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Bayesian Statistics and Data Analysis
Lecture 6

Måns Magnusson
Department of Statistics, Uppsala University
Thanks to Aki Vehtari, Aalto University

Recap: MCMC, Gibbs and Metropolis

- Markov Chain Monte Carlo
  - A transition distribution $T(\theta_0 \to \theta_1)$ with a unique stationary distribution
  - Target: setup T so that $p(\theta|y)$ is the stationary distribution

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  - Conditional (or block) sampling of θ

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  - Proposal distribution J (i.e. T)
  - \+ better for correlated posteriors
  - \- scale need to be tuned for efficient sampling
  - \- hard to propose in high dimensions (many small steps or many rejections)

Section 2

Hamiltonian Monte Carlo

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Why Hamiltonian Monte Carlo?

- Want to build an efficient Markov Chain
    - We want to sample jointly all θ
    - We know the unnormalized posterior $q(\theta|y) = Z \cdot p(\theta|y)$, were Z is the normalization constant.
    - Can we use this to create a good proposal distribution J?

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  - Can we use this to create a good proposal distribution J?
  - Hamiltonian Monte Carlo!

What is Hamiltonian Monte Carlo?

- Add momentum variables to our posterior (canonical distribution)

$$p(\psi, \theta | y) = p(\psi | \theta, y) \cdot p(\theta | y)\,,$$

in practice we let $p(\psi | \theta, y) = p(\psi)$

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  - θ: position
  - ψ: momentum

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- Idea from Physics (Mechanics):
  - θ: position
  - ψ: momentum
- Define the Hamiltonian as

$$\begin{aligned} H(\psi, \theta) &= -\log(p(\psi)) - \log(p(\theta|y)) && (1) \\ &= K(\psi) + V(\theta)\,, && (2) \end{aligned}$$

  where $K(\psi)$ is the kinetic energy and $V(\theta)$ is the potential energy

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What is Hamiltonian Monte Carlo?

- Hamiltonian Dynamics (preserve energy)

$$\frac{d\theta}{dt} = \frac{\partial H}{\partial \psi} = \frac{\partial K}{\partial \psi} \tag{3}$$

$$\frac{d\psi}{dt} = -\frac{\partial H}{\partial \theta} = \frac{\partial V}{\partial \theta} \tag{4}$$

- Let $V(\theta) = -\log(q(\theta|y)) = -\log p(\theta) - \log p(y|\theta)$
- Let $\psi \sim N(0, M)$ where M is the mass matrix
- Hence, $K(\psi) = -\log p(\psi) \propto 0.5\psi^T M^{-1}\psi + C$

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- Hence, $K(\psi) = -\log p(\psi) \propto 0.5\psi^T M^{-1}\psi + C$
- We need to choose M in a smart way.
  1. Ideally, $M^{-1} = Cov(\theta|y)$
  2. In practice, $M^{-1} = V(\theta|y)$

The leapfrog integrator

- We want to simulate Hamiltonian dynamics

$$\frac{d\theta}{dt} = M^{-1}\psi \tag{5}$$

$$\frac{d\psi}{dt} = \frac{\partial \log q(\theta|y)}{\partial \theta} \tag{6}$$

- A discrete approximation: the leapfrog integrator

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- A discrete approximation: the leapfrog integrator
- We take L leapfrog steps with step size ϵ as

$$\psi \leftarrow \psi + \frac{1}{2}\epsilon \frac{d \log q(\theta|y)}{d\theta} \tag{7}$$

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$$\psi \leftarrow \psi + \frac{1}{2}\epsilon \frac{d \log q(\theta|y)}{d\theta} \tag{9}$$

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- Discretization introduce a error depending on ϵ (not $L\epsilon$)

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Hamiltonian Monte Carlo Algorithm

1. Sample momentum

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Hamiltonian Monte Carlo Algorithm

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2. Simulate values $(\theta^\star, \psi^\star)$ using the leapfrog integrator L steps with stepsize ϵ, starting from (θ_{t-1}, ψ_0)
3. Accept the proposed values $(\theta^\star, \psi^\star)$ with probability

$$r = \min\left(1, \frac{q(\theta^\star|y)}{q(\theta_{t-1}|y)} \frac{p(\psi^\star)}{p(\psi_0)}\right)$$

Hamiltonian Monte Carlo

- Bivariate Normal HMC example

Hamiltonian Monte Carlo

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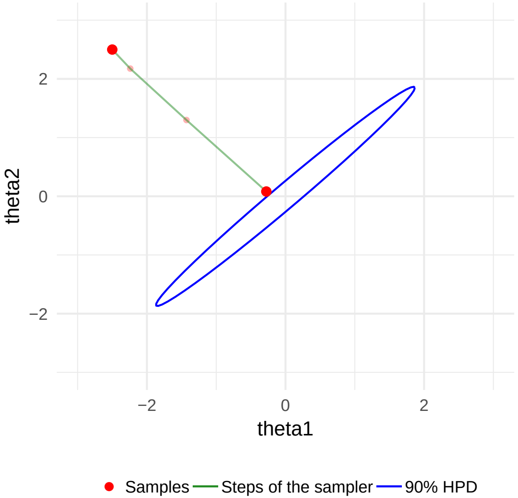
- Bivariate Normal HMC example



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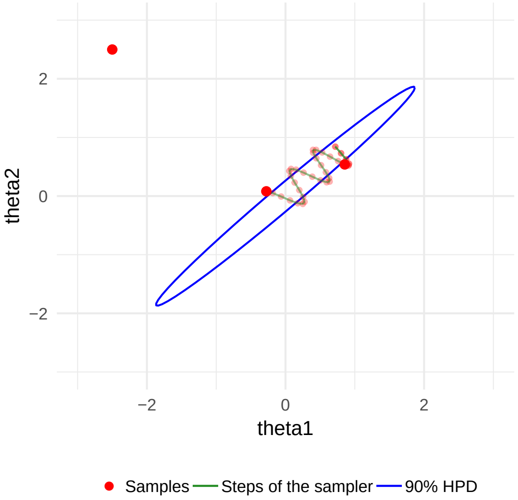

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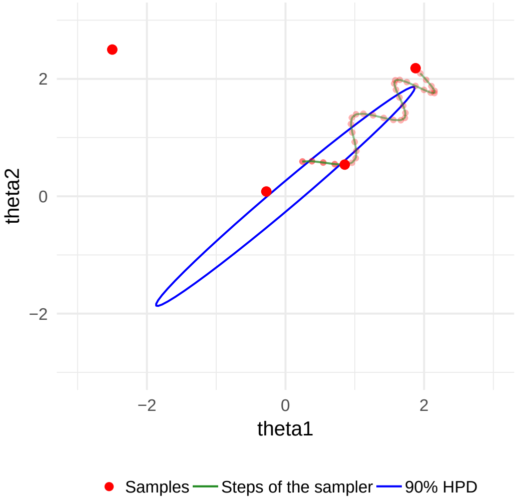

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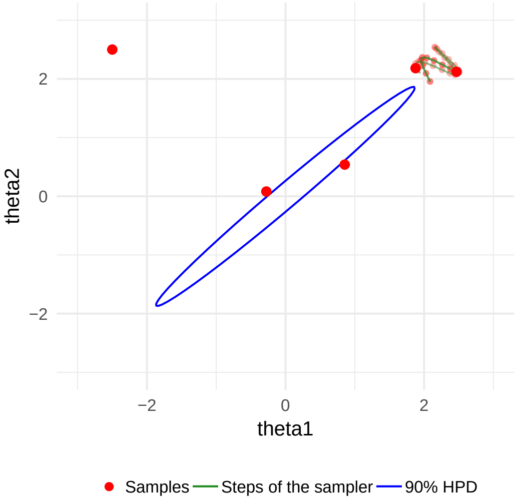

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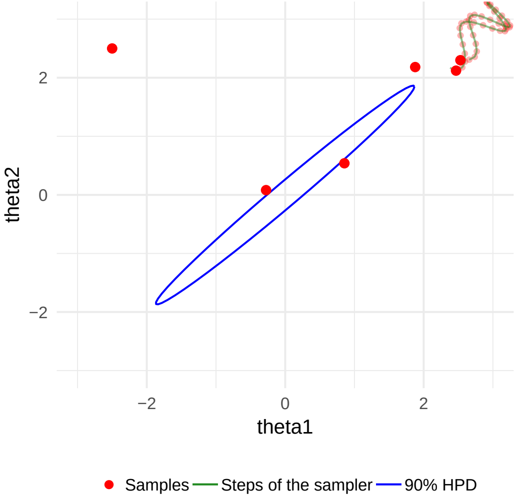

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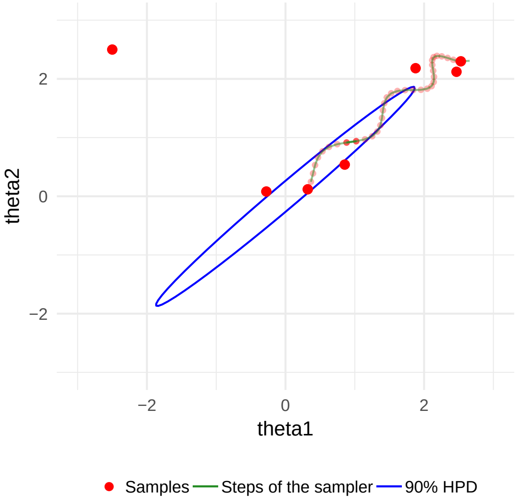

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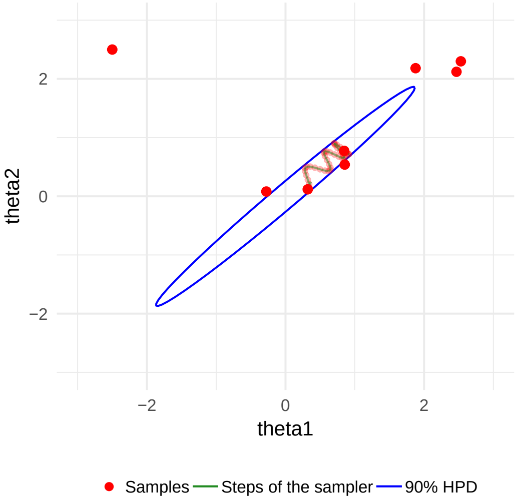

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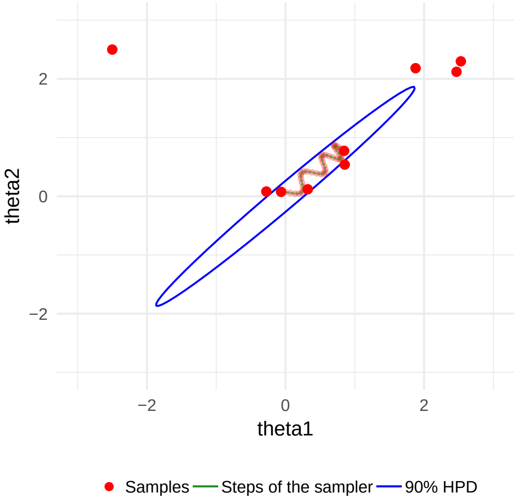

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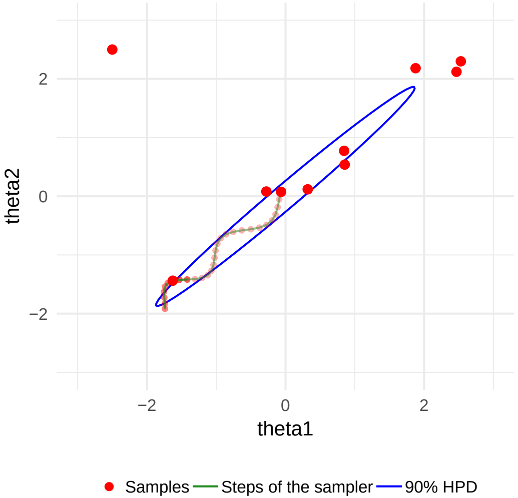

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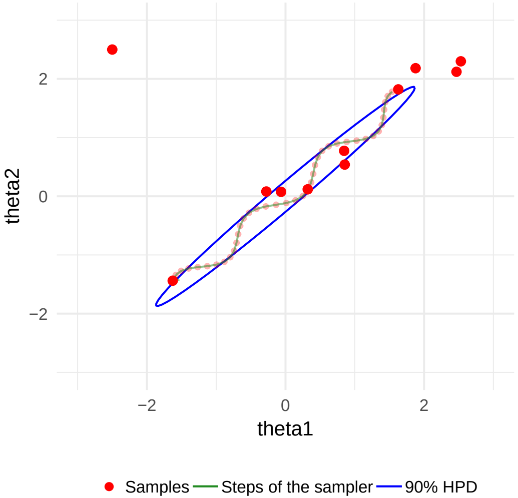

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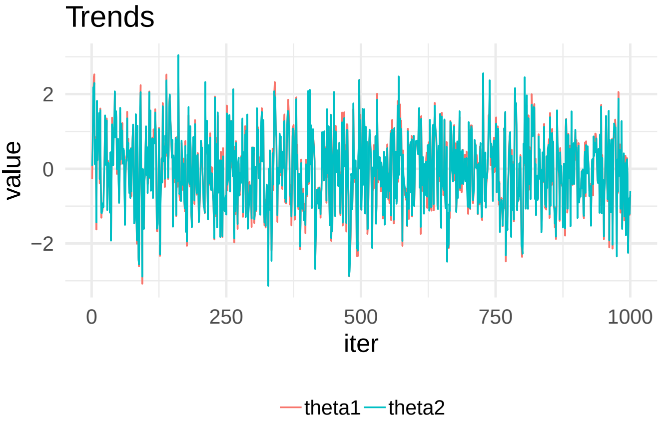

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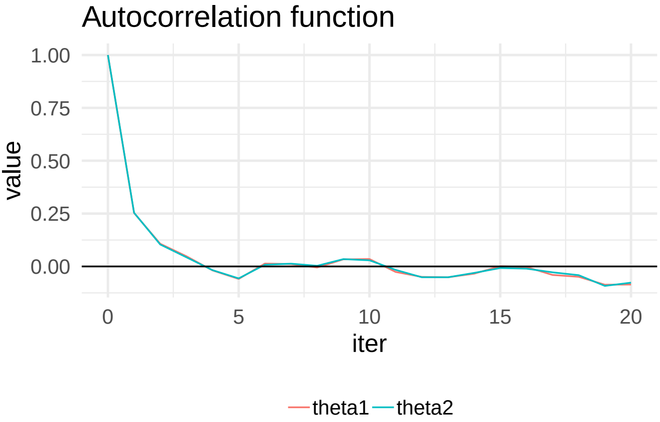

Hamiltonian Monte Carlo Summary

- Parameters:
  - ϵ step size

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- \- Ideally, we should adapt ϵL
- \- Costly to run each iteration (L log density gradient evaluations)

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- Goal: Simplify/adapt the tuning of HMC
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  2. Grow (randomly) in two directions (to keep reversibility of Markov chain)
  3. Stop to grow tree when encounter a U-turn

$$(\theta_{start} - \theta_L) \cdot \psi_L < 0$$

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- Dynamic simulation is discretized
  - small ϵ gives accurate simulation, but requires more log density evaluations
  - large ϵ reduces computation, but increases simulation error

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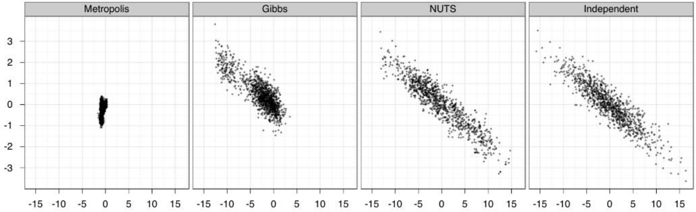
HMC / NUTS

Comparison of algorithms on **highly correlated** 250-dimensional Gaussian distribution

- Do **1,000,000** draws with both Random Walk Metropolis and Gibbs, thinning by 1000
- Do **1,000** draws using Stan's NUTS algorithm (no thinning)
- Do 1,000 independent draws (we can do this for multivariate normal)



Source: Jonah Gabry

Section 4

HMC diagnostics

Max tree depth

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

Divergences

- HMC specific diagnostic
- indicates that Hamiltonian dynamic simulation has problems with unexpected fast changes in log-density
  - indicates possibility of biased estimates
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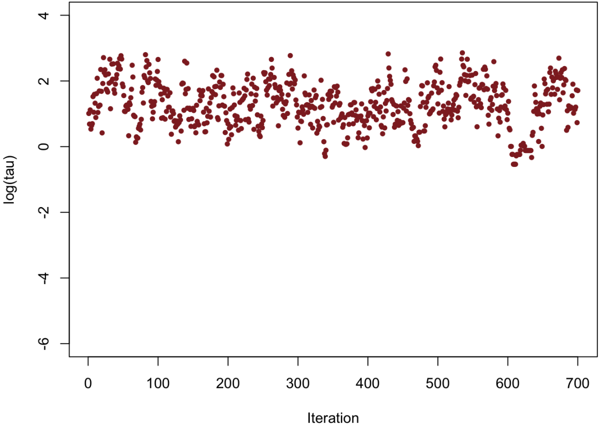

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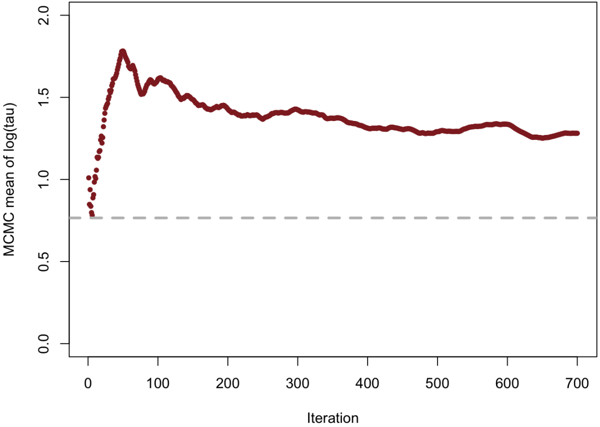

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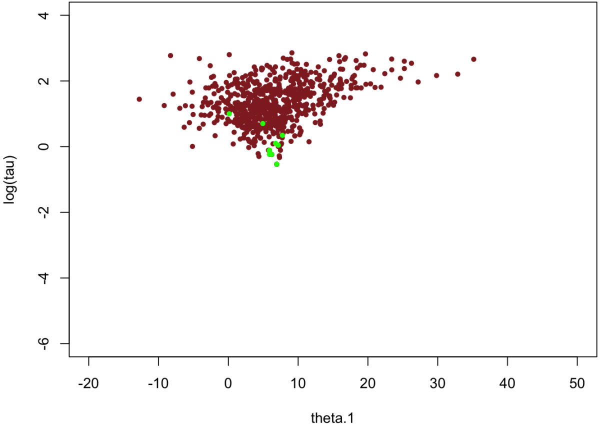

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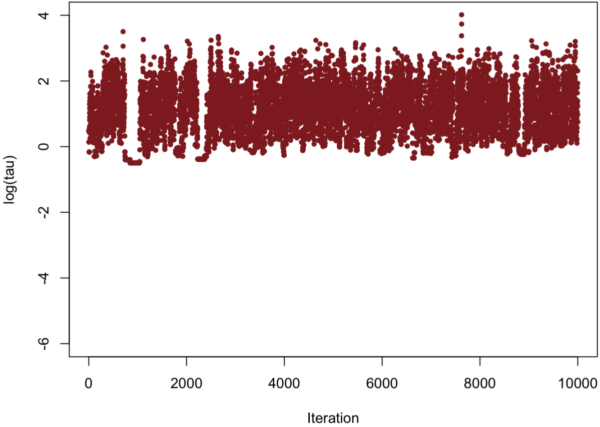

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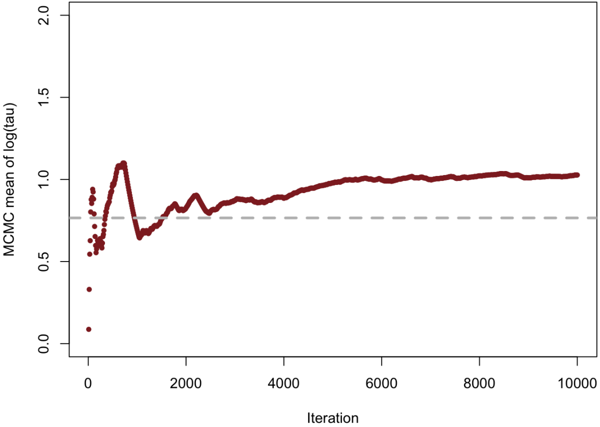

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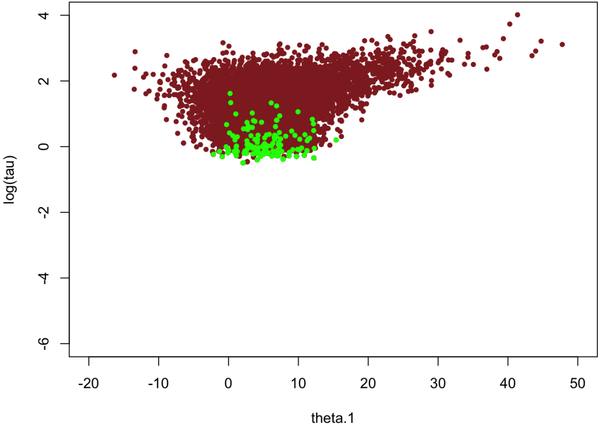

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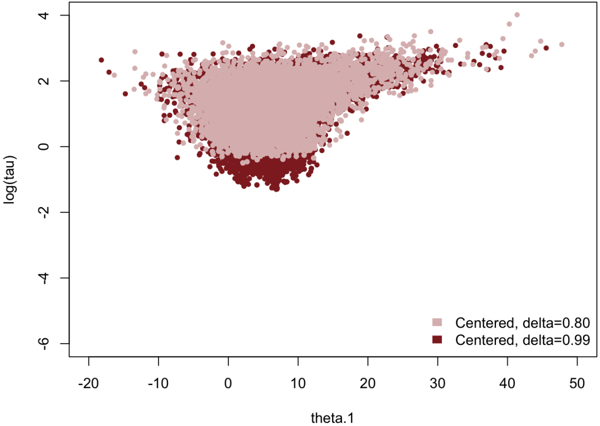

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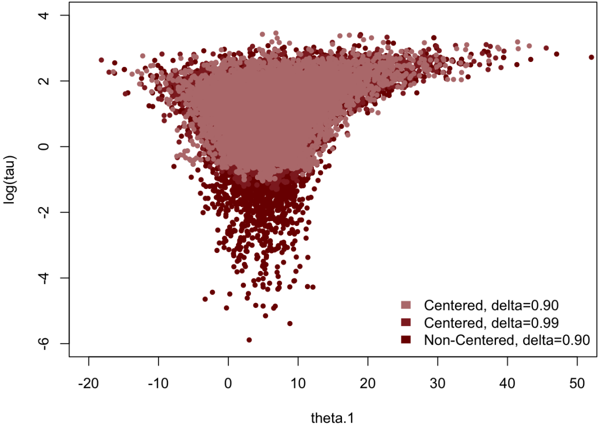

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Problematic distributions

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  - 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

Extra (optional) material for HMC

- Michael Betancourt (2018). A Conceptual Introduction to Hamiltonian Monte Carlo. https://arxiv.org/abs/1701.02434
- Michael Betancourt (2017). Diagnosing Biased Inference with Divergences. https://mc-stan.org/users/documentation/case-studies/divergences_and_bias.html

Section 5

Probabilistic Programming

The Box process: Probabilistic modeling

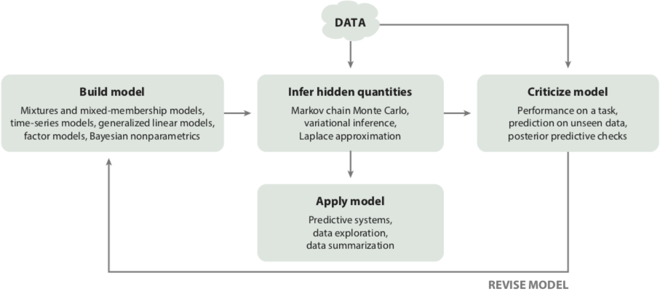

Figure: The Box approach (Box, 1976, Blei, 2014)

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Probabilistic programming languages

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

Probabilistic programming languages

- 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
  - easy workflow to build and revise models
  - inference has to be as automatic as possible
  - diagnostics for telling if the automatic inference doesn't work

Probabilistic programming

- Enables agile (incremental) workflow for developing probabilistic models
  - language
  - automated inference
  - diagnostics
- Many frameworks Stan, PyMC3, Pyro (Uber), Edward (Google), Birch (Uppsala), ...

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Section 6

Stan

Stan - probabilistic programming framework

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

mc-stan.org

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

mc-stan.org

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- 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

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

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  - mass matrix refers to having different scaling for different parameters and optionally also rotation to reduce correlations

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- After adaptation the algorithm parameters are fixed
- After warmup store iterations for inference
- See more details in Stan reference manual

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

- MCMC recap
- Hamiltonian Monte Carlo
- Dynamic HMC and NUTS
- HMC diagnostics
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- Stan

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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

Binomial model - Stan code

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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>`

Binomial model - Stan code

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- 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)

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model {
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}
```

- $\sim$ is syntactic sugar and this is equivalent to

```
model {
  target += beta_lpdf(theta | 1, 1);
  target += binomial_lpmf(y | N, theta);
}
```

Binomial model - Stan code

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- `target` is the log posterior density

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- `_lpdf` for continuous, `_lpmf` for discrete distributions (discrete for the left hand side of |)

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- `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)

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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

```r
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)
```

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)
```

PyStan

PyStan

```
import pystan
import stan_utility

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

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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-theta
}
```

Difference between proportions

```
data {
  int<lower=0> N1;
  int<lower=0> y1;
  int<lower=0> N2;
  int<lower=0> y2;
}
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  real<lower=0,upper=1> theta1;
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model {
  theta1 ~ beta(1,1);
  theta2 ~ beta(1,1);
  y1 ~ binomial(N1,theta1);
  y2 ~ binomial(N2,theta2);
}

generated quantities {
  real oddsratio;
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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 = 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 chair
convergence, Rhat=1).
```

Difference between proportions

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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 chair
convergence, Rhat=1).
```

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

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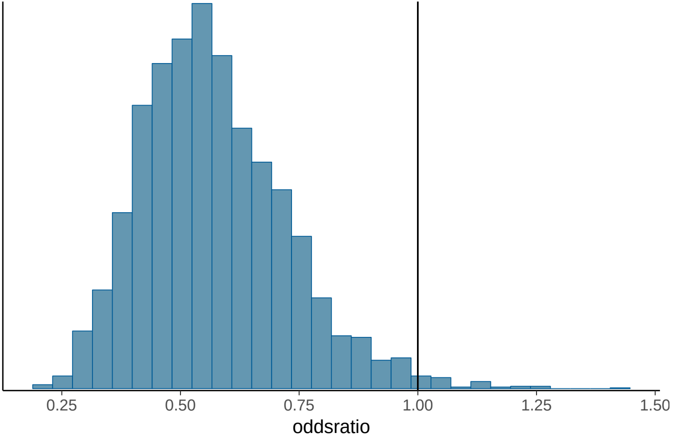
Difference between proportions

```
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_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%)"

get_num_leapfrog_per_iteration(fit_bin2)
```

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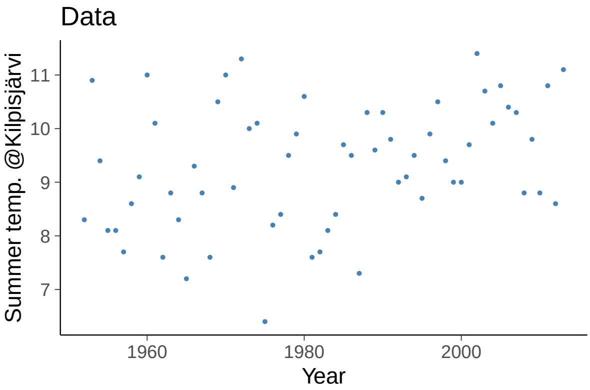
Shinystan

- 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?



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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 `real x[N]`

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

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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);
}
```

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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?

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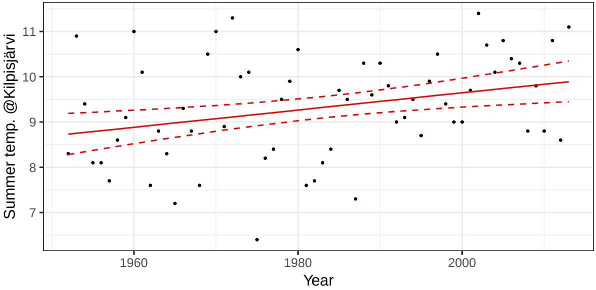
Kilpisjärvi summer temperature

Posterior fit



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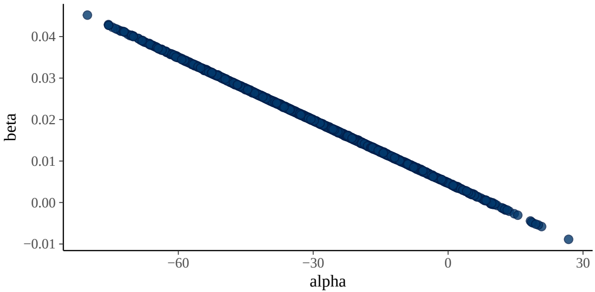
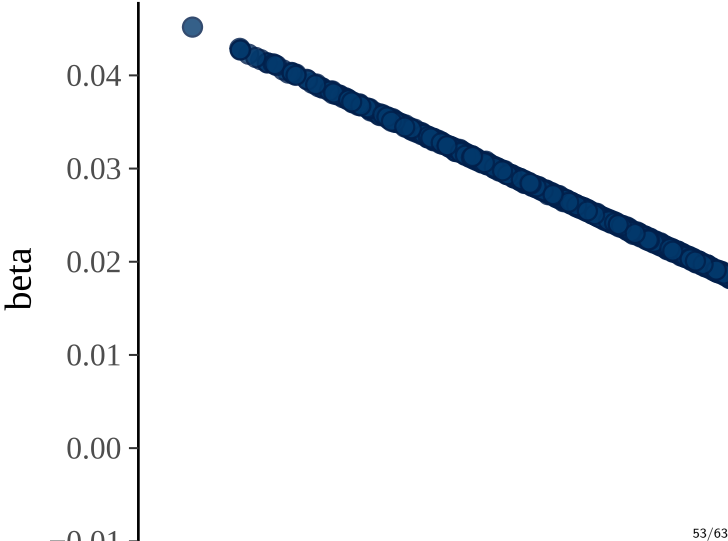
Kilpisjärvi summer temperature

Posterior draws of alpha and beta



Kilpisjärvi summer temperature

Posterior draws of alpha and beta



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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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

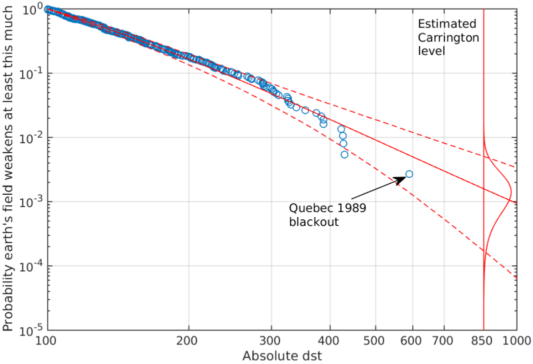
- BRMS provides simplified model description
    - a larger set of models than RStanARM, but still restricted
    - need to wait for the compilation

```
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->(
  }
  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

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