

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 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>
- Michael Betancourt (2018). Scalable Bayesian Inference with Hamiltonian Monte Carlo
<https://www.youtube.com/watch?v=jUSZboSq1zg>

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_jebbs_2.pdf
- Carpenter et al (2017). Stan: A probabilistic programming language. Journal of Statistical Software 76(1). <https://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

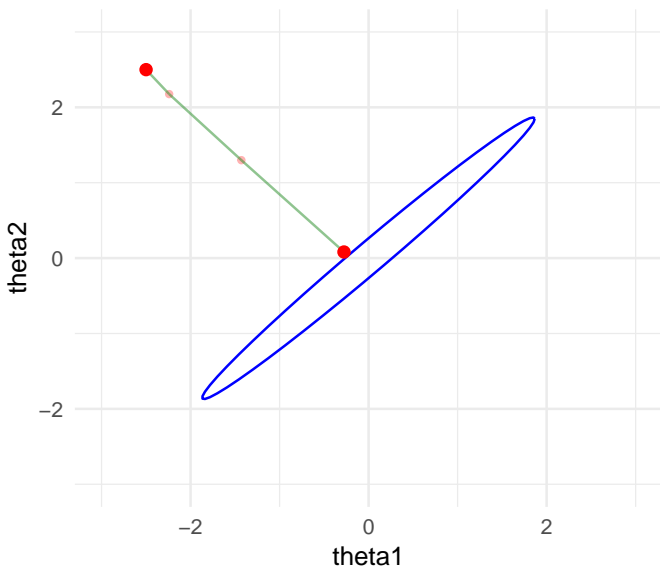
- demo12_1: HMC
- <http://elevanth.org/blog/2017/11/28/build-a-better-markov-chain/>
- rstan_demo
- rstanarm_demo
- <http://sumsar.net/blog/2017/01/bayesian-computation-with-stan-and-farmer-jons/>
- <http://mc-stan.org/documentation/case-studies.html>
- <https://cran.r-project.org/package=rstan>
- <https://cran.r-project.org/package=rstanarm>

Hamiltonian Monte Carlo

- Uses gradient information for more efficient sampling
- Augments parameter space with momentum variables

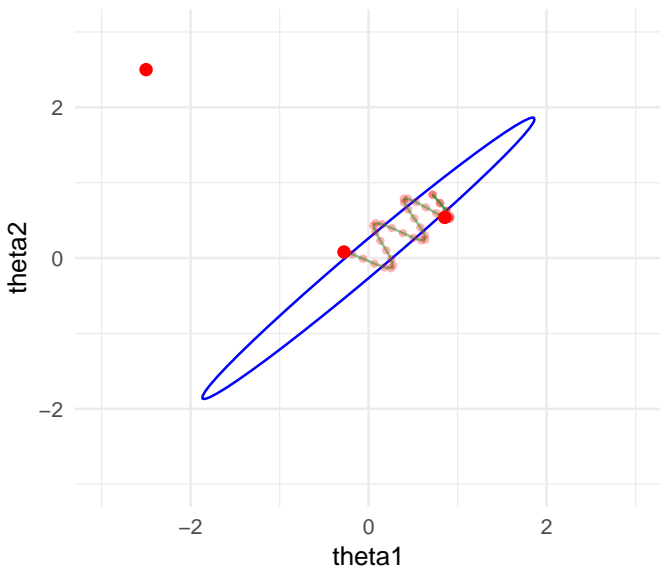
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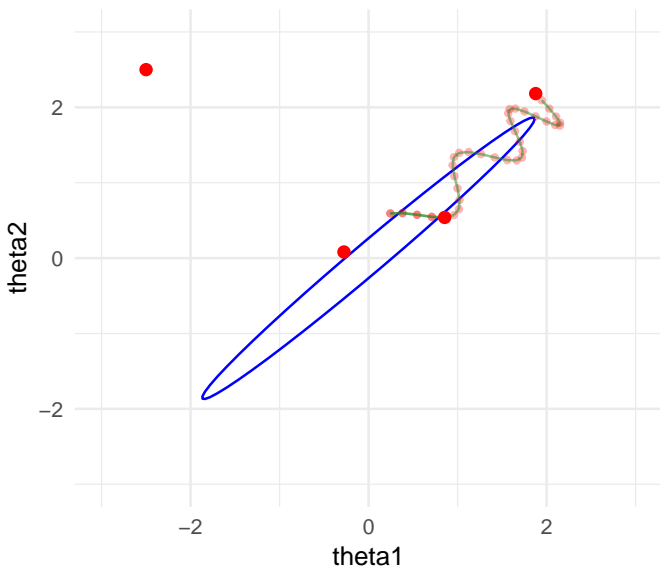
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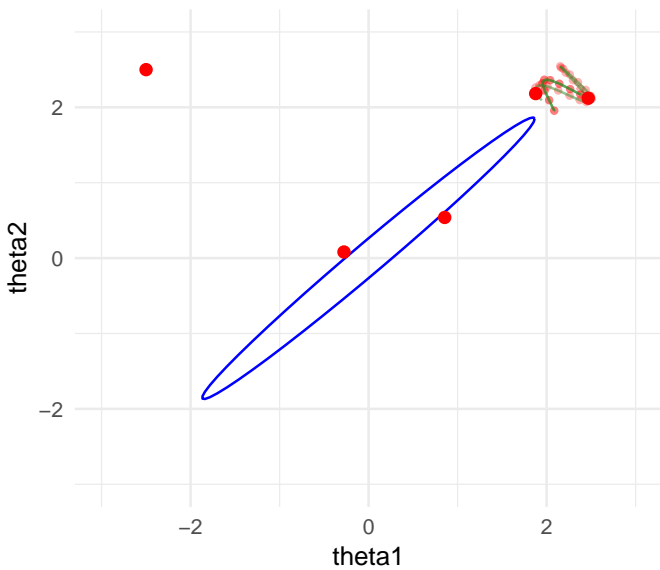
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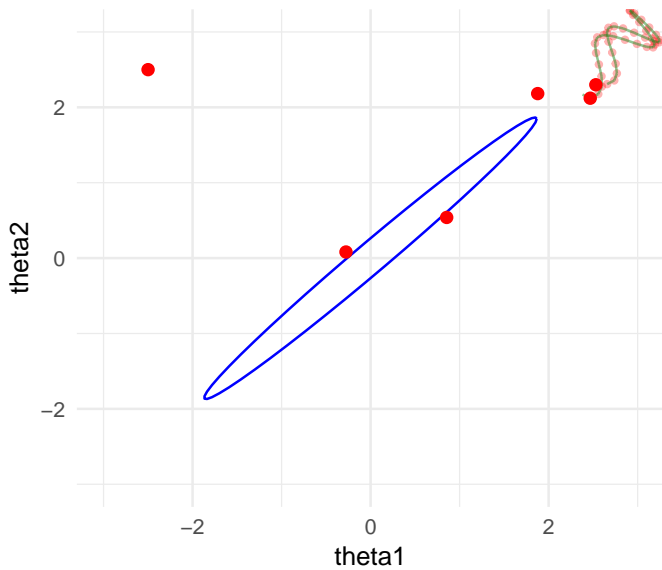
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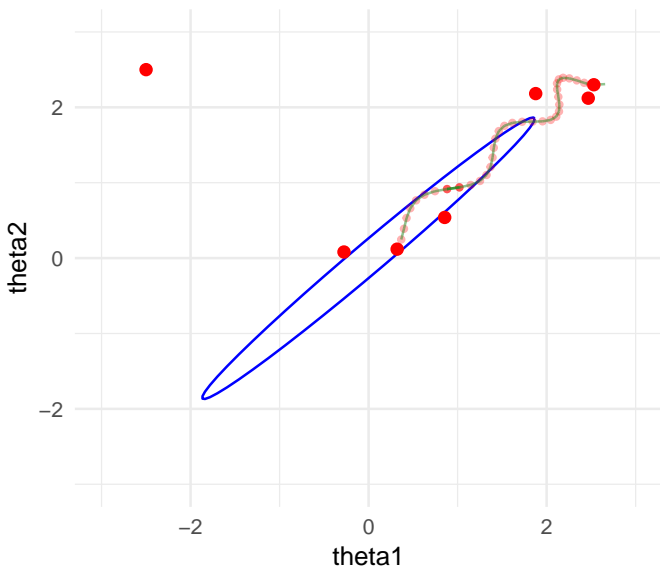
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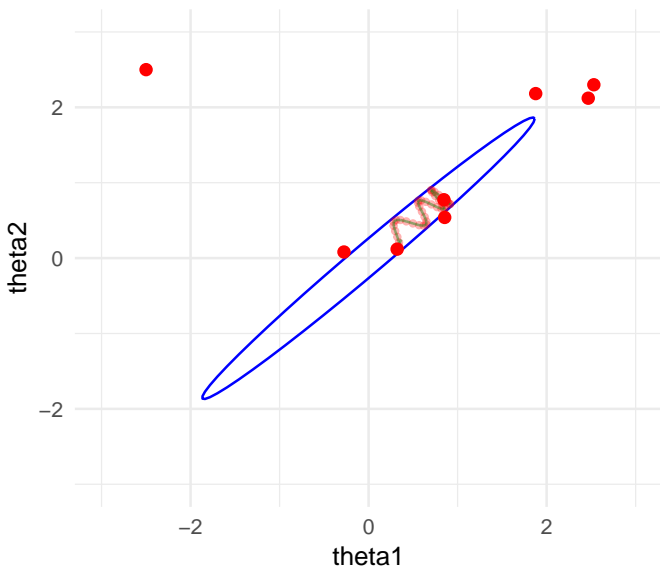
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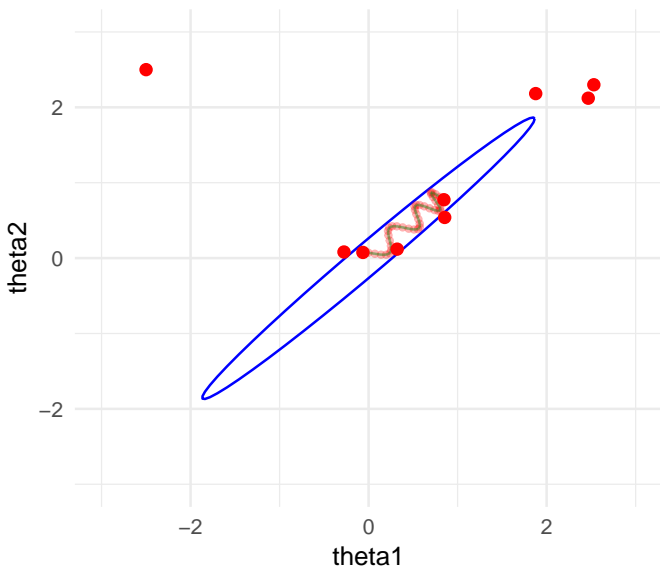
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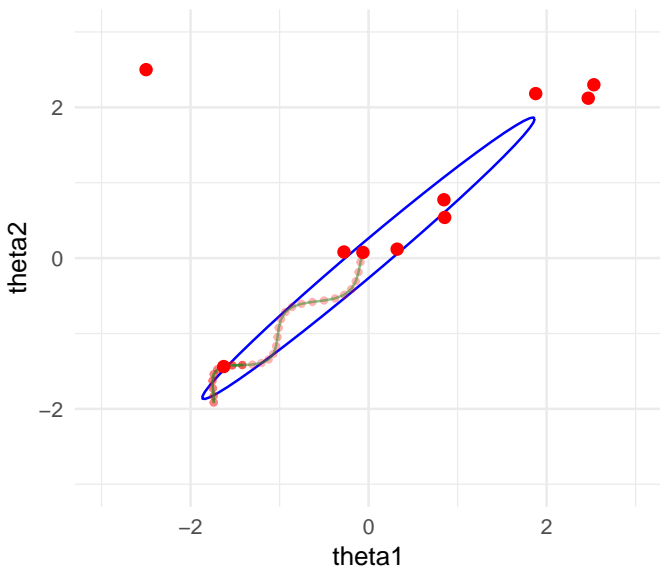
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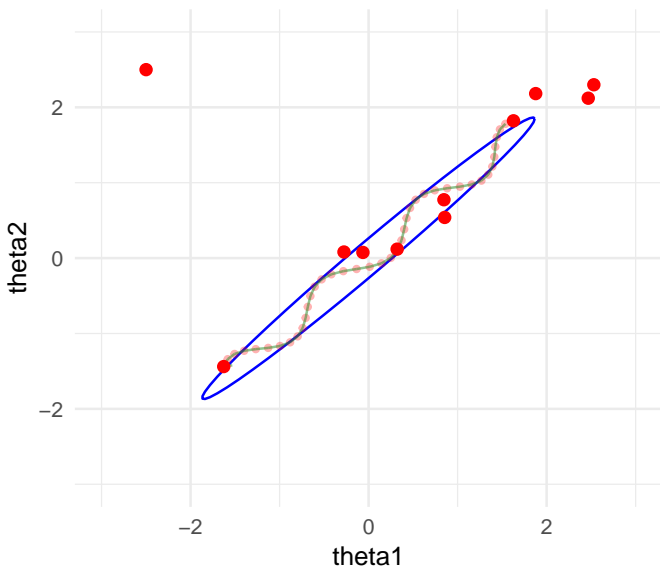
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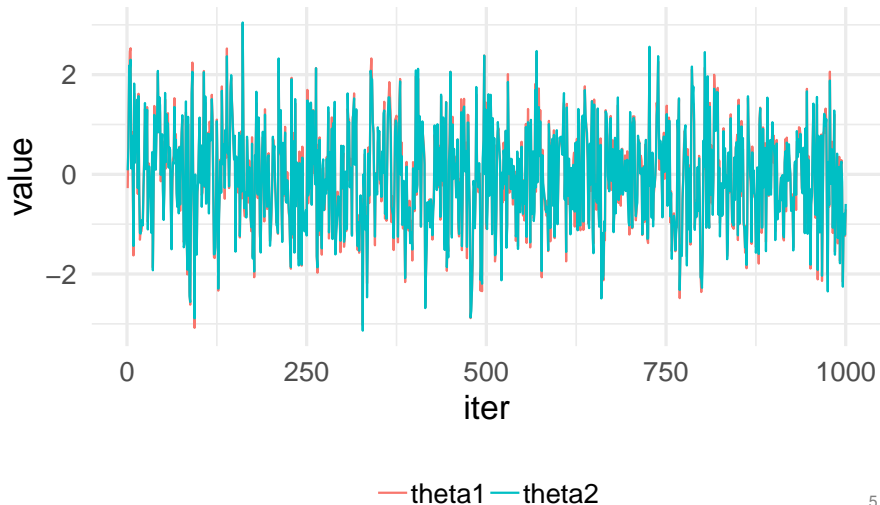
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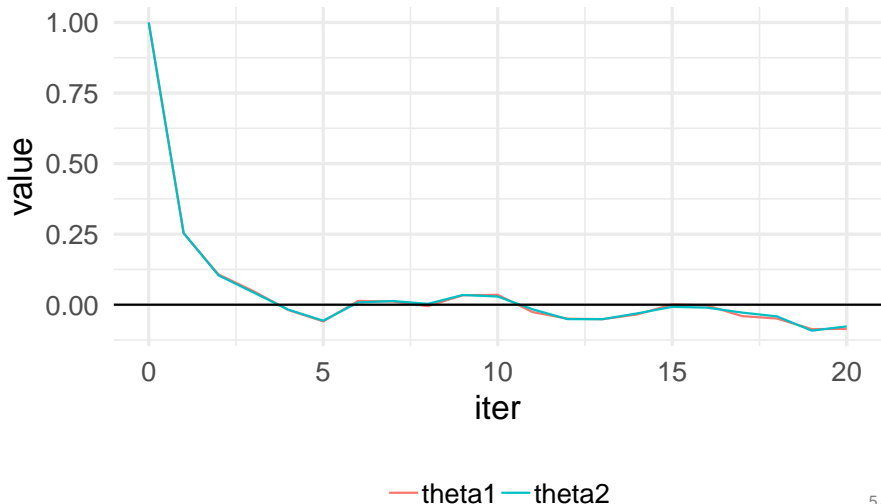
Trends



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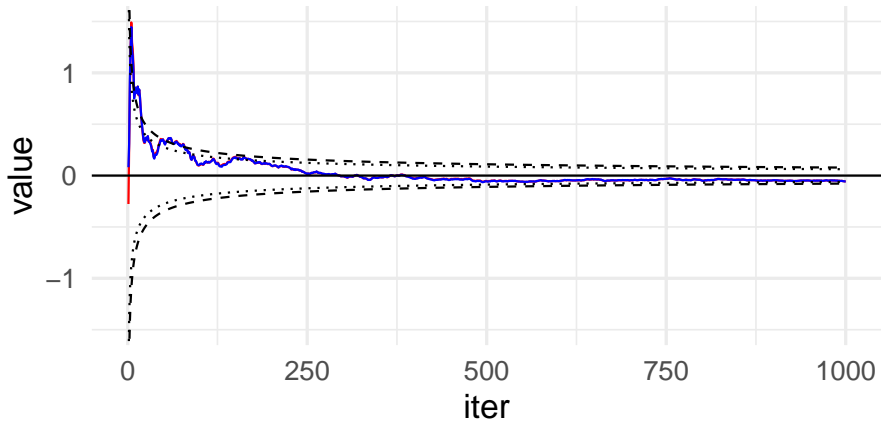
Autocorrelation function



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Cumulative averages



- theta1 — theta2 - - 95% interval for MCMC error ··· 95% interval for independent sampling

Hamiltonian Monte Carlo

- Uses gradient information for more efficient sampling
- Augments parameter space with momentum variables
- Simulation of Hamiltonian dynamics reduces random walk
 - Explanation of HMC with black board
 - <http://elevarth.org/blog/2017/11/28/build-a-better-markov-chain/>

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- 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
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- 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

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- See more details in Stan reference manual

Max tree depth diagnostic

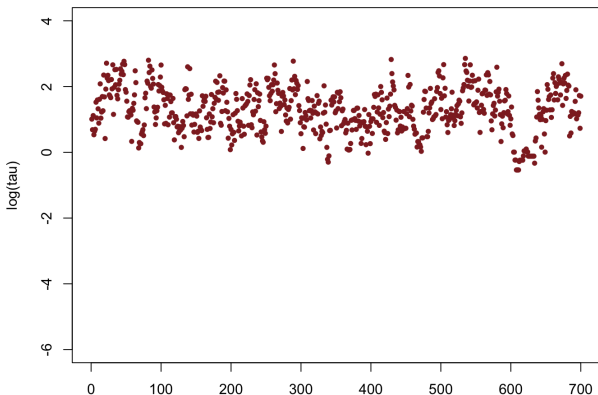
- Dynamic HMC specific diagnostic
- Indicates inefficiency in sampling leading to higher autocorrelations and lower ESS (n_{eff})
- Different parameterizations matter

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

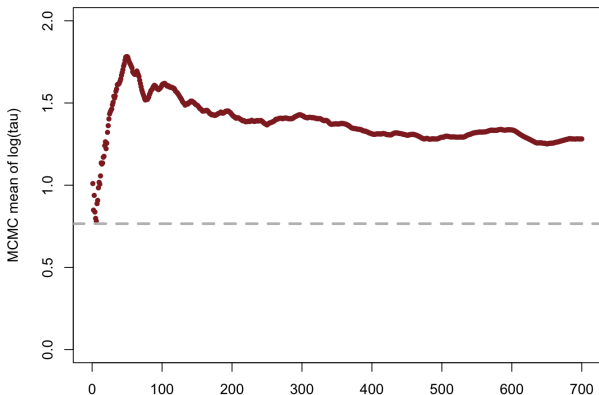
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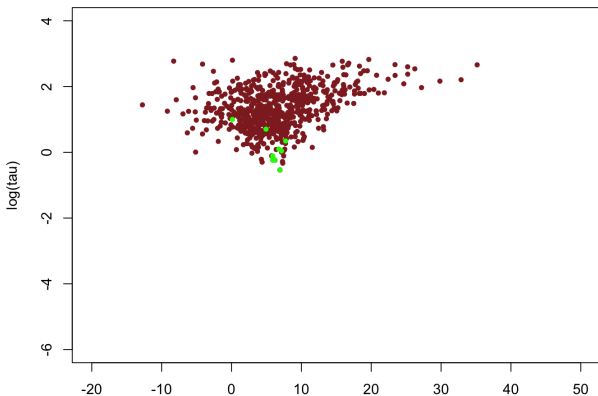
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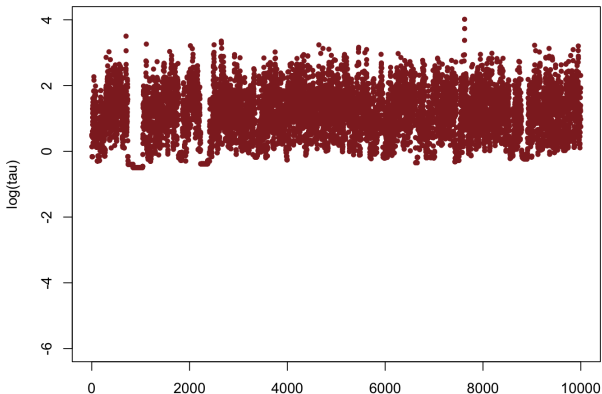
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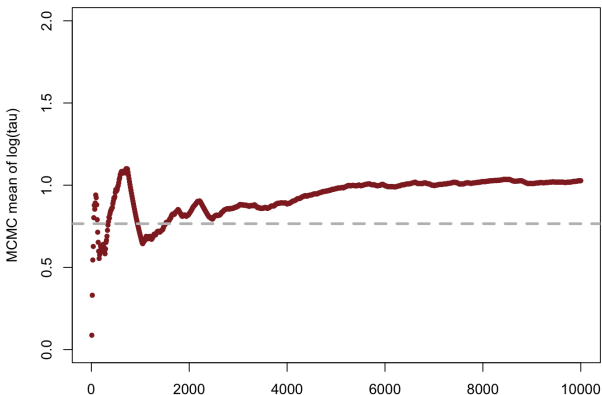
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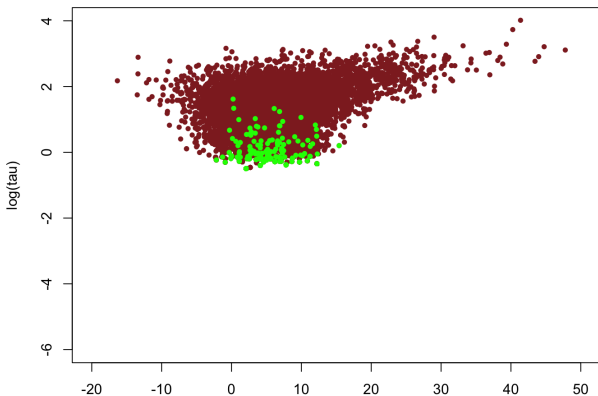
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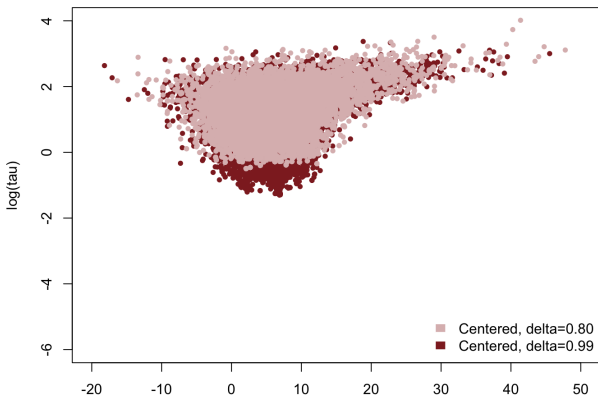
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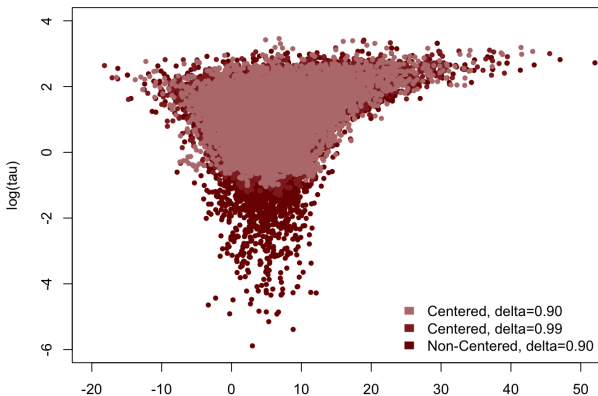
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 - simple mass matrix scaling doesn't help
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 - optimal step size depends on location
- Multimodal
 - difficult to move from one mode to another
- Long-tailed with non-finite variance and mean
 - efficiency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

Probabilistic programming language

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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



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- Language, inference engine, user interfaces, documentation, case studies, diagnostics, packages, ...
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- More than ten thousand users in social, biological, and physical sciences, medicine, engineering, and business



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- R, Python, Julia, Scala, Stata, Matlab, command line interfaces
- More than 100 R packages using Stan



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Stan

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

Binomial model - Stan code

```
data {  
  int<lower=0> N;      // number of experiments  
  int<lower=0,upper=N> y; // number of successes  
}  
  
parameters {  
  real<lower=0,upper=1> theta; // parameter of the binomial  
}  
  
model {  
  theta ~ beta(1,1); //prior  
  y ~ binomial(N,theta); // observation model  
}
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- Stan checks that given data matches type and constraints

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

Binomial model - Stan code

```
parameters {  
  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>

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- For these declared transformation Stan automatically takes into account the Jacobian of the transformation (see BDA3 p. 21)

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- \sim is syntactic sugar and this is equivalent to

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model {  
  target += beta_lpdf(theta | 1, 1);  
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(discrete for the left hand side of `|`)

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- 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 (transpiles) 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())
source('stan_utility.R')

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

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PyStan

PyStan

```
import pystan
import stan_utility

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

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Stan

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

```
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

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

- generated quantities is run after the sampling

Difference between proportions

```
d_bin2 <- list(N1 = 674, y1 = 39, N2 = 680, y2 = 22)
fit_bin2 <- stan(file = 'binom2.stan', data = d_bin2)
```

```
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 sample size, and `Rhat` is the potential scale reduction factor on split chains (at convergence, `Rhat=1`).

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):

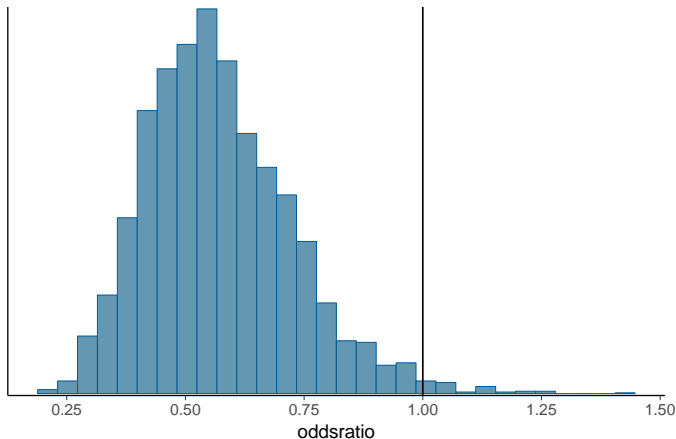
	mean	se_mean	sd	10%	50%	90%	n_eff	Rhat
theta1	0.1	0	0.0	0.0	0.1	0.1	3280	1
theta2	0.0	0	0.0	0.0	0.0	0.0	3171	1
oddsratio	0.6	0	0.2	0.4	0.6	0.8	3108	1
lp__	-253.5	0	1.0	-254.8	-253.2	-252.6	1922	1

For each parameter, `n_eff` is a crude measure of effective sample size, and `Rhat` is the potential scale reduction factor on split chains (at 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=0.25)))
```



HMC specific diagnostics

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

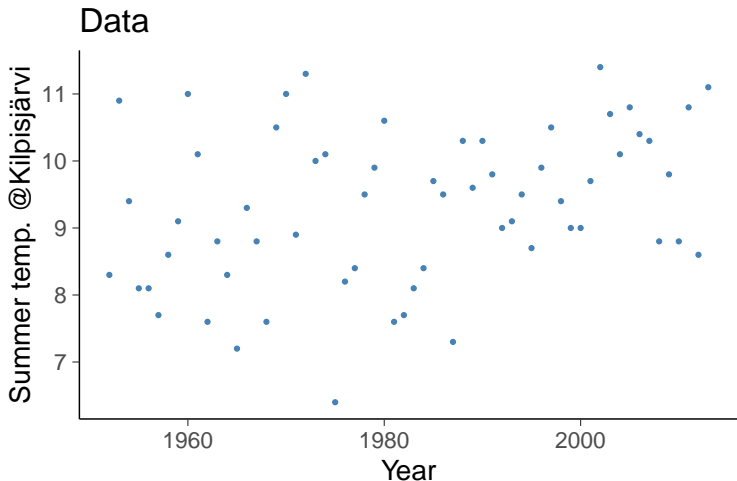
```
[1] "0 of 4000 iterations saturated the maximum tree depth of 10 (0%)"  
[1] "0 of 4000 iterations ended with a divergence (0%)"
```

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?



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

Priors for Gaussian linear model

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


Student-t linear model

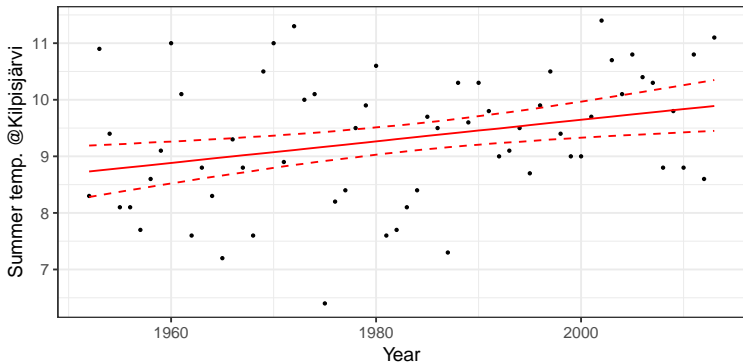
```
...
parameters {
  real alpha;
  real beta;
  real<lower=0> sigma;
  real<lower=1,upper=80> nu;
}
transformed parameters {
  vector[N] mu;
  mu <- alpha + beta*x;
}
model {
  nu ~ gamma(2,0.1);
  y ~ student_t(nu, mu, sigma);
}
```

Priors

- Prior for temperature increase?

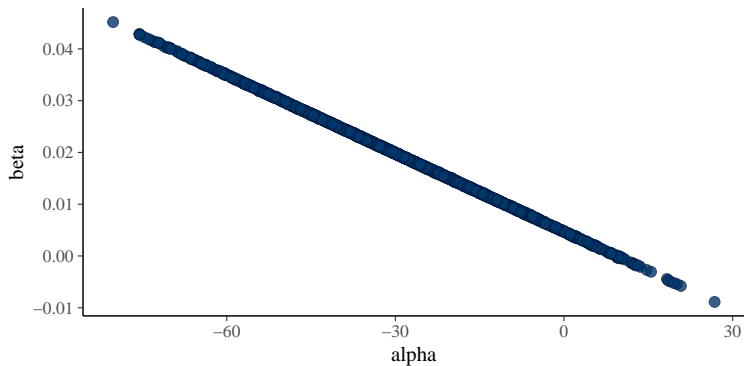
Kilpisjärvi summer temperature

Posterior fit



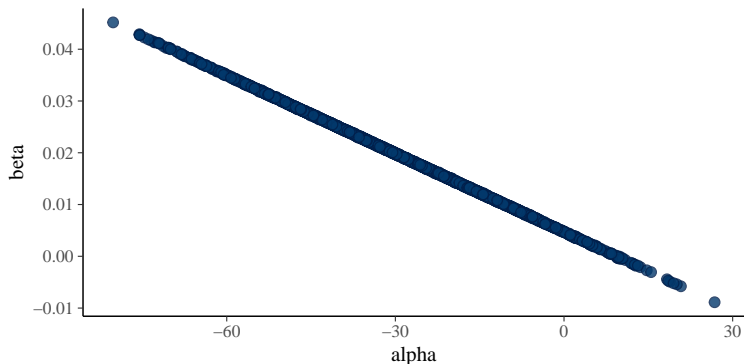
Kilpisjärvi summer temperature

Posterior draws of alpha and beta



Kilpisjärvi summer temperature

Posterior draws of alpha and beta



There were 14 transitions after warmup that exceeded the maximum treedepth. Increase `max_treedepth` above 10. See <http://mc-stan.org/misc/warnings.html#maximum-treedepth-exceeded>
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(0,1))  
fit_bin2 <- stan_glm(y/N ~ grp2, family = binomial(), data = d_bin2,  
                    weights = N)
```

RStanARM

- RStanARM provides simplified model description with pre-compiled models
 - no need to wait for compilation
 - a restricted set of models

Two group Binomial model:

```
d_bin2 <- data.frame(N = c(674, 680), y = c(39,22), grp2 = c(0,1))  
fit_bin2 <- stan_glm(y/N ~ grp2, family = binomial(), data = d_bin2,  
                    weights = N)
```

Gaussian linear model

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


BRMS

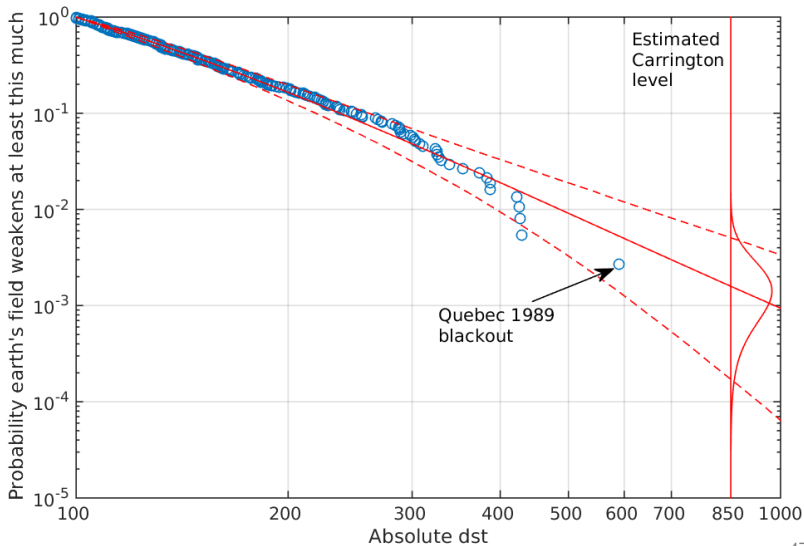
- BRMS provides simplified model description
 - a larger set of models than RStanARM, but still restricted
 - need to wait for the compilation

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

```
fit_lin_t <- brm(temp ~ year, data = d_lin, family = student())
```

Extreme value analysis

Geomagnetic storms



Extreme value analysis

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

Functions

```
functions {  
  real gpareto_lpdf(vector y, real k, real sigma) {  
    // generalised Pareto log pdf with mu=0  
    // should check and give error if k<0  
    // and max(y)/sigma > -1/k  
    int N;  
    N <- dims(y)[1];  
    if (fabs(k) > 1e-15)  
      return -(1+1/k)*sum(log1pv(y*k/sigma)) -N*log(sigma);  
    else  
      return -sum(y/sigma) -N*log(sigma); // limit k->0  
  }  
  vector gpareto_ccdf(vector y, real k, real sigma) {  
    // generalised Pareto log ccdf with mu=0  
    // should check and give error if k<0  
    // and max(y)/sigma < -1/k  
    if (fabs(k) > 1e-15)  
      return exp((-1/k)*log1pv(y/sigma*k));  
    else  
      return exp(-y/sigma); // limit k->0  
  }  
}
```

Other packages

- R
 - 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)