Writing Models in Stan

Why write models in Stan

- Clarity you know exactly what the model is doing and what each parameter represents (simplifies interpretation and model assessment).
- Flexibility you can build a truly *bespoke* model that fits your data structure perfectly and estimates exactly what you want it to (especially useful for complex models and/or assessing comparisons or summaries of parameters, e.g., differences between group means).

Why not write models in Stan

- Speed with some small changes to the formula, brms can probably fit the collection of models that you are interested in, even quite complex models.
- Safety with great power, comes great responsibilty
 - Extra important to follow a careful workflow, including prior predictive checks, fitting the model to simulated data and confirming it recovers the true parameter values, convergence diagnostics, and posterior predictive checks.

Warning: package 'kableExtra' was built under R version 4.4.2

Structure of a Stan model

A stan program is divided into "blocks". Three blocks are almost always included (not technically necessary, but you're on thin ice if you don't have at least these three blocks).

1. "data" block: where you declare the data types, their dimensions, any restrictions (i.e. upper= or lower= , which act as checks for Stan), and their names. Each named data object represents a named element of the list that you will create in R.

- 2. "parameters" block: This is where you declare the parameters you want to model, their dimensions, restrictions, and name. For example, in a simple linear regression, you'll need three parameters, the intercept, a slope, and the standard deviation of the errors around the regression line.
- 3. "model" block: This is where you include any sampling statements, including the "like-lihood" (the log probability calculations). This is where the distributions are defined, including the priors. You can restrict priors using upper or lower when declaring the parameters (i.e. <lower=0> to make sure a parameter is positive think standard deviation terms)

Four blocks are optional:

• "functions"

You can define a custom function for use in the model. You probably won't use this at first, but it's very flexible. It can be a function to sample from a custom distribution, a complex calculation that needs to be run multiple times, etc.

• "transformed data"

Can be very simple calculations (e.g., defining an n-1 value) or re-ordering or grouping of data. This also may not be necessary at first.

• "transformed parameters"

 Summaries of parameters and data that are necessary to calculate the likelihood, or that you want to use later in the model (in the model or generated quantities blocks), or that you want to save for accessing after sampling.

• "generated quantities"

 Derived quantities based on parameters, data, and random numbers (e.g., posterior predictions or some random variate from a normal distribution with a mean and sd based on parameters).

Comments are indicated by "//" and are ignored by Stan, and vital to future-you.

An example Stan model from Chapter 11 in Statistical Rethinking. Here I've taken some of the code from Chapter 11 to set up model m11.4: the logistic regression model that estimates the treatment effects and separate intercepts for each chimpanzee (actor) on the pulled_left binary response.

Data setup, including defining a list in R (dat_list), that has three components, named to match the data variable names.

```
## R code 11.1 - taken directly from the book
library(rethinking)
```

```
data(chimpanzees)
d <- chimpanzees

## R code 11.2
d$treatment <- 1 + d$prosoc_left + 2*d$condition

## R code 11.10
# trimmed data list
dat_list <- list(
  pulled_left = d$pulled_left,
  actor = d$actor,
  treatment = as.integer(d$treatment) )</pre>
```

Then we define and fit the model with ulam.

```
## R code 11.11
m11.4 <- ulam(
  alist(
    pulled_left ~ dbinom( 1 , p ) ,
    logit(p) <- a[actor] + b[treatment] ,
    a[actor] ~ dnorm( 0 , 1.5 ),
    b[treatment] ~ dnorm( 0 , 0.5 )
) , data=dat_list , chains=4 , log_lik=TRUE ,
    messages = FALSE)</pre>
```

Then we'll use the **rethinking** function **stancode** to extract the model as it was written in Stan. The output of the function is a character vector, that we can write to a text file with a *.stan* extension.

```
m11.4_stan_code <- stancode(m11.4)

data{
    array[504] int pulled_left;
    array[504] int treatment;
    array[504] int actor;
}

parameters{
    vector[7] a;
    vector[4] b;
}

model{
    vector[504] p;</pre>
```

```
b ~ normal( 0 , 0.5 );
    a ~ normal( 0 , 1.5 );
    for ( i in 1:504 ) {
        p[i] = a[actor[i]] + b[treatment[i]];
        p[i] = inv_logit(p[i]);
    pulled_left ~ binomial( 1 , p );
generated quantities{
    vector[504] log_lik;
    vector[504] p;
    for ( i in 1:504 ) {
        p[i] = a[actor[i]] + b[treatment[i]];
        p[i] = inv_logit(p[i]);
    for ( i in 1:504 ) log_lik[i] = binomial_lpmf( pulled_left[i] | 1 , p[i] );
}
  cat(m11.4_stan_code,
      file = "m11.4 Stan code.stan")
```

The model includes four blocks, each defined by the curly braces. Here's the data block with some added annotation, where the three data variables are defined (everything between the curly braces that follow the key word data.

```
data{
    array[504] int pulled_left; // the response variable 0 or 1 (1 = pulled left)
    array[504] int treatment; // the indicator for each treatment 1 through 4.
    array[504] int actor; // the indicator for each chimpanzee (1 through 7)
}
```

Notice that these are the same names and dimensions of the dat_list

```
str(dat_list)

List of 3
$ pulled_left: int [1:504] 0 1 0 0 1 1 0 0 0 0 ...
$ actor : int [1:504] 1 1 1 1 1 1 1 1 1 1 ...
$ treatment : int [1:504] 1 1 2 1 2 2 2 2 1 1 ...
```

The overthinking box on page 334 in Section 11.1.1 explains more of the components of the Stan model.

An elaboration of the Stan model.

If I was writing this Stan model for my own use, I would generalise some of the components so that I could run it on different datasets. In this case, that means defining some of the dimensions (number of observations, number of actors, number of treatments) as data in the model. First, add three components to the data list.

```
dat_list[["n_observations"]] <- length(dat_list[["pulled_left"]])
dat_list[["n_actors"]] <- max(dat_list[["actor"]]) #number of actors
dat_list[["n_treatments"]] <- max(dat_list[["treatment"]]) #number of treatments</pre>
```

Then we can re-write the Stan code so that it will work with any size of dataset and any collection of actors and treatments. We can use these dimensions in the variable declaration lines in the data, parameters, and models blocks, as well as the loops in the model and generated quantities blocks.

```
data{
    int<lower=1> n_observations; // number of observations
    int<lower=1> n_actors;// number of actors
    int<lower=1> n treatments;// number of treatments
    array[n_observations] int pulled_left; // the response variable 0 or 1 (1 = pulled lef
    array[n_observations] int treatment; // the indicator for each treatment 1 through 4.
    array[n_observations] int actor; // the indicator for each chimpanzee (1 through 7)
}
parameters{
     vector[n_actors] a;
     vector[n_treatments] b;
}
model{
     vector[n observations] p;
    b ~ normal( 0 , 0.5 );
    a ~ normal( 0 , 1.5 );
    for ( i in 1:n_observations ) {
        p[i] = a[actor[i]] + b[treatment[i]];
        p[i] = inv_logit(p[i]);
    pulled_left ~ binomial( 1 , p );
generated quantities{
    vector[n_observations] log_lik;
     vector[n_observations] p;
```

```
for ( i in 1:n_observations ) {
    p[i] = a[actor[i]] + b[treatment[i]];
    p[i] = inv_logit(p[i]);
}
for ( i in 1:n_observations ) log_lik[i] = binomial_lpmf( pulled_left[i] | 1 , p[i] );
}
```

I'll write that model to another .stan text file to save it.

```
write("
data{
    int<lower=1> n_observations; // number of observations
    int<lower=1> n_actors;// number of actors
    int<lower=1> n_treatments;// number of treatments
    array[n_observations] int pulled_left; // the response variable 0 or 1 (1 = pulled lef
    array[n observations] int treatment; // the indicator for each treatment 1 through 4.
    array[n_observations] int actor; // the indicator for each chimpanzee (1 through 7)
}
parameters{
     vector[n_actors] a;
     vector[n_treatments] b;
}
model{
    vector[n_observations] p;
    b ~ normal( 0 , 0.5 );
    a ~ normal( 0 , 1.5 );
    for ( i in 1:n_observations ) {
        p[i] = a[actor[i]] + b[treatment[i]];
        p[i] = inv_logit(p[i]);
    pulled_left ~ binomial( 1 , p );
}
generated quantities{
   vector[n_observations] log_lik;
    vector[n_observations] p;
    for ( i in 1:n_observations ) {
        p[i] = a[actor[i]] + b[treatment[i]];
        p[i] = inv_logit(p[i]);
    for ( i in 1:n_observations ) log_lik[i] = binomial_lpmf( pulled_left[i] | 1 , p[i] );
ጉ"
```

```
"m11.4_modified_Stan_code.stan")
```

Fitting the model using cmdstanr

The R package cmdstanr is the go-to package for using Stan from within R. It's used in the backend of the packages rethinking and brms. The package rstan has much of the same functionality, but because it is housed on CRAN, it runs an older version of Stan.

If you haven't already installed cmndstanr, the package has great set-up documentation and tools built into the package to make sure your set-up works.

There are three basic steps to fitting a model.

1 - Compile the model

```
library(cmdstanr)
m11.4_stan <- cmdstanr::cmdstan_model("m11.4_modified_Stan_code.stan")</pre>
```

2 - Sample

```
stan_fit <- m11.4_stan$sample(
  data = dat_list,
  seed = 1999, # not necessary
  chains = 4,
  parallel_chains = 4,
  refresh = 1000, # reduces the number of messages
  iter_warmup = 1000,
  iter_sampling = 1000
)</pre>
```

Running MCMC with 4 parallel chains...

```
Chain 1 Iteration: 1 / 2000 [ 0%] (Warmup)
Chain 1 Iteration: 1000 / 2000 [ 50%] (Warmup)
Chain 1 Iteration: 1001 / 2000 [ 50%] (Sampling)
Chain 2 Iteration: 1 / 2000 [ 0%] (Warmup)
Chain 3 Iteration: 1 / 2000 [ 0%] (Warmup)
```

```
Chain 2 Iteration: 1000 / 2000 [ 50%]
                                        (Warmup)
Chain 2 Iteration: 1001 / 2000 [ 50%]
                                        (Sampling)
Chain 3 Iteration: 1000 / 2000 [ 50%]
                                        (Warmup)
Chain 3 Iteration: 1001 / 2000 [ 50%]
                                        (Sampling)
Chain 4 Iteration:
                      1 / 2000 [ 0%]
                                        (Warmup)
Chain 4 Iteration: 1000 / 2000 [ 50%]
                                        (Warmup)
Chain 4 Iteration: 1001 / 2000 [ 50%]
                                        (Sampling)
Chain 1 Iteration: 2000 / 2000 [100%]
                                        (Sampling)
Chain 2 Iteration: 2000 / 2000 [100%]
                                        (Sampling)
Chain 1 finished in 0.6 seconds.
Chain 2 finished in 0.6 seconds.
Chain 3 Iteration: 2000 / 2000 [100%]
                                        (Sampling)
Chain 4 Iteration: 2000 / 2000 [100%]
                                        (Sampling)
Chain 3 finished in 0.6 seconds.
Chain 4 finished in 0.6 seconds.
```

All 4 chains finished successfully.

Mean chain execution time: 0.6 seconds.

Total execution time: 2.7 seconds.

3 - Summarise

The \$summary() function built into the fitted model object provides parameter summaries as well as convergence diagnostics

variable	mean	median	sd	mad	q5	q95	rhat	ess_bulk	ess_tail
lp	-	-	2.360	2.254	-	-	1.003	1804.284	2576.485
	268.381	268.052			272.704	265.115			
a[1]	-0.455	-0.453	0.329	0.331	-1.001	0.071	1.005	1446.445	2153.997
a[2]	3.872	3.812	0.757	0.732	2.738	5.217	1.002	3702.480	2458.456
a[3]	-0.752	-0.748	0.335	0.332	-1.299	-0.202	1.003	1626.247	2519.966
a[4]	-0.752	-0.743	0.340	0.336	-1.316	-0.203	1.004	1543.525	2438.514
a[5]	-0.445	-0.449	0.325	0.331	-0.973	0.079	1.003	1402.022	2506.169
a[6]	0.475	0.473	0.341	0.342	-0.086	1.048	1.003	1589.370	2060.532
a[7]	1.959	1.944	0.414	0.403	1.300	2.660	1.002	2316.522	2666.182
b[1]	-0.039	-0.035	0.283	0.282	-0.507	0.417	1.007	1307.736	1979.435
b[2]	0.481	0.483	0.285	0.279	0.024	0.953	1.005	1327.208	2088.818

Save the output from cmdstarr. Stan saves each iteration in a series of csv files while it's simulating things (by default in a temporary directory), but to ensure that everything is saved (all posterior draws and diagnostics) use the save_object function.

```
stan_fit$save_object("saved_stan_fit.rds") #must add the .rds
```

Assessing model fit (WAIC and PSISloo)

The cmdstanr includes the psis_loo calculations (this works because the model includes a derived parameter name log_lik.

```
loo_psis <- stan_fit$loo()
loo_psis</pre>
```

Computed from 4000 by 504 log-likelihood matrix.

```
Estimate SE

elpd_loo -266.2 9.5

p_loo 8.5 0.4

looic 532.4 19.0

-----

MCSE of elpd_loo is 0.0.

MCSE and ESS estimates assume MCMC draws (r_eff in [1.3, 2.3]).

All Pareto k estimates are good (k < 0.7).

See help('pareto-k-diagnostic') for details.
```

But if you want to calculate waic, you'll have to extract the posterior draws and use the loo package functions.

```
library(loo)
```

This is loo version 2.8.0

- Online documentation and vignettes at mc-stan.org/loo
- As of v2.0.0 loo defaults to 1 core but we recommend using as many as possible. Use the 'c

- Windows 10 users: loo may be very slow if 'mc.cores' is set in your .Rprofile file (see ht

```
Attaching package: 'loo'
```

The following object is masked from 'package:rethinking':

```
compare
```

```
log_lik_draws <- stan_fit$draws("log_lik")
loo_waic <- waic(log_lik_draws)
loo_waic</pre>
```

Computed from 4000 by 504 log-likelihood matrix.

```
Estimate SE
elpd_waic -266.2 9.5
p_waic 8.5 0.4
waic 532.4 19.0
```

Resources

The main Stan website has lots of useful information.

The Stan user guide has a huge collection of example models. For example, here's the section that covers regression models.

The Stan Forums, including the questions tagged with #Ecology.