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

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

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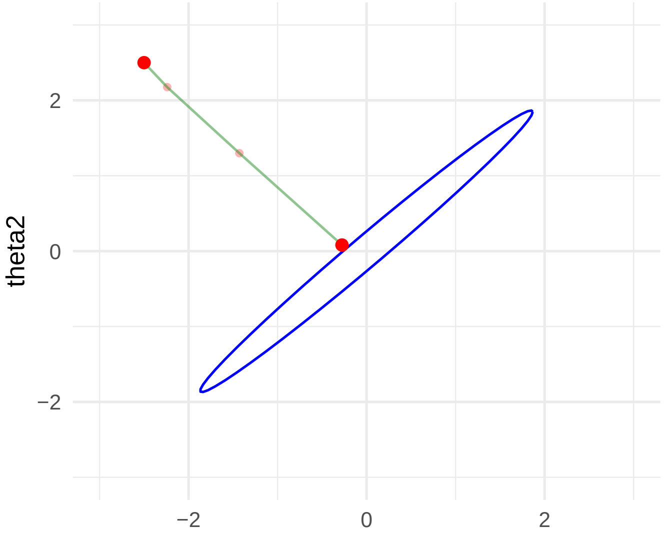

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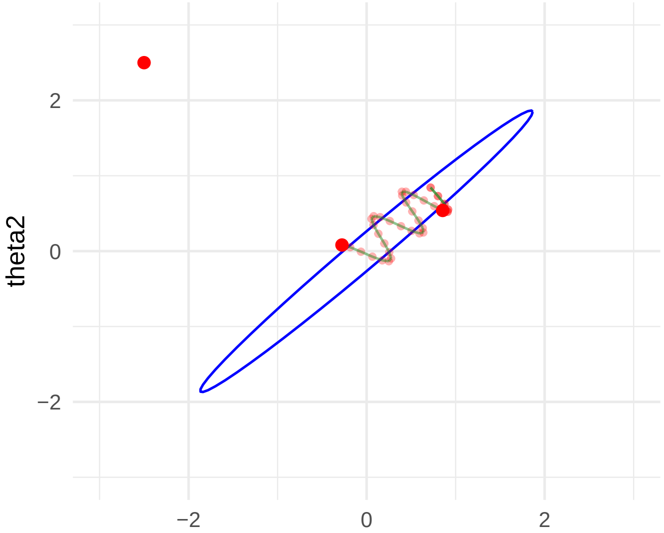

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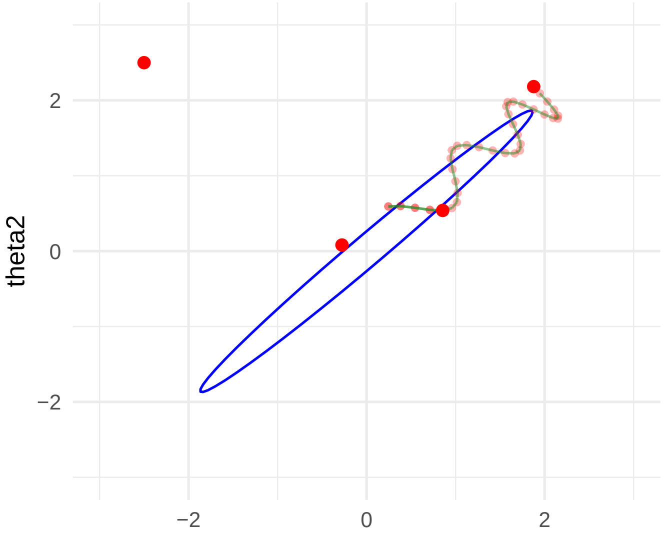

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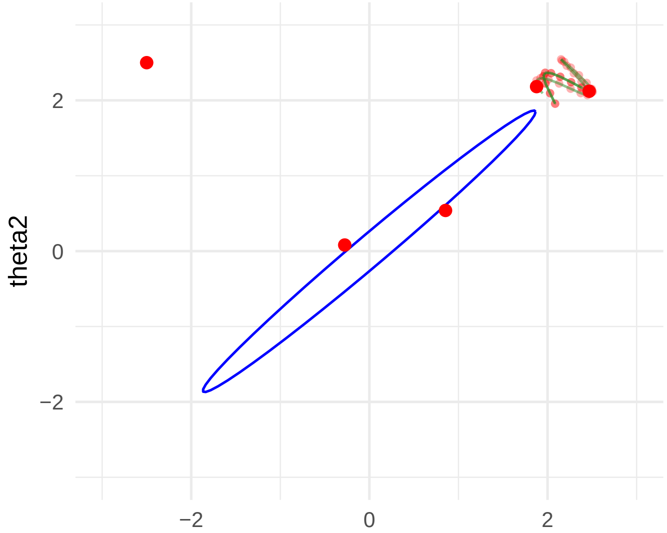

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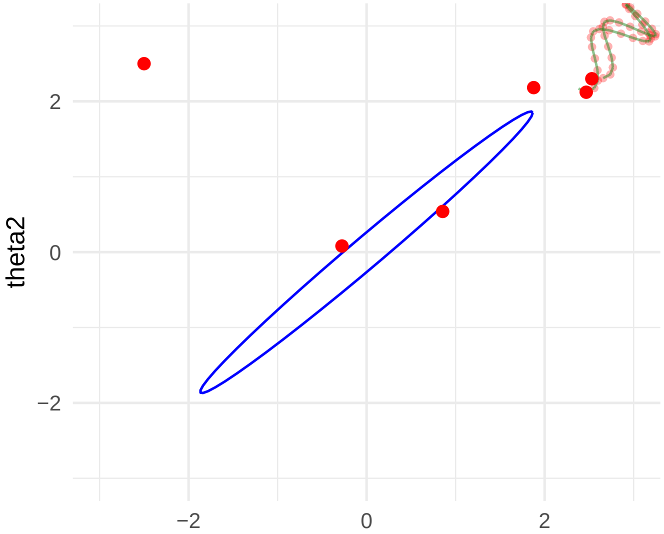

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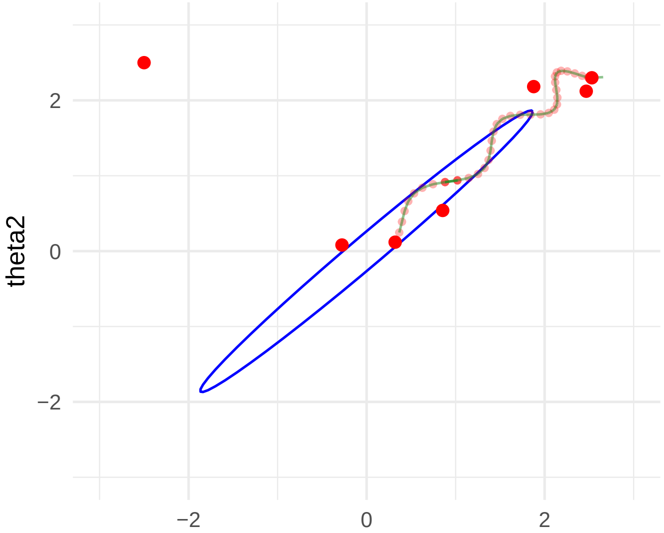

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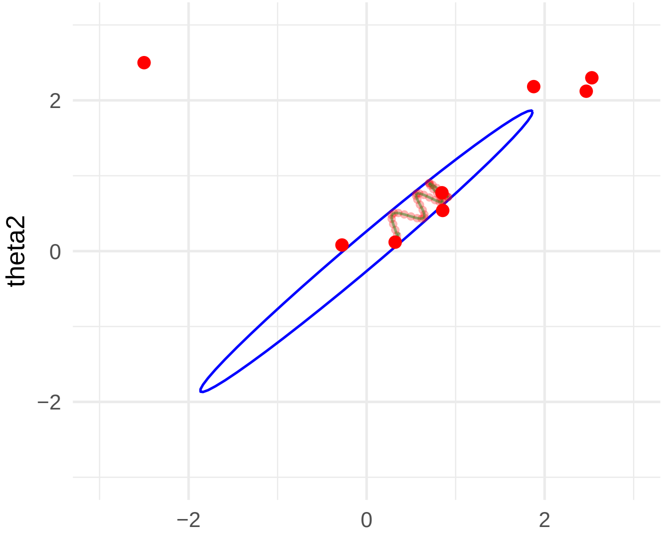

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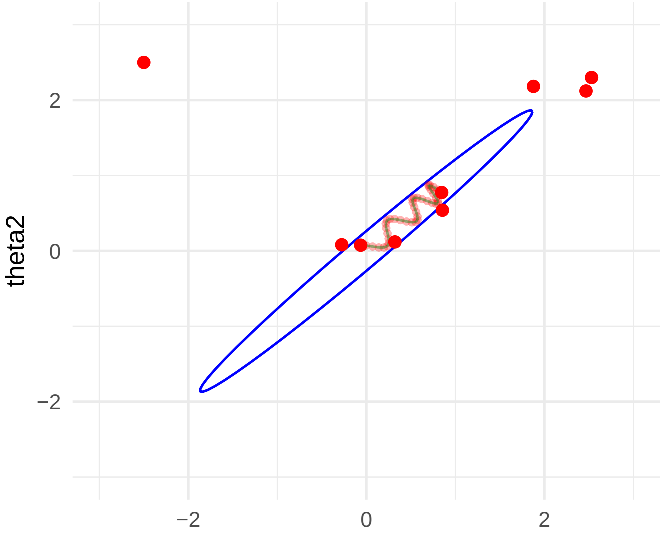

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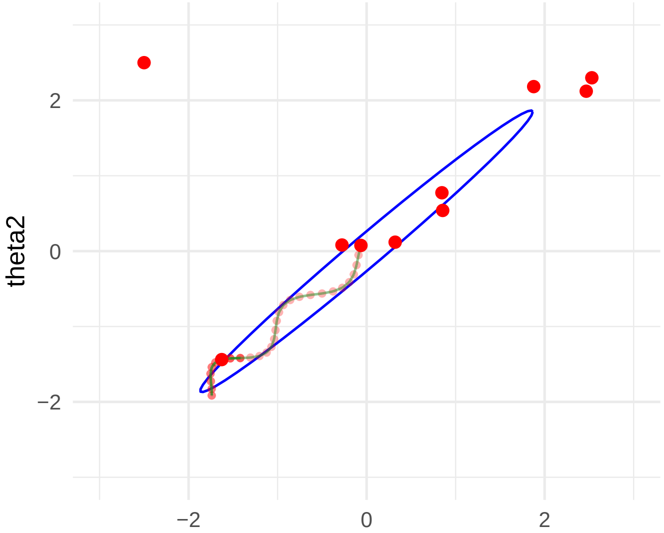

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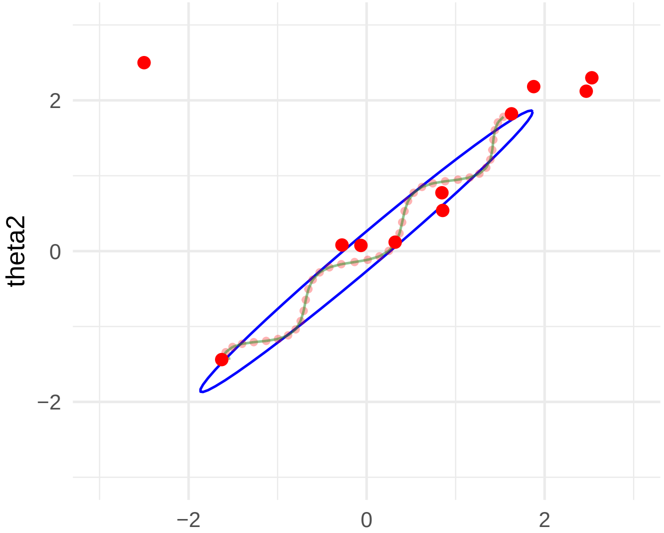

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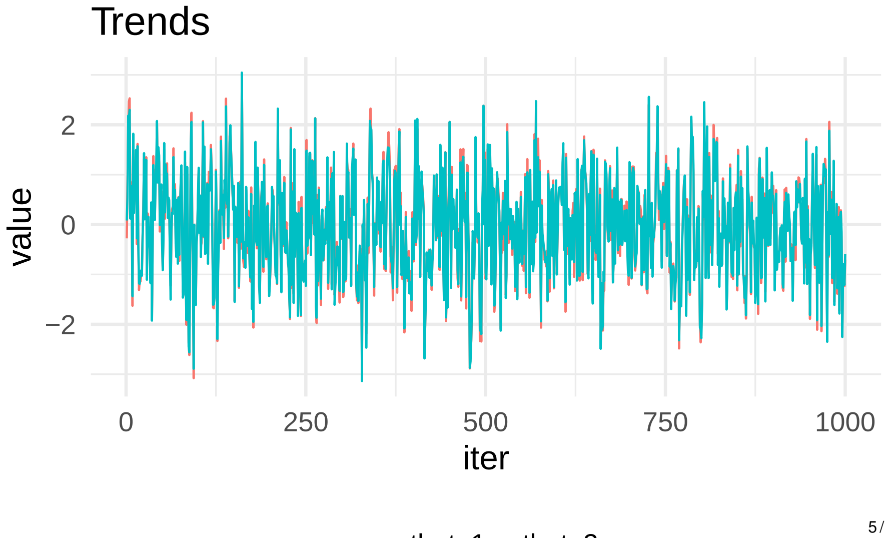

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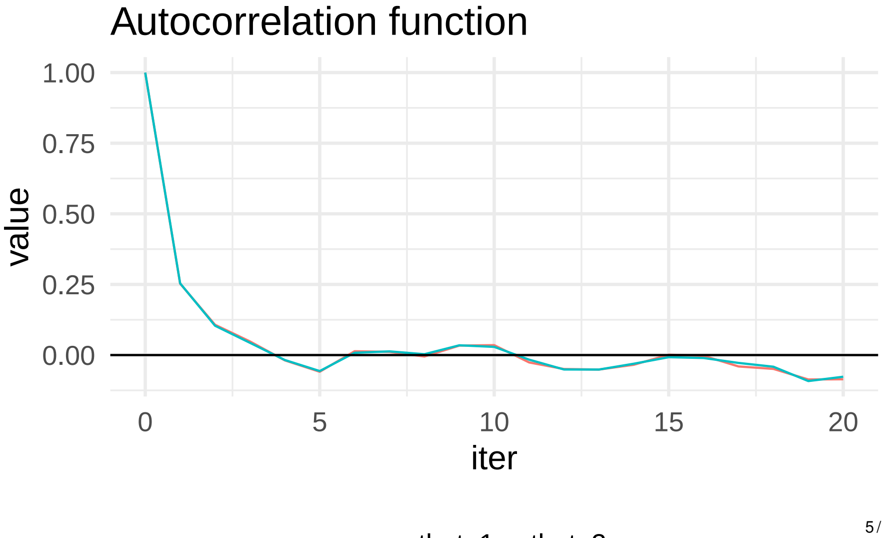

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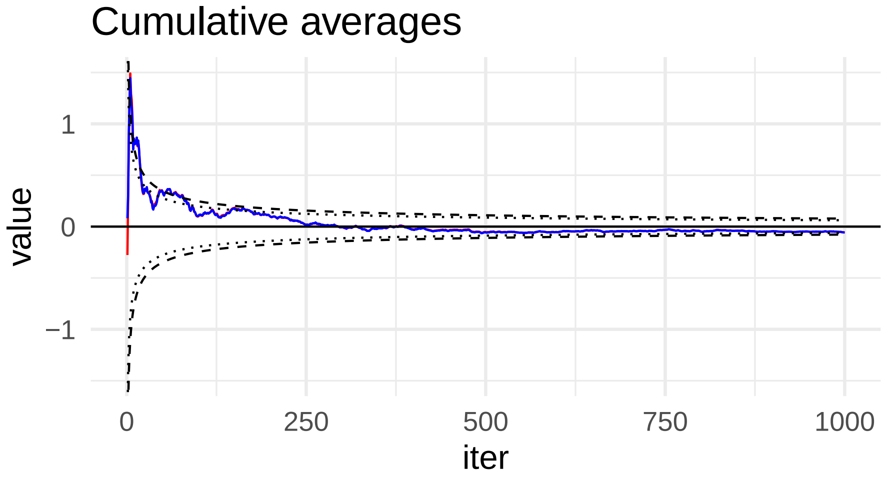

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- Simulation of Hamiltonian dynamics reduces random walk
    - Explanation of HMC with black board
    - http://elevanth.org/blog/2017/11/28/build-a-better-markov-chain/

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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
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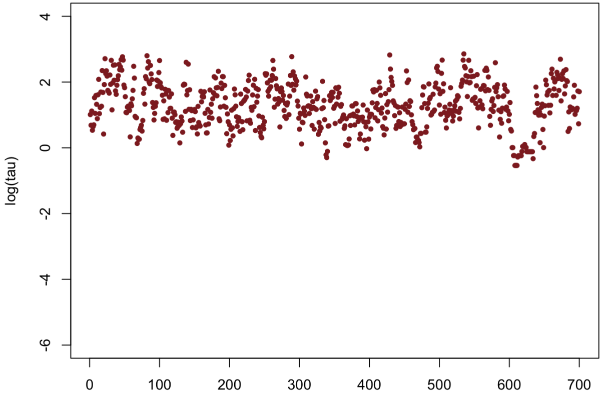

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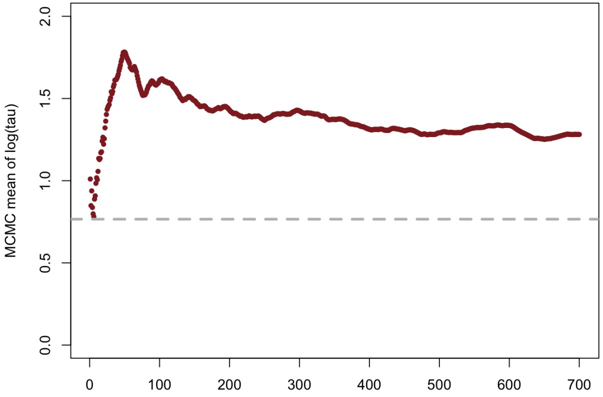

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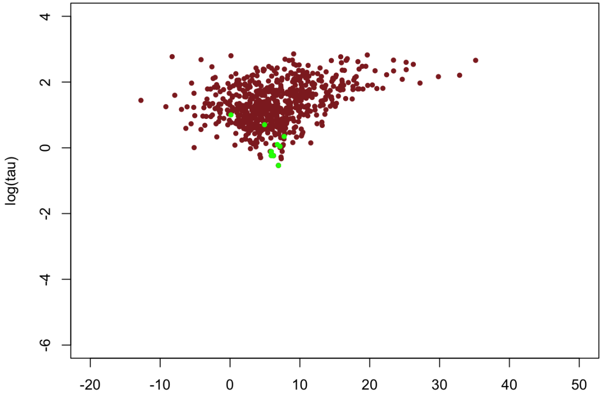

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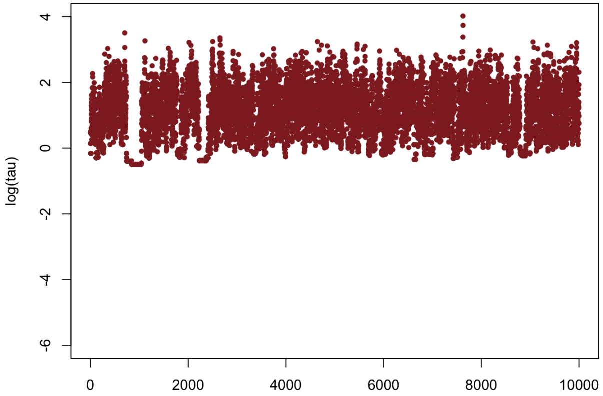

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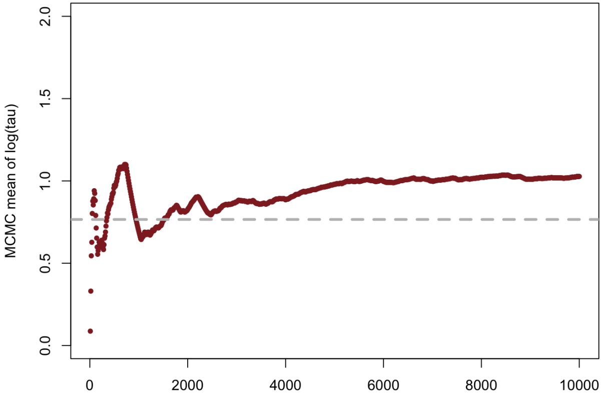

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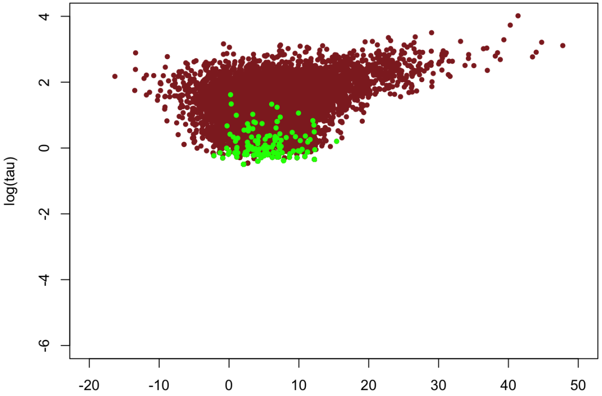

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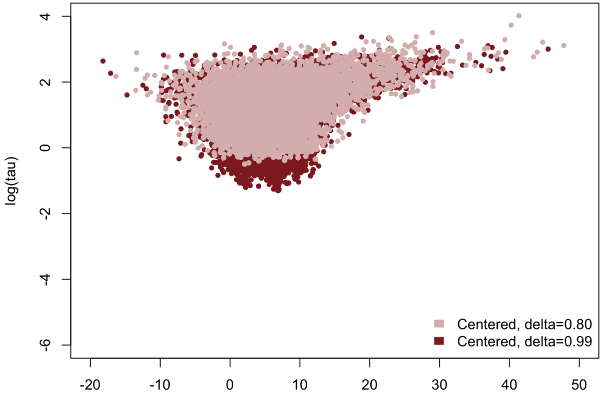

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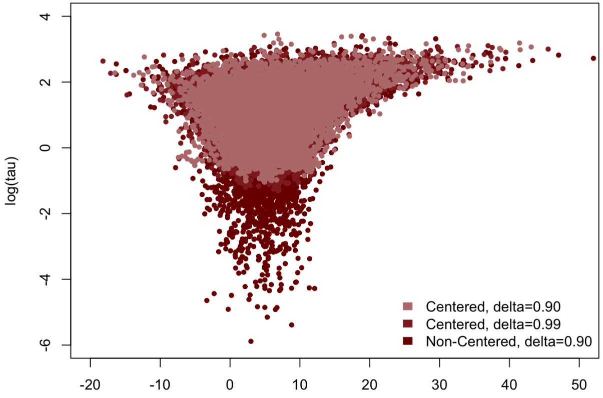

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- Multimodal
  - difficult to move from one mode to another
- Long-tailed with non-finite variance and mean
  - efficiency of exploration is reduced
  - central limit theorem doesn’t hold for mean and variance

Probabilistic programming language

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- 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, ...
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- R, Python, Julia, Scala, Stata, Matlab, command line interfaces
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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 binon
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model {
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  - 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

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- Stan makes transformation to unconstrained space and samples in unconstrained space
    - e.g. log transformation for <lower=a>
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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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- `_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)
```

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')
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

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
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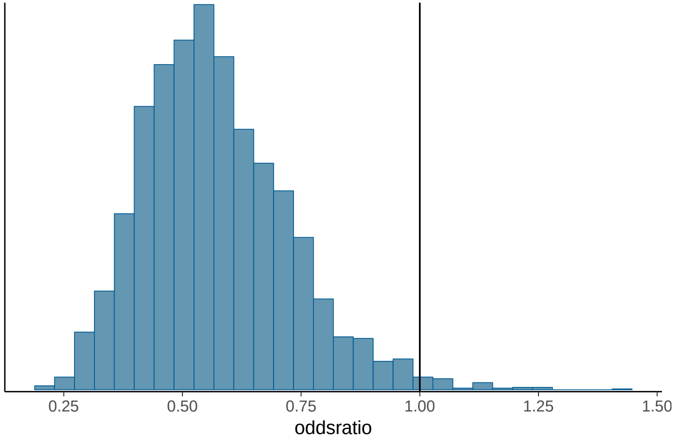
oddsratio    0.6       0 0.2    0.4    0.6    0.8  3108    1
lp__      -253.5       0 1.0 -254.8 -253.2 -252.6  1922    1

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)
```

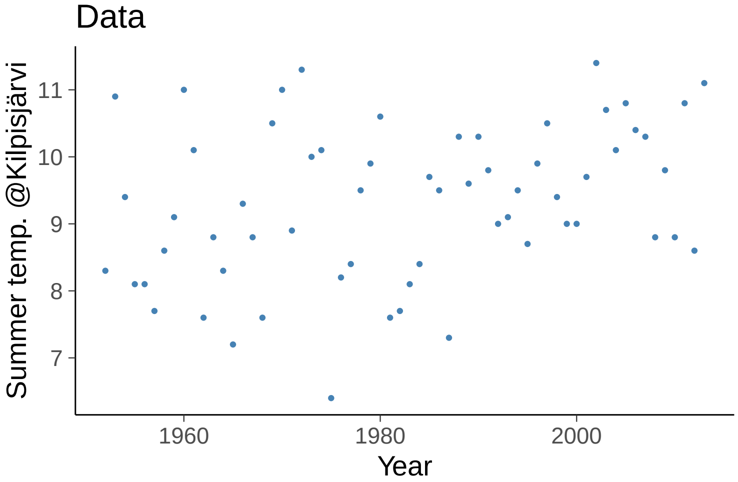
```
[1] "0 of 4000 iterations saturated the maximum tree depth of 10 (0%)"
[1] "0 of 4000 iterations ended with a divergence (0%)"
```

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

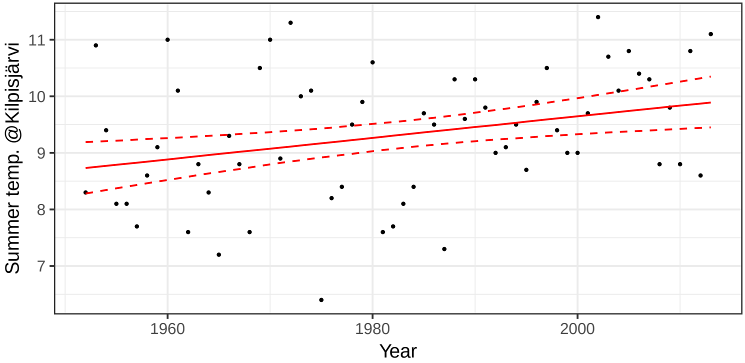
```
...
parameters {
  real alpha;
  real beta;
  real<lower=0> sigma;
  real<lower=1,upper=80> nu;
}
transformed parameters {
  vector[N] mu;
  mu <- alpha + beta*x;
}
model {
  nu ~ gamma(2,0.1);
  y ~ student_t(nu, mu, sigma);
}
```

Priors

- Prior for temperature increase?

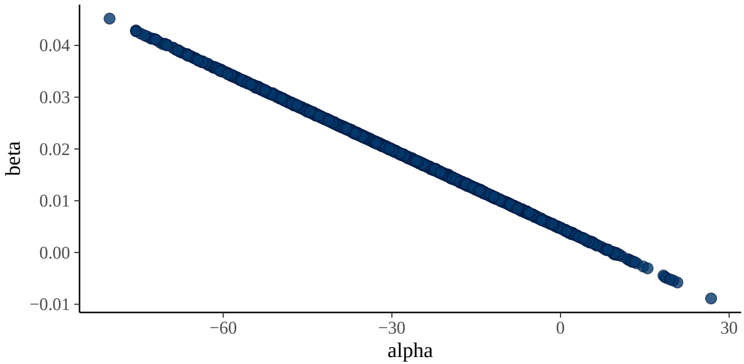
Kilpisjärvi summer temperature

Posterior fit



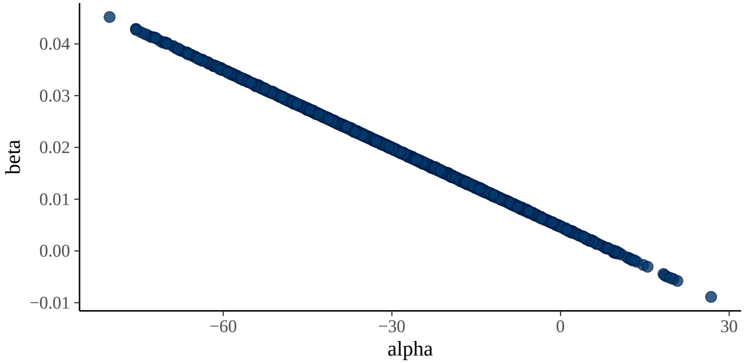
Kilpisjärvi summer temperature

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

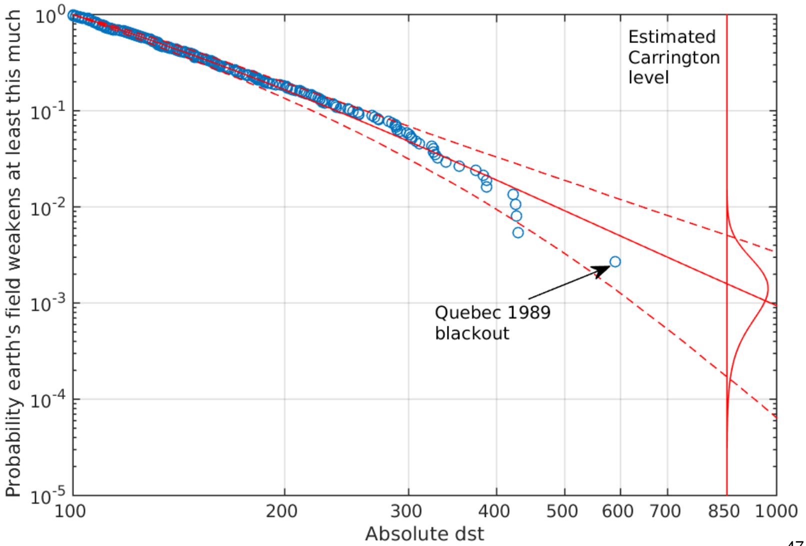
- BRMS provides simplified model description
  - a larger set of models than RStanARM, but still restricted
  - need to wait for the compilation

```
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)

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