynamic HMC

- Michael Betancourt (2018). A Conceptual Introduction to Hamiltonian Monte Carlo.
  https://arxiv.org/abs/1701.02434
- Cole C. Monnahan, James T. Thorson, and Trevor A. Branch (2016) Faster estimation of Bayesian models in ecology using Hamiltonian Monte Carlo.
  https://dx.doi.org/10.1111/2041-210X.12681

Extra material for Stan

- Andrew Gelman, Daniel Lee, and Jiqiang 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
- http://elevanth.org/blog/2017/11/28/build-a-better-markov-chain/
- rstan_demo
- rstanarm_demo
- http://sumsar.net/blog/2017/01/bayesian-computation-with-stan-and-farmer-jons/
- http://mc-stan.org/documentation/case-studies.html
- https://cran.r-project.org/package=rstan
- https://cran.r-project.org/package=rstanarm

Hamiltonian Monte Carlo

- Uses log density (negative log density is called energy)
- Uses gradient of log density for more efficient sampling
- Augments parameter space with momentum variables

Hamiltonian Monte Carlo

- Uses log density (negative log density is called energy)
- Uses gradient of log density for more efficient sampling
- Augments parameter space with momentum variables
- Simulation of Hamiltonian dynamics reduces random walk
  - Explanation of HMC with black board
  - http://elevanth.org/blog/2017/11/28/
    build-a-better-markov-chain/

Hamiltonian Monte Carlo

- Uses gradient of log density for more efficient sampling
- Alternating dynamic simulation and sampling energy level
- Parameters: step size, number of steps in each chain
- No U-Turn Sampling (NUTS) and dynamic HMC
  - adaptively selects number of steps to improve robustness and efficiency
  - dynamic HMC refers to dynamic trajectory length
  - to keep reversibility of Markov chain, need to simulate in two directions
  - http://elevanth.org/blog/2017/11/28/build-a-better-markov-chain/
- Dynamic simulation is discretized
  - small step size gives accurate simulation, but requires more log density evaluations
  - large step size reduces computation, but increases simulation error which needs to be taken into account in the Markov chain
  - black board explanation of the effect of step size

Adaptive dynamic HMC in Stan

- Dynamic HMC using growing tree to increase simulation trajectory until no-U-turn criterion stopping
  - max treedepth to keep computation in control
  - pick a draw along the trajectory with probabilities adjusted to take into account the error in the discretized dynamic simulation
  - give bigger weight for tree parts further away to increase probability of jumping further away
- Mass matrix and step size adaptation in Stan
  - mass matrix refers to having different scaling for different parameters and optionally also rotation to reduce correlations
  - mass matrix and step size adjustment and are estimated during initial adaptation phase
  - step size is adjusted to be as big as possible while keeping discretization error in control (adapt_delta)
- After adaptation the algorithm parameters are fixed
- After warmup store iterations for inference
- See more details in Stan reference manual

Max tree depth diagnostic

- Dynamic HMC specific diagnostic
- Indicates inefficiency in sampling leading to higher autocorrelations and lower ESS (n_{eff})
- Different parameterizations matter

Divergences

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

Problematic distributions

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

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, PyMC3, Pyro (Uber), Edward (Google), Birch, ELFI, ...

Stan - probabilistic programming framework

- Language, inference engine, user interfaces, documentation, case studies, diagnostics, packages, ...
  - autodiff to compute gradients of the log density
- More than ten thousand 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, Matlab, command line interfaces
- More than 100 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
}

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

Binomial model - Stan code

```
data {
  int<lower=0> N;          // number of experiments
  int<lower=0, upper=N> y; // number of successes
}
```

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

Binomial model - Stan code

```
parameters {
  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)

Binomial model - Stan code

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

Binomial model - Stan code

```
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);
}
```

• 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

RStan

RStan

```
library(rstan)
rstan_options(auto_write = TRUE)
options(mc.cores = parallel::detectCores())

d_bin <- list(N = 10, y = 7)
fit_bin <- stan(file = 'binom.stan', 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)
```

Stan

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

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

```stan
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 = 2
fit_bin2 <- stan(file = 'binom2.stan', data = d_bin
```

```
starting worker pid=10151 on localhost:11783 at 10:03:27.872
starting worker pid=10164 on localhost:11783 at 10:03:28.087
starting worker pid=10176 on localhost:11783 at 10:03:28.295
starting worker pid=10185 on localhost:11783 at 10:03:28.461

SAMPLING FOR MODEL 'binom2' NOW (CHAIN 1).

Gradient evaluation took 6e-06 seconds
1000 transitions using 10 leapfrog steps per transition would take 0.06 seconds.
Adjust your expectations accordingly!


Iteration:    1 / 2000 [  0%]  (Warmup)
Iteration:  200 / 2000 [ 10%]  (Warmup)
...
Iteration: 1000 / 2000 [ 50%]  (Warmup)
Iteration: 1001 / 2000 [ 50%]  (Sampling)
...
Iteration: 2000 / 2000 [100%]  (Sampling)

 Elapsed Time: 0.012908 seconds (Warm-up)
               0.017027 seconds (Sampling)
               0.029935 seconds (Total)


SAMPLING FOR MODEL 'binom2' NOW (CHAIN 2).
...
```

Difference between proportions

```
monitor(fit_bin2, probs = c(0.1, 0.5, 0.9))
```

```
Inference for the input samples
(4 chains: each with iter=1000; warmup=0):
```

	mean	se_mean	sd	10%	50%	90%	n_eff	Rhat
theta1	0.1	0	0.0	0.0	0.1	0.1	3280	1
theta2	0.0	0	0.0	0.0	0.0	0.0	3171	1
oddsratio	0.6	0	0.2	0.4	0.6	0.8	3108	1
lp__	−253.5	0	1.0	−254.8	−253.2	−252.6	1922	1

```
For each parameter, n_eff is a crude measure of effective samp
and Rhat is the potential scale reduction factor on split chain
convergence, Rhat=1).
```

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

Difference between proportions

```
draws <- as.data.frame(fit_bin2)
mcmc_hist(draws, pars = 'oddsratio') +
  geom_vline(xintercept = 1) +
  scale_x_continuous(breaks = c(seq(0.25,1.5,by=0.
```
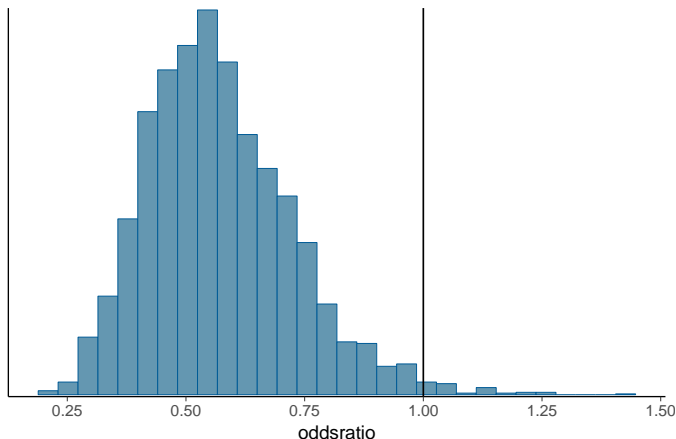
HMC specific diagnostics

```
check_treedepth(fit_bin2)
check_energy(fit_bin2)
check_div(fit_bin2)

[1] "0 of 4000 iterations saturated the maximum tree depth of 1
[1] "0 of 4000 iterations ended with a divergence (0%)"
```
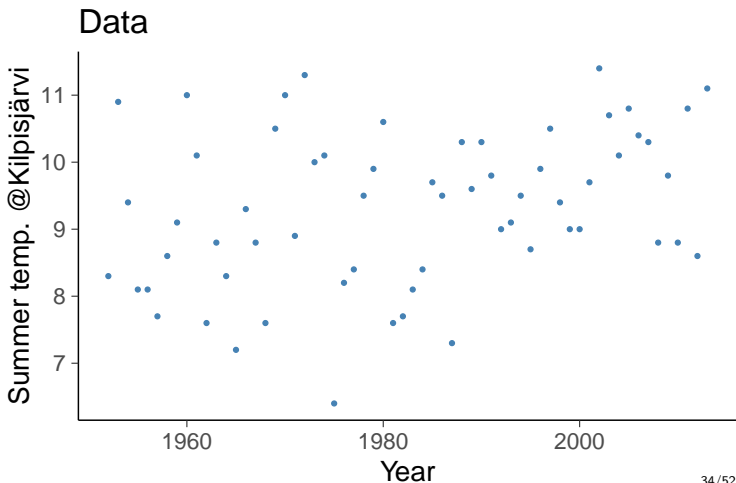
Shinystan

- 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?

Data

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

• Introduction

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

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

Gaussian linear model

• Introduction

```
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);
}
```
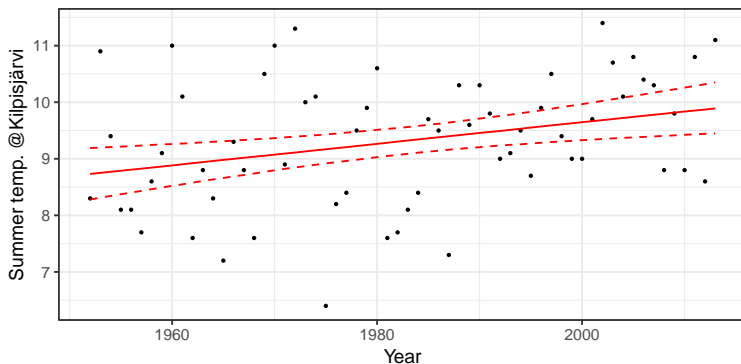
Priors

- Prior for temperature increase?

Kilpisjärvi summer temperature

UPPSALA
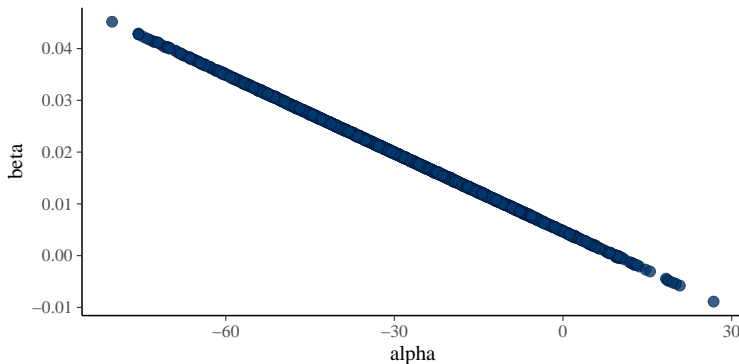UNIVERSITET

· Introduction

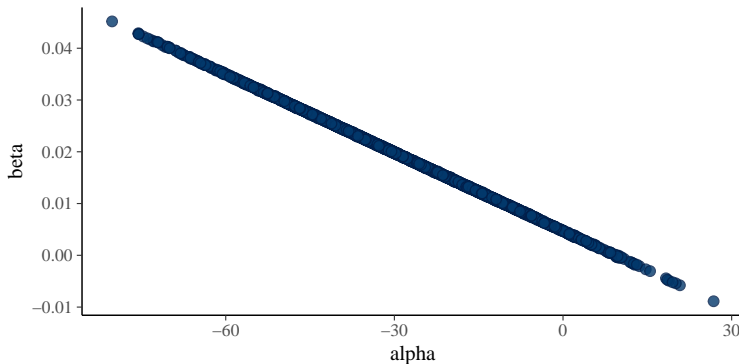Posterior fit

Kilpisjärvi summer temperature

Posterior draws of alpha and beta

Kilpisjärvi summer temperature

Posterior draws of alpha and beta

There were 14 transitions after warmup that exceeded the maximu
treedepth. Increase max_treedepth above 10. See
http://mc-stan.org/misc/warnings.html#maximum-treedepth-exceede
Examine the pairs() plot to diagnose sampling problems

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

RStanARM

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  - no need to wait for compilation
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Two group Binomial model:

```
d_bin2 <- data.frame(N = c(674, 680), y = c(39,22), grp2 = c(0
fit_bin2 <- stan_glm(y/N ~ grp2, family = binomial(), data = d.
                     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
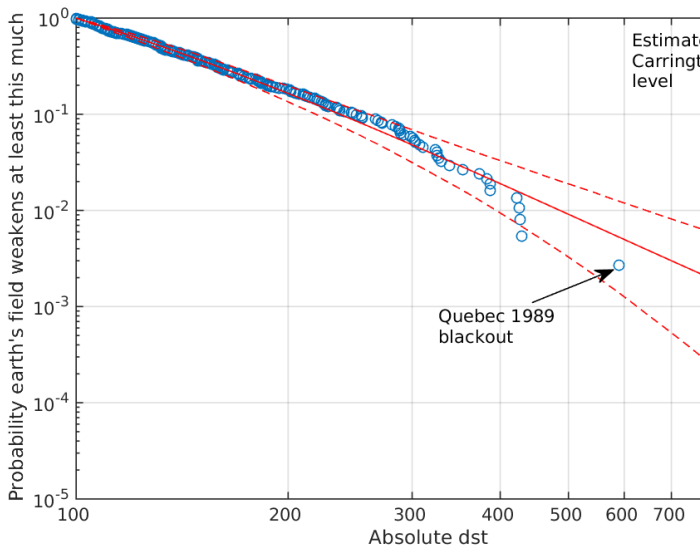 - need to wait for the compilation

```
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(sig
    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
  - shinystan — interactive diagnostics
  - bayesplot — visualization and model checking (see model checking in Ch 6)
  - loo — cross-validation model assessment, comparison and averaging (see Ch 7)
  - projpred — projection predictive variable selection

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

Different interfaces

- 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
- 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
- More recent useful R packages
    - posterior: for handling posterior draws, convergence diagnostics, and summaries
    - tidybayes + ggdist: pretty plots