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_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 development team (2018). Modeling Language User's Guide and Reference Manual https://github.com/stan-dev/stan/releases/download/v2.17.0/stan-reference-2.17.0.pdf
  - easiest to start from Part III Example Models
- Basics of Bayesian inference and Stan, part 1 Jonah Gabry & Lauren Kennedy
  - 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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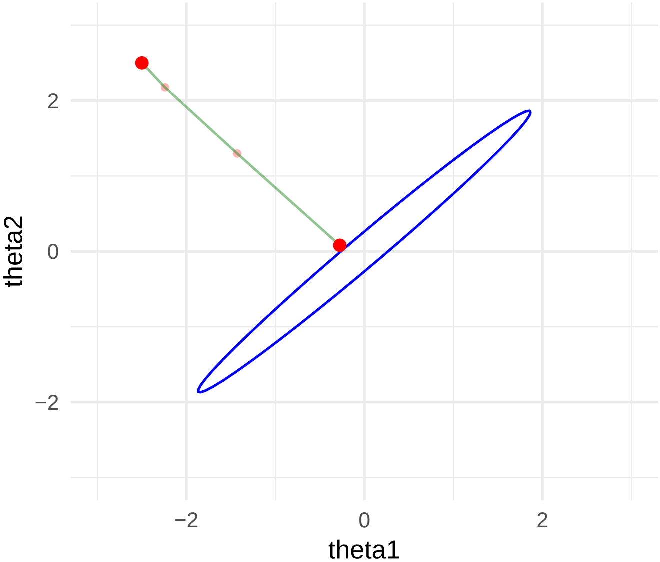

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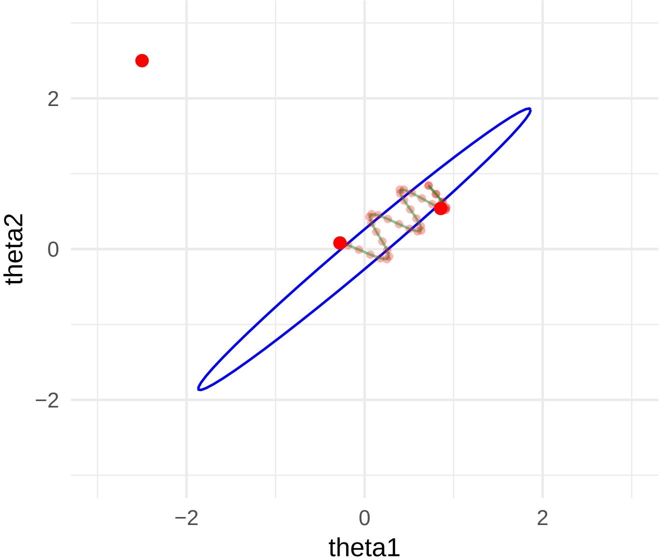

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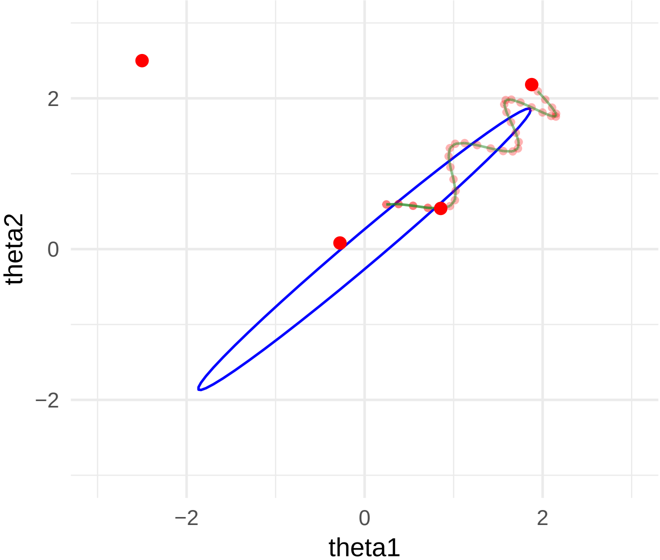

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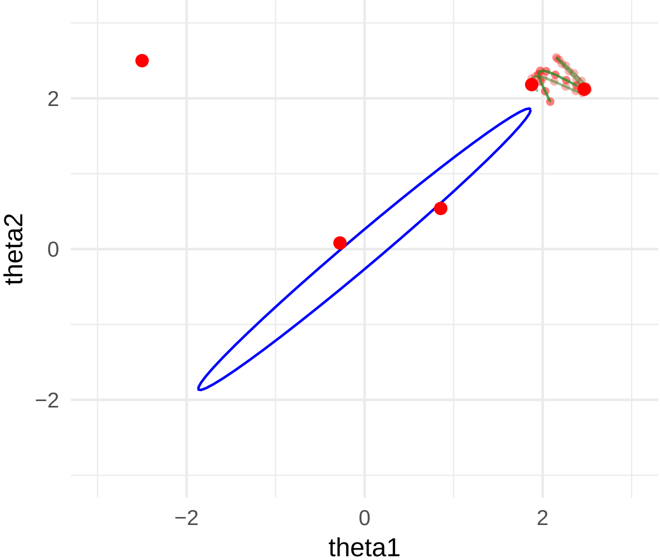

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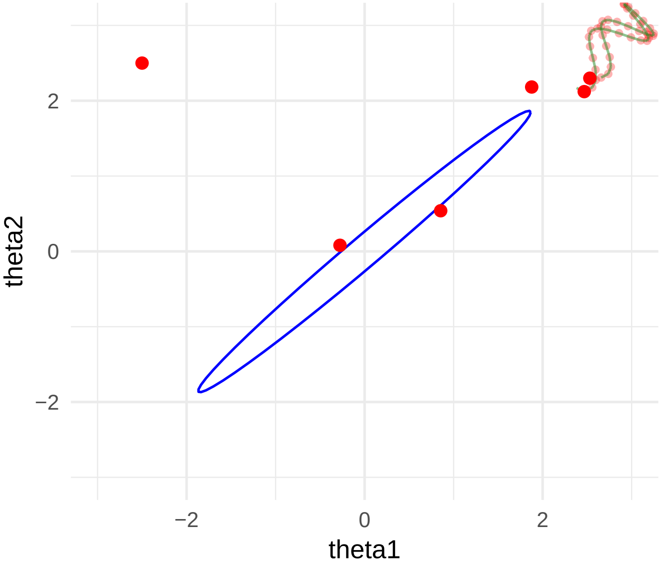

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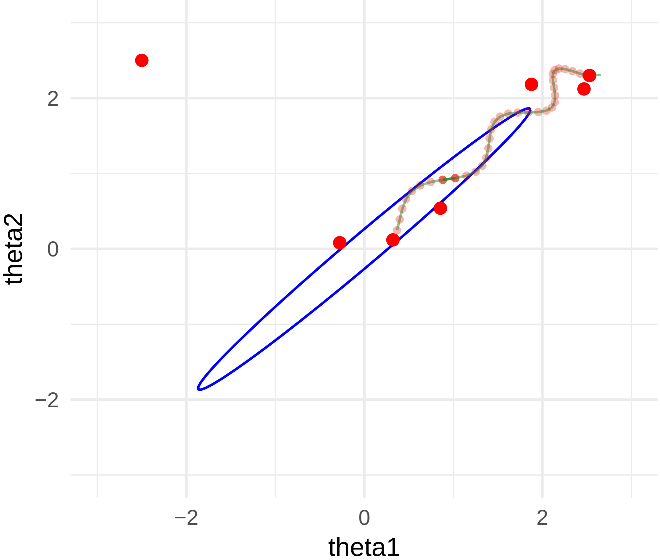

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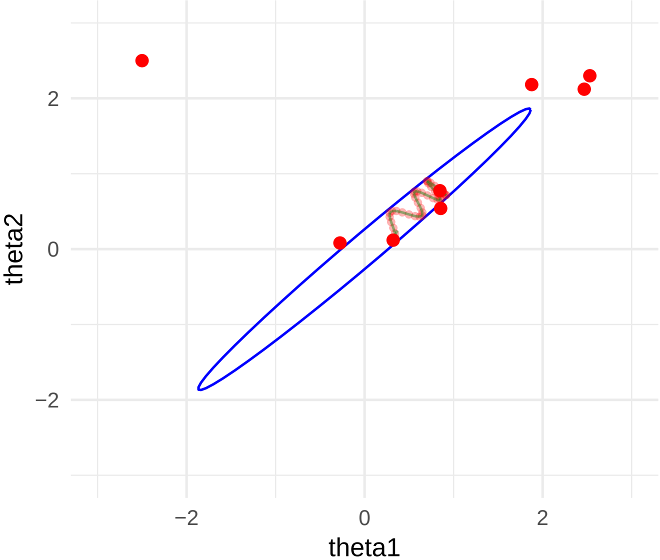

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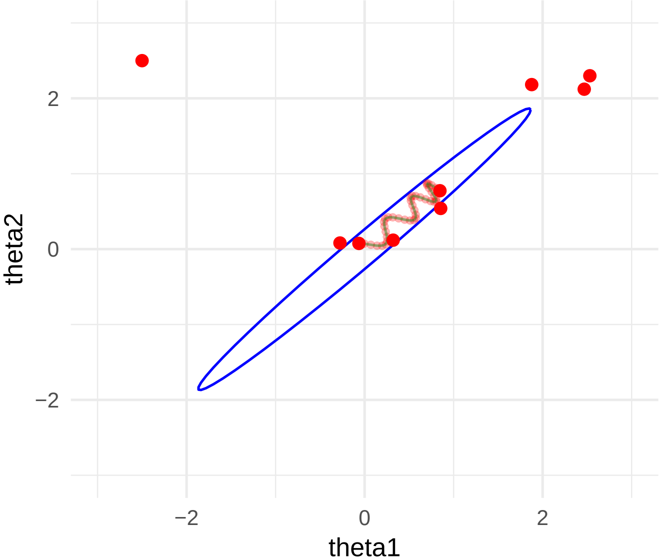

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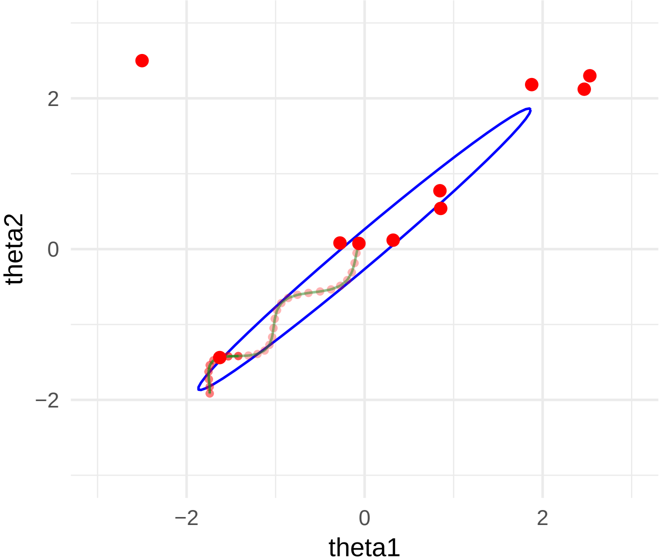

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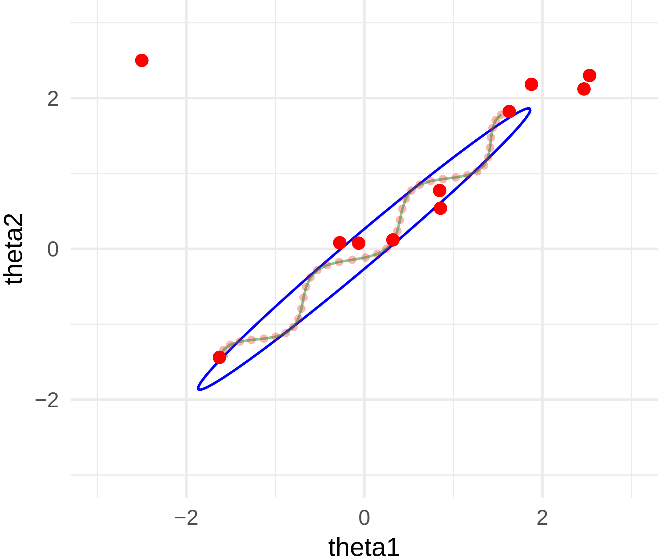

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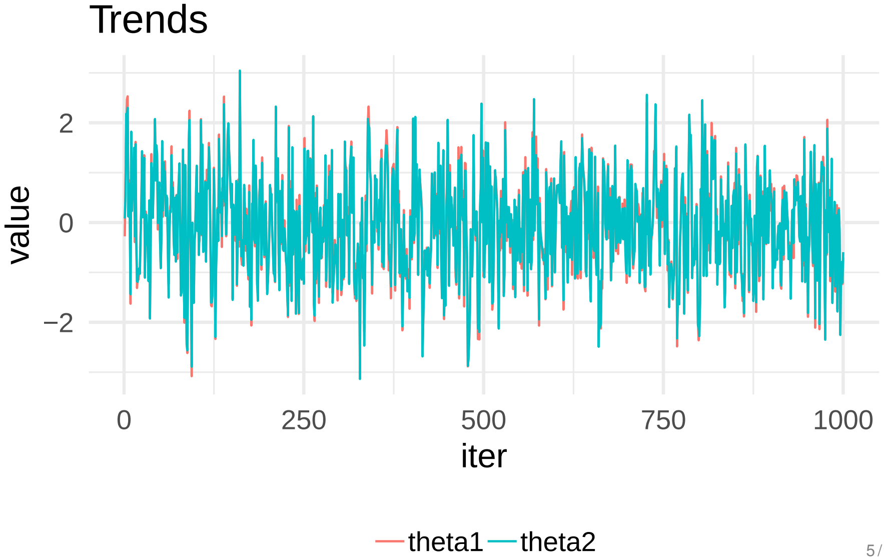

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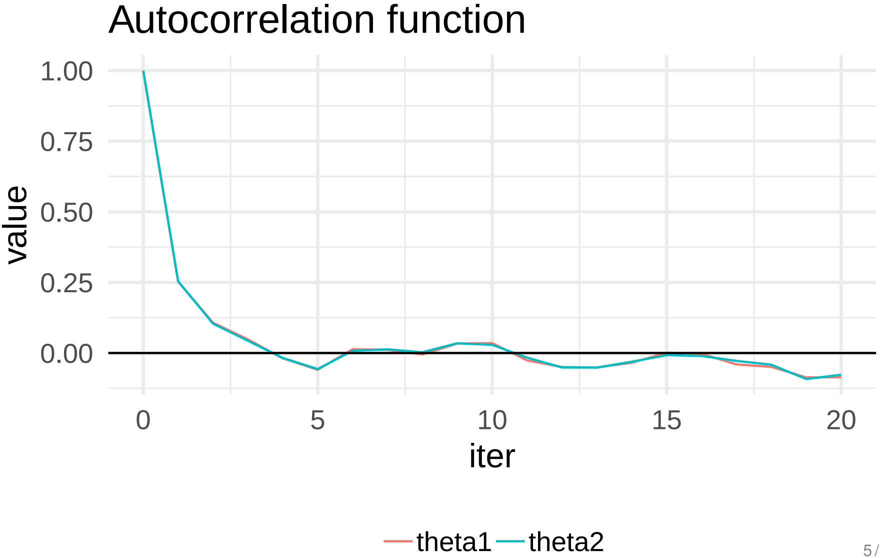

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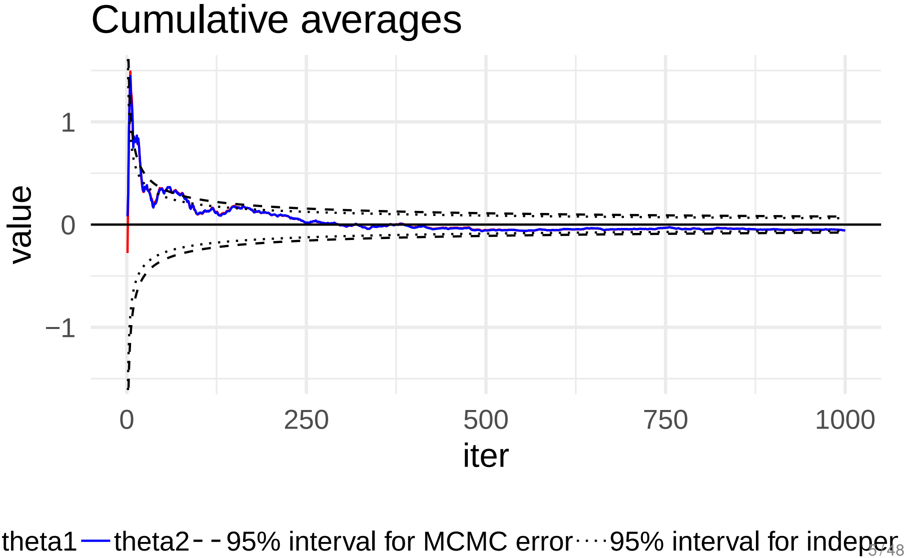

Hamiltonian Monte Carlo

- 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://elevanth.org/blog/2017/11/28/build-a-better-markov-chain/

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- 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
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  - 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

Adaptive dynamic HMC in Stan

- Dynamic HMC using growing tree to increase simulation trajectory until no-U-turn criterion stopping
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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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- 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 n_{eff}
- Different parameterizations matter

Divergences

- HMC specific: Indicates that Hamiltonian dynamic simulation has problems going to narrow places
  - indicates possibility of biased estimates
- Different parameterizations matter
- http://mc-stan.org/users/documentation/case-studies/divergences_and_bias.html

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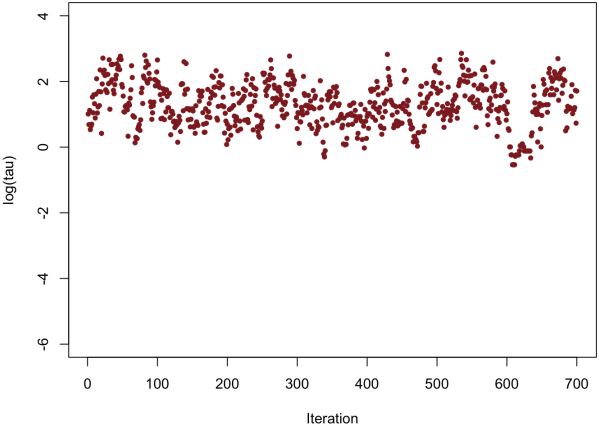

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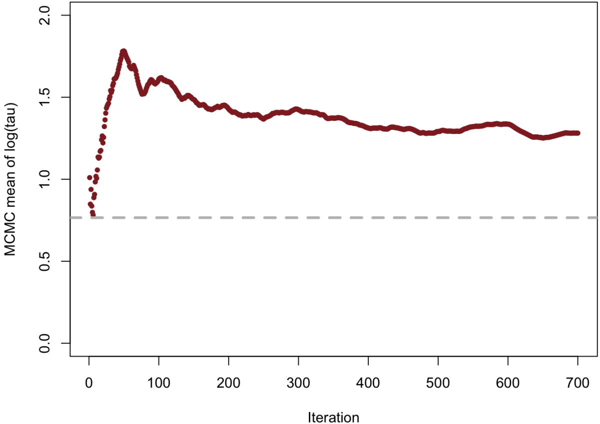

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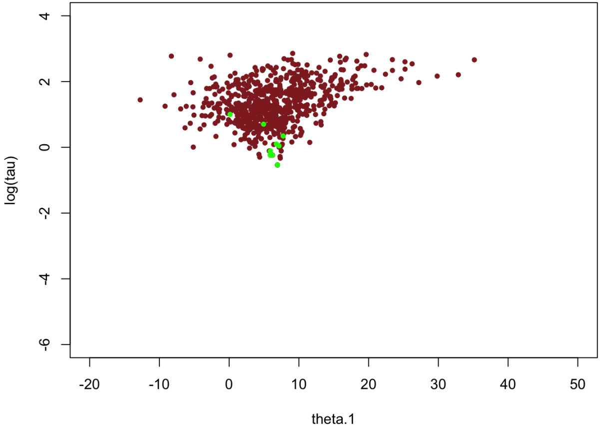

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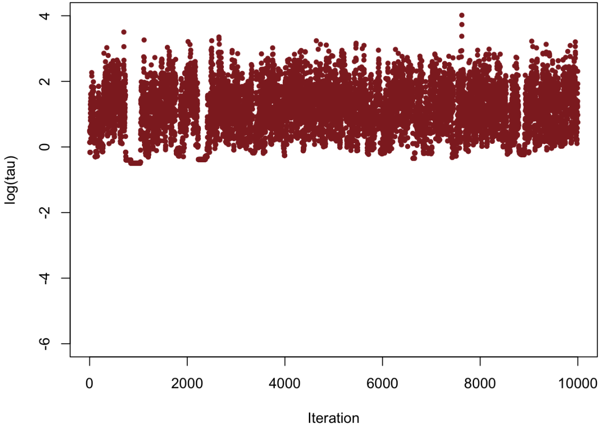

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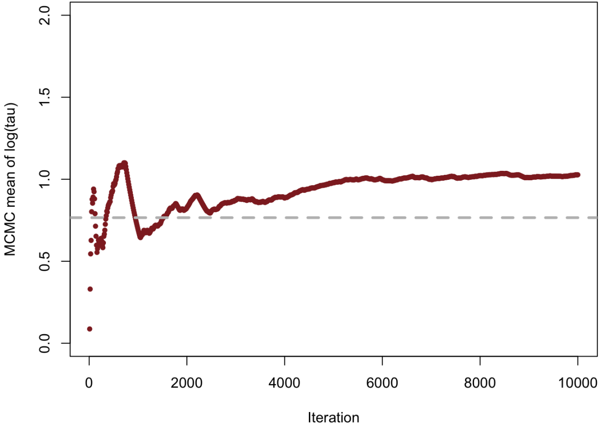

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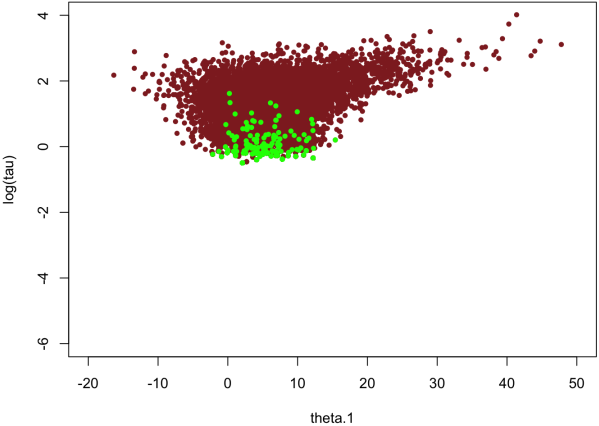

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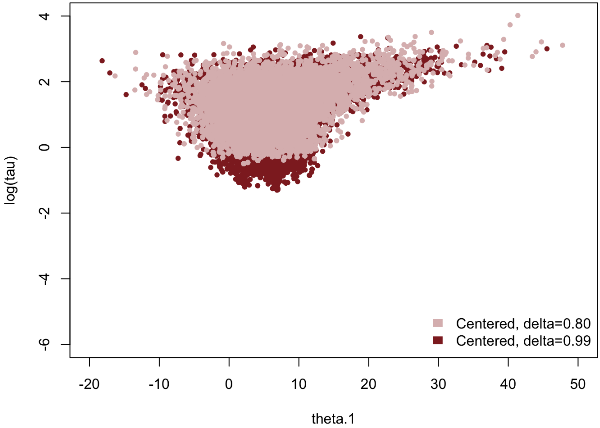

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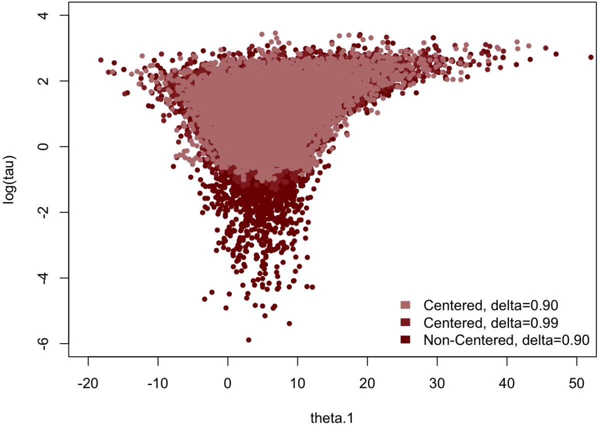

Probabilistic programming language

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

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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- 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 binon
}

model {
  theta ~ beta(1,1);        //prior
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```

- Data type and size are declared
- Stan checks that given data matches type and constraints

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)

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- $\sim$ is syntactic sugar and this could be also written as

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

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- `target` is the log posterior density (usually)
- `_lpdf` for continuous, `_lpmf` for discrete distributions

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 and PyStan

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)
```

RStan and PyStan

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Stan

- Compilation (unless previously compiled model available)
- Adaptation
- Warm-up
- 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;
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Difference between proportions

```
generated quantities {
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}
```

- generated quantities is run after the sampling

Difference between proportions

```r
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).
```

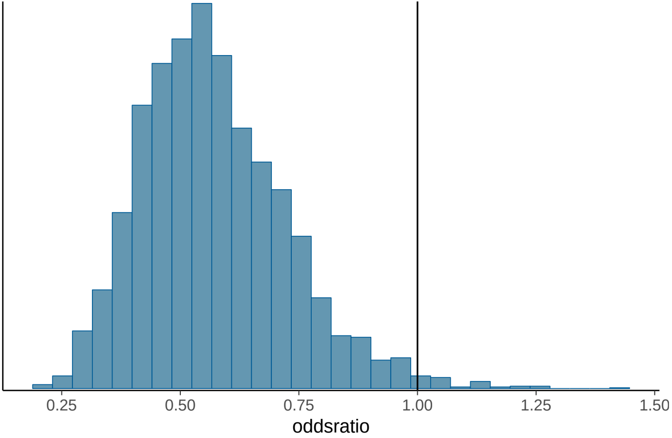
Difference between proportions

```
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

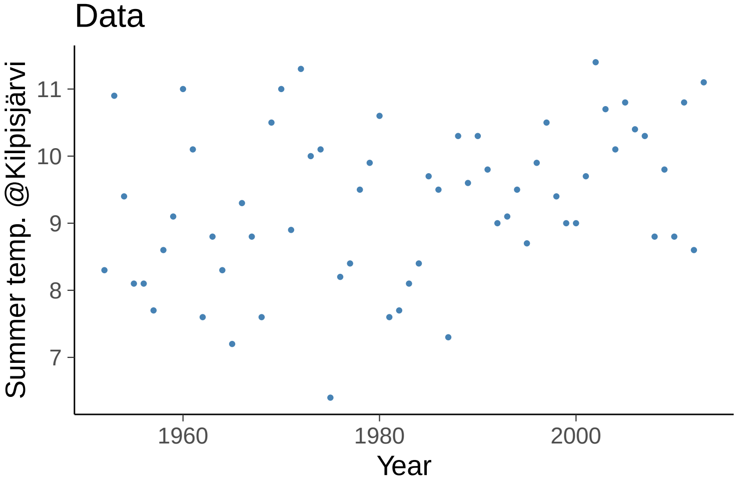
```
check_treedepth(fit_bin2)
check_energy(fit_bin2)
check_div(fit_bin2)

[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);
}
```

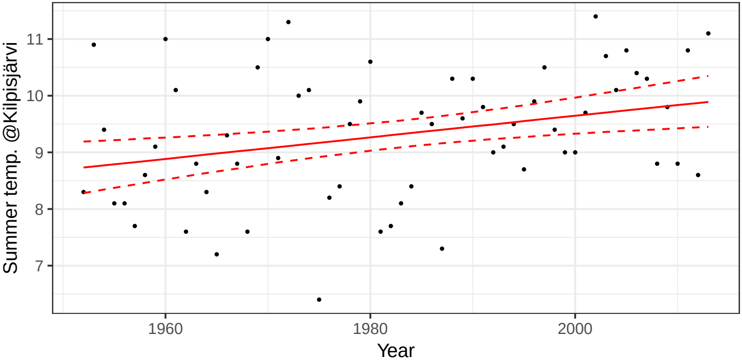
Student-t linear model

```
...
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);
}
```

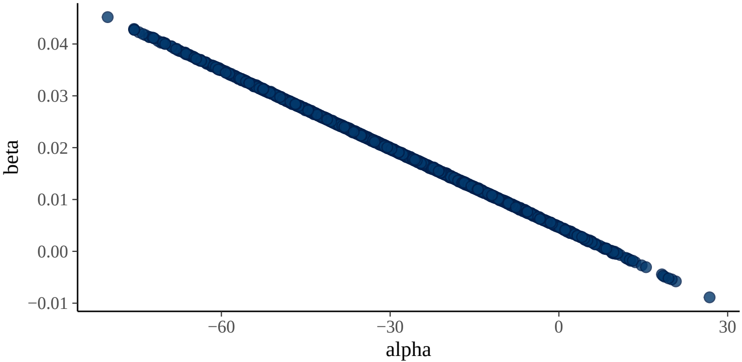
Priors

- Prior for temperature increase?

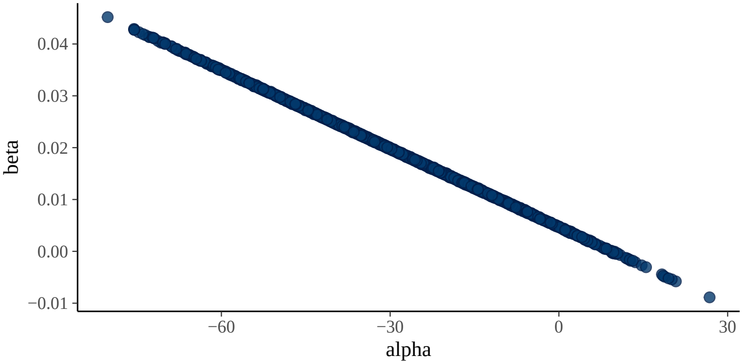
Kilpisjärvi summer temperature



Kilpisjärvi summer temperature



Kilpisjärvi summer temperature



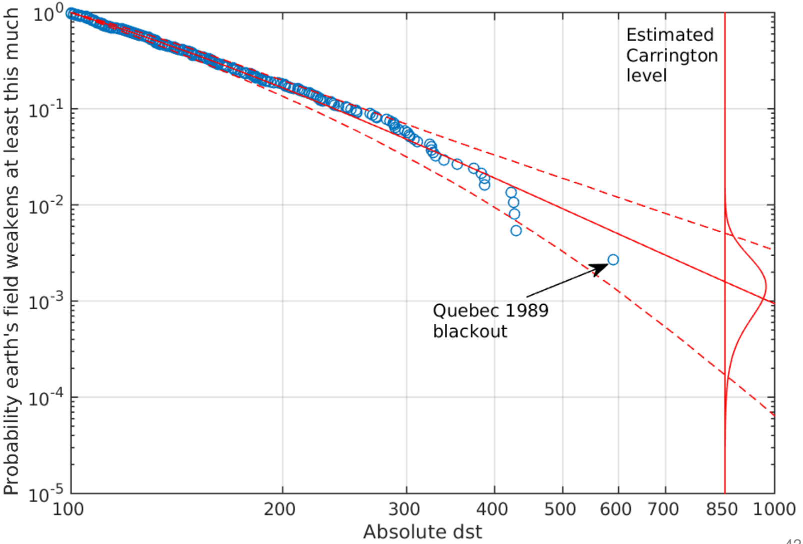

```
There were 14 transitions after warmup that exceeded the maximum
treedepth. Increase max_treedepth above 10. See
http://mc-stan.org/misc/warnings.html#maximum-treedepth-exceeded
Examine the pairs() plot to diagnose sampling problems
```

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);
}
```

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
  }
}
```

RStanARM

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

```
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)

draws_bin2 <- as.data.frame(fit_bin2) %>%
  mutate(theta1 = plogis(`(Intercept)`),
         theta2 = plogis(`(Intercept)` + grp2),
         oddsratio = (theta2/(1-theta2))/(theta1/(1-theta1)))

mcmc_hist(draws_bin2, pars='oddsratio')
```

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())
```

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)