Class 10: Moving from rstanarm to rstan

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Learning outcomes:

- Start using `rstan` instead of `rstanarm`
- Be able to fit more flexible models
- Interpret output from `rstan` models
- Do some model comparison using LOO and WAIC

Main differences

- `rstanarm` fits most models in one line very quickly, but it only fits a few of the main types of models (mainly regression models)
- `rstan` can fit a much wider variety of models
- `rstan` gives you much more control over prior distributions
- `rstan` takes a long time to compile each model before it starts running

Modelling set-up in `rstan`

1. Write some stan code and save it in a `rstan` file or in a text string
2. Save your data in a list with all the named components matching the `data` part of the stan code
3. Use the `stan` function to fit the model
4. Use `plot`, `summary`, etc to look at the output

Linear regression in rstan

```
stan_code = '
data {
  int N;
  vector[N] x;
  vector[N] y;
}
parameters {
  real intercept;
  real slope;
  real<lower=0> residual_sd;
}
model {
  // Likelihood
  y ~ normal(intercept + slope * x, residual_sd);
  // Priors
  intercept ~ normal(0, 100);
  slope ~ normal(0, 100);
  residual_sd ~ uniform(0, 100);
}
'
```

Key features of `rstan` code

- Three blocks for most models
  - `data` must declare all the objects that are fixed throughout the code
  - `parameters` can only include objects which are given prior distributions
  - `model` contains the priors and the likelihoods
- Other blocks we will use later

Fitting the models

```r
earnings = read.csv('../data/earnings.csv')
library(rstan)
#options(mc.cores = parallel::detectCores())
stan_run = stan(data = list(N = nrow(earnings),
                            y = earnings$y,
                            x = earnings$x_centered),
                model_code = stan_code)
```

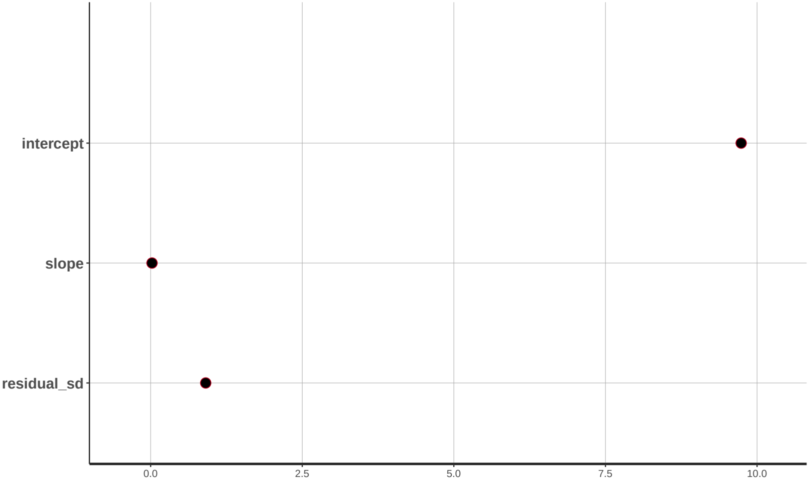
Looking at output

```r
print(stan_run)
```

```
## Inference for Stan model: ec2a1d3ccd2ba93b4b1df3b0cecf11b9.
## 4 chains, each with iter=2000; warmup=1000; thin=1;
## post-warmup draws per chain=1000, total post-warmup draws=4000.
##
##                mean se_mean   sd    2.5%     25%     50%     75%   97.5%
## intercept      9.74    0.00 0.03    9.68    9.72    9.74    9.76    9.79
## slope          0.02    0.00 0.00    0.02    0.02    0.02    0.02    0.03
## residual_sd    0.91    0.00 0.02    0.87    0.89    0.91    0.92    0.95
## lp__        -426.20    0.03 1.18 -429.21 -426.75 -425.90 -425.33 -424.84
##             n_eff Rhat
## intercept    2720    1
## slope        4000    1
## residual_sd  2939    1
## lp__         2205    1
##
## Samples were drawn using NUTS(diag_e) at Mon Oct  8 15:03:04 2018.
## 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).
```

Looking at output 2

```r
plot(stan_run)
```



An alternative way of setting the model up

```
stan_code = '
data {
  int N;
  vector[N] x;
  vector[N] y;
}
parameters {
  real intercept;
  real slope;
  real<lower=0> residual_sd;
}
transformed parameters {
  vector[N] fits;
  for (i in 1:N) {
    fits[i] = intercept + slope * x[i];
  }
}
model {
  // Likelihood
  y ~ normal(fits, residual_sd);
  // Priors
  intercept ~ normal(0, 100);
  slope ~ normal(0, 100);
  residual_sd ~ uniform(0, 100);
}
'
```

Flexibility in prior distributions

- Because we are writing out the model directly we can change the priors exactly how we want them
- For example, if we wanted to force the slope to be positive we could put a `gamma` prior on the slope, or change the declaration to `real<lower=0> slope;`
- A popular prior for standard deviation parameters is the half-cuachy. You will see this lots in the `rstanarm` and `rstan` examples

Quirks of the stan language

- Each line must finish with a semi-colon
- The declarations are a minefield. There seems to be at least 2 ways to specify vectors, and multiple ways to specify matrices. Hopefully they will tidy up in a future version
- However you can declare other variables on the fly in e.g. the `model` or `transformed parameters` sections
- Within block it doesn't seem to matter hugely the order the code is in, but the declarations need to be at the top
- Unlike most or R, everything is strongly typed. You cannot miss anything out of the `parameters` or `data` parts
- If you can vectorise the likelihood stan will run much faster

Mixed effects models in rstan

```
stan_code_mm = '
data {
  int N;
  int N_eth;
  vector[N] x;
  vector[N] y;
  int eth[N];
}
parameters {
  real intercept[N_eth];
  real slope;
  real mean_intercept;
  real<lower=0> residual_sd;
  real<lower=0> sigma_slope;
}
model {
  // Likelihood
  for (i in 1:N) {
    y[i] ~ normal(intercept[eth[i]] + slope * x[i], residual_sd);
  }
  // Priors
  slope ~ normal(0, 0.1);
  for (j in 1:N_eth) {
    intercept[j] ~ normal(mean_intercept, sigma_slope);
  }
  mean_intercept ~ normal(11, 2);
  sigma_slope ~ cauchy(0, 10);
  residual_sd ~ cauchy(0, 10);
}
'
```

Running the hierarchical model

```r
stan_run_2 = stan(data = list(N = nrow(earnings),
                              y = earnings$y,
                              x = earnings$x_centered,
                              eth = earnings$eth,
                              N_eth = length(unique(earning
                model_code = stan_code_mm)
```

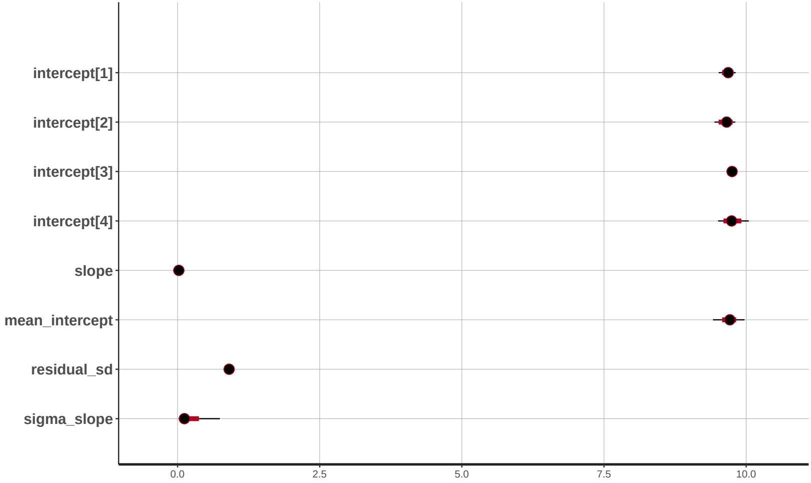
Output 1

```r
print(stan_run_2)
```

```
## Inference for Stan model: 90c73485e3cd793d3c411fc380ed2c1f.
## 4 chains, each with iter=2000; warmup=1000; thin=1;
## post-warmup draws per chain=1000, total post-warmup draws=4000.
##
##                   mean se_mean   sd    2.5%     25%     50%     75%
## intercept[1]      9.68    0.00 0.08    9.52    9.63    9.68    9.73
## intercept[2]      9.65    0.00 0.10    9.44    9.59    9.66    9.71
## intercept[3]      9.75    0.00 0.03    9.69    9.73    9.75    9.77
## intercept[4]      9.75    0.00 0.13    9.51    9.67    9.74    9.81
## slope             0.02    0.00 0.00    0.02    0.02    0.02    0.02
## mean_intercept    9.71    0.00 0.13    9.42    9.65    9.71    9.77
## residual_sd       0.91    0.00 0.02    0.87    0.89    0.91    0.92
## sigma_slope       0.18    0.01 0.23    0.02    0.07    0.12    0.22
## lp__           -421.10    0.18 2.94 -427.43 -422.93 -420.94 -419.09
##                  97.5% n_eff Rhat
## intercept[1]      9.82  1100 1.01
## intercept[2]      9.81   650 1.01
## intercept[3]      9.81  1539 1.00
## intercept[4]     10.05  2281 1.00
## slope             0.03   732 1.00
## mean_intercept    9.97  1552 1.00
## residual_sd       0.94  1941 1.00
## sigma_slope       0.74   930 1.00
## lp__           -415.69   275 1.01
##
## Samples were drawn using NUTS(diag_e) at Mon Oct  8 15:03:33 2018.
## 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).
```

Output 2

```r
plot(stan_run_2)
```



Getting directly at the posterior distribution

```r
post = as.data.frame(stan_run_2)
head(post)
```

```
##   intercept[1] intercept[2] intercept[3] intercept[4]
## 1     9.587808     9.618257     9.752213     9.704414 0.
## 2     9.603065     9.550718     9.785447     9.840273 0.
## 3     9.652886     9.561738     9.752084     9.721791 0.
## 4     9.717656     9.761773     9.762135     9.784466 0.
## 5     9.698116     9.693098     9.763895     9.747191 0.
## 6     9.698116     9.693098     9.763895     9.747191 0.
##   mean_intercept residual_sd sigma_slope      lp__
## 1       9.680109   0.8852871  0.11053914 -423.2668
## 2       9.730371   0.8659221  0.19622963 -422.2908
## 3       9.660946   0.8897362  0.15178171 -419.9416
## 4       9.700114   0.9228407  0.08869739 -418.9574
## 5       9.767824   0.9171940  0.04259593 -418.8286
## 6       9.767824   0.9171940  0.04259593 -418.8286
```

Creating predictions by hand

```
stan_code_3 = '
data {
  int N;
  int N_pred;
  vector[N] x;
  vector[N] y;
  vector[N_pred] x_pred;
}
parameters {
  real intercept;
  real slope;
  real<lower=0> residual_sd;
}
model {
  // Likelihood
  y ~ normal(intercept + slope * x, residual_sd);
  // Priors
  intercept ~ normal(0, 100);
  slope ~ normal(0, 100);
  residual_sd ~ uniform(0, 100);
}
generated quantities {
  vector[N_pred] y_pred;
  for (j in 1:N_pred)
    y_pred[j] = intercept + slope * x[j];
}
'
```

Fitting the new model

```r
stan_run_3 = stan(data = list(N = nrow(earnings),
                              N_pred = 5,
                              y = earnings$y,
                              x = earnings$x_centered,
                              x_pred = seq(-3,3, length = 5
                model_code = stan_code_3)
```

Extract out the predictions

```r
preds = extract(stan_run_3, 'y_pred')
head(preds$y_pred)
```

```
##           
## iterations     [,1]     [,2]     [,3]     [,4]     [,5]
##       [1,] 10.18138 9.693234 9.571198 9.510179 9.571198
##       [2,] 10.13474 9.680057 9.566386 9.509551 9.566386
##       [3,] 10.06657 9.659494 9.557726 9.506842 9.557726
##       [4,] 10.18562 9.623705 9.483225 9.412985 9.483225
##       [5,] 10.08883 9.675997 9.572789 9.521185 9.572789
##       [6,] 10.16509 9.658379 9.531702 9.468364 9.531702
```

Creating posterior predictive values by hand

```
stan_code_4 = '
data {
  int N;
  vector[N] x;
  vector[N] y;
  vector[N_pred] y_pred;
}
parameters {
  real intercept;
  real slope;
  real<lower=0> residual_sd;
}
model {
  // Likelihood
  y ~ normal(intercept + slope * x, residual_sd);
  // Priors
  intercept ~ normal(0, 100);
  slope ~ normal(0, 100);
  residual_sd ~ uniform(0, 100);
}
generated quantities {
  vector[N] y_pred;
  for (j in 1:N)
    y_pred[j] = normal_rng(intercept + slope * x[j], residual_sd);
}
'
```

A stan glmm

```
stan_code_od_pois = '
data {
  int<lower=0> N;
  int<lower=0> N_trt;
  int<lower=0> y[N];
  int trt[N];
}
parameters {
  real beta_trt[N_trt];
  real trt_mean;
  real<lower=0> trt_sd;
}
model {
  for (i in 1:N)
    y[i] ~ poisson_log(beta_trt[trt[i]]);

  // Priors on coefficients
  for(j in 1:N_trt)
    beta_trt[j] ~ normal(trt_mean, trt_sd);

  trt_mean ~ normal(0, 10);
  trt_sd ~ cauchy(0, 5);
}
'
```

Model comparison in `rstan` (and `rstanarm`)

- These two have their own model comparison criteria called WAIC (Widely Applicable Information Criterion) and LOO (Leave one out)
- We will use both. Philosphically WAIC is the more satisfactory but practically LOO seems to work better
- WAIC falls under the framework of *Information Criterion*, LOO is slightly different

Model comparison: an introduction

- We can come up with the fanciest model in the world but if it does not meet our desired goals (either prediction or causation) then we cannot publish or use it
- You can broadly split model comparison into two parts: *absolute* model comparison and *relative* model comparison
- In absolute model comparison, we are looking at how well a specific model fits the data at hand
- In relative model comparison, we can only look at how well a set of models performs on the same data with the goal of choosing the best one (or group)

Relative model comparison: model information criteria

- You might have come across these before: Akaike Information Criterion (AIC), Bayesian Information Criterion (BIC)
- The general idea is that the score on the likelihood is a good measure of model fit, except for the fact that more complex models will generally have higher likelihood scores
- If we penalise these scores by some measure of the complexity of the model then we can compare models across complexities
- The usual measure of complexity is some function of the number of parameters
- Because these are relative model comparisons, the best model acording to an IC might still be useless!

Different types of information criteria

- For various historical reasons, people tend to transform the likelihood score into the *deviance*, which is minus twice the log-likelihood score
- They then add a model complexity term onto it
- The two most common ICs are:

  $$\text{AIC} : -2 \log L + 2p$$

  $$\text{BIC} : -2 \log L + p \log n$$

  where p is the number of parameters and n is the number of observations
- We usually pick the smallest values of these across different models

Information criteria for Hierarchical models

- For Bayesian models it's hard to know which value of L to use, seeing as at each iteration we get a different likelihood score.
- Two specific versions of IC have been developed for these situations
- The first, called the *Deviance Information Criteria* (DIC) is calculated via:

  $$\text{DIC} : -2 \log L_{\text{max}} + 2p_D$$

  where p_D is the *effective number of parameters*
- The second called the Widely Applicable Information Criterion (WAIC) which is calculated as:

  $$\text{WAIC} : -2 \log L_{\text{max}} + p_{\text{WAIC}}$$

- Here p_{WAIC} is a measure of the variability of the likelihood scores

Which information criterion should I use?

- WAIC and DIC are built for Bayesian hierarchical models
- DIC was traditionally used everywhere but has fallen out of favour
- WAIC is included in the `loo` package which is installed alongside Stan
- WAIC is considered superior as it also provides uncertainties on the values. Most of the others just give a single value
- More generally there is a philosophical argument about whether we ever want to choose a single best model

An alternative: cross validation

- Cross validation (CV) works by:

1. Removing part of the data,
2. Fitting the model to the remaining part,
3. Predicting the values of the removed part,
4. Comparing the predictions with the true (left-out) values

- It's often fitted repeatedly, as in k-fold CV where the data are divided up into k groups, and each group is left out in turn
- In smaller data sets, people perform leave-one-out cross-validation (LOO-CV)

Pros and cons of CV

- We might also run the 5-fold CV on the previous slide for different complexity models and see which had the smallest root mean square error of prediction (RMSEP), i.e. use it as a relative criteria
- CV is great because it actually directly measures the performance of the model on real data, based on data the model hasn't seen
- However, it's computationally expensive, and problems occur in hierarchical models if some groups are small, and therefore might get left out of a fold
- The `loo` function (in the `loo` package) gives an approximation of LOO-CV

Absolute model comparison

- We've already met posterior predictive distributions, which is essentially leave none out CV.
- Another popular one is something called the *Bayes Factor*. This is created by first calculating the posterior distribution of a model given the data, a measure of absolute model fit. The ratios of these can be compared for different models to create a relative model criteria.
- However, Bayes Factors are really hard to calculate and often overly sensitive to irrelevant prior choices

Continuous model expansion

- There are lots of clever ways to set up prior distributions so that a model choice step is part of the model fit itself
- One way is partial pooling, by which we force e.g. varying slope and intercept parameters to the same value (or not)
- Another way is to put shrinkage or selection priors on the parameters in the model, possibly setting them to zero
- More on all of these later in the course

Example: computing loo and waic on an rstanarm regression model

```
library(loo)
prostate = read.csv('../data/prostate.csv')
mod_1 = stan_lmer(lpsa ~ lcavol+ ( 1| gleason), data = pros
mod_2 = stan_lmer(lpsa ~ (lcavol | gleason), data = prostat
```

```
loo_1 = loo(mod_1)
loo_2 = loo(mod_2)
compare_models(loo_1, loo_2)
```

```
##
## Model comparison:
## (negative 'elpd_diff' favors 1st model, positive favors
##
## elpd_diff        se
##      -0.3       1.8
```

Now with WAIC

```
library(loo)
prostate = read.csv('../data/prostate.csv')
waic_1 = waic(mod_1)
waic_2 = waic(mod_2)
compare_models(waic_1, waic_2)
```

```
##
## Model comparison:
## (negative 'elpd_diff' favors 1st model, positive favors
##
## elpd_diff        se
##      -0.3       1.8
```

Summary

- We have now seen a number of different types of hierarchical GLM in rstan
- Many of the ideas of hierarchical linear models transfer over, but we can explore richer behaviour with hierarchical GLMs
- These have all used the normal, binomial or Poisson distribution at the top level, and have allowed for over-dispersion, robustness, and ordinal data, to name just three