From BRMS to Stan

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My Questions for You

- What kinds of models do you use for research? For teaching?
- BRMS
 - How often do you use it: never, sometimes, always?
 - What do you like/dislike/find confusing about BRMS?
- Stan
 - Have you run Stan models through an interface, RStan, CmdStanR, CmdStanPy?
 - Have you written / tried to write or modify Stan models?
 - What do you like/dislike/find confusing about Stan?

Talk Outline

- Brief discussion of BRMS
- Stan from 0 to 60 in 30 minutes
 - Model 1: "Hello World"
 - Model 2: black diamond varying-slope / varying intercept
- Notebook: brms2stan.qmd

BRMS: Bayesian Regression and Multilevelmodeling in Stan

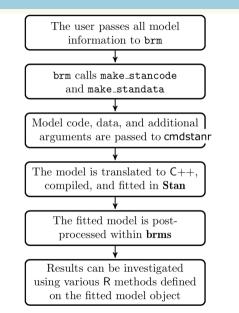


- Fit Bayesian generalized linear / non-linear multivariate multilevel models using Stan.
- Specify model via 1me4-like formula syntax.

```
sleep_mlm_brmsfit <-
   brm(Reaction ~ Days + (Days|Subject),
   data = sleepstudy)</pre>
```

https://paul-buerkner.github.io/brms/

BRMS Processing



BRMS Processing

Pass all information to BRMS

```
brm(Reaction ~ Days + (Days Subject), data = sleepstudy)
```

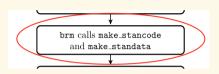
Get results

```
Family: gaussian
 Links: mu = identity; sigma = identity
Formula: Reaction ~ Days + (Days | Subject)
  Data: sleepstudy (Number of observations: 180)
Multilevel Hyperparameters:
                                         Regression Coefficients:
~Subject (Number of levels: 18)
                                              Estimate Est.Error
                 Estimate Est Error
                                         Intercept
                                                   251.31
                                                              7.40
                                         Days 10.45 1.70
sd(Intercept)
                    27.27 7.03
sd(Davs)
            6.60 1.51
                                         sigma
                                                    25.87
                                                             1.52
cor(Intercept, Days) 0.07 0.30
```

Reasons to Use BRMS

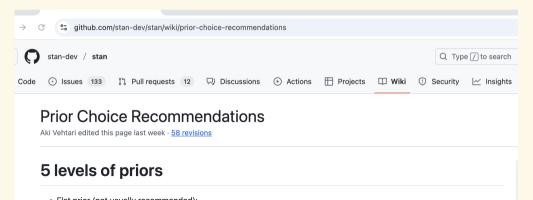
- Familiar syntax (for R users).
- Handles many common models: IRT, zero-inflated, additive distributional, phylogenetic, missing data imputation.
 - See Vignettes and Articles
- Sound and robust implementations, e.g.
 - Zero-centers predictors (like RStanARM).
 - Makes varying slope/ varying intercept models easy.
- Large community of users
 - Majority of questions on Stan mailing list are BRMS.
 - Many helpful community experts to answer them!

BRMS Drawbacks



- Generated Stan code is hard to read/modify.
- Priors used may be suboptimal.

See github/stan-dev/stan wiki page Prior Choice Recommendations



BRMS Priors

Prior Definitions for brms Models

```
> prior_summary(sleep_mlm_brmsfit)
                      prior
                                class
                                            coef
                                                   group resp dpar nlpar lb ub
                                                                                       source
                     (flat)
                                                                                      default.
                                     h
                     (flat)
                                    b
                                                                                 (vectorized)
                                            Days
 student t(3, 288.7, 59.3) Intercept
                                                                                      default
      lkj_corr_cholesky(1)
                                                                                      default.
      lkj_corr_cholesky(1)
                                                                                 (vectorized)
                                                 Subject
     student t(3, 0, 59.3)
                                   sd
                                                                                      default
     student t(3, 0, 59.3)
                                   sd
                                                 Subject
                                                                                 (vectorized)
     student_t(3, 0, 59.3)
                                   sd
                                                                                 (vectorized)
                                            Days Subject
     student_t(3, 0, 59.3)
                                                                                 (vectorized)
                                    sd Intercept Subject
     student t(3, 0, 59.3)
                                                                                      default
                                sigma
```

- To change the priors you must understand the model structure.
- If you understand the model structure, you can code it in Stan!

Changing BRMS Priors

Easy to get wrong - cf. questions on discourse.mc-stan.org, e.g.: recent discussion

Equally complicated - custom families, custom link functions.

From BRMS to Stan

When model specification in BRMS is long / complicated / not quite possible - try Stan.

- How do you write a Stan program?
- BRMS Formula provides structure of regression and data inputs.
- Mapping BRMS elements to a Stan program
 - data block defines all data inputs outcomes and predictors, plus dimensions.
 - parameters block defines all distributional parameters.
 - model block specifies the likelihood and priors.

Stan Program Structure

A Stan program consists of one or more named program blocks, strictly ordered.

```
functions {
  // declare, define functions
} data {
  // declare input data
} transformed data {
   // transform inputs, define program data
} parameters {
   // declare (continuous) parameters
} transformed parameters {
   // define derived parameters
} model {
   // compute the log joint distribution
} generated quantities {
   // define quantities of interest
```

Stan Program Execution

- NUTS-HMC sampler discretizes Hamiltonian dynamics into steps.
 - 1 sampler iteration is comprised of many steps.
 - Good NUTS-HMC sampler intro: Faster estimation of Bayesian models in ecology using Hamiltonian Monte Carlo
- data, transformed data blocks executed once on startup cheap
- parameters
 - on startup: initialize parameters
 - at every step of inference algorithm: validate constraints
- transformed parameters, model blocks executed every step of the sampler expensive
- generated quantities executed every iteration of the sampler less expensive

Stepwise Model Development: Hello, World!

- A "Hello, World!" program is the name given to the first, simplest possible program written when learning a new programming language.
 - Pro tip: always start with "Hello, World!"
- End goal is a efficient and maintainable multi-level model
 - Reaction ~ Days + (Days|Subject)
- Initial goal is a simple linear model ignore difference between subjects
 - BRMS formula: Reaction ~ Days
- Simple linear regression: $y \sim alpha + beta * x$,
 - where reaction time is y and day is x.

Initial Stan Model sleep_simple.stan

```
data {
  int<lower=0> N:
 vector[N] day;
  vector[N] v: // reaction time
parameters {
 real alpha; // intercept
 real b_day; // slope
 real<lower=0> sigma; // residual standard deviation
model {
  y ~ normal(alpha + day * b_day, sigma);
  alpha ~ normal(250, 50); // informed prior for human reaction times in ms
  b day ~ normal(10, 10); // weakly informed prior for per-day effect
  sigma ~ normal(0, 10); // very weakly informative prior
```

Improved Stan Model sleep_simple.stan - Mean-center Data

This decreases the correlation between the intercept and slope. (BRMS, RStanArm do this automatically.)

```
data {
  int<lower=0> N; vector[N] day; vector[N] y;
transformed data {
 real day mean = mean(day);
  vector[N] day centered = day - day mean: // mean-center data
parameters {
 real alpha; real b_day; real<lower=0> sigma;
model {
  y ~ normal(alpha + day_centered * b_day, sigma);
  alpha ~ normal(250, 50); b_day ~ normal(10, 10); sigma ~ normal(0, 10);
generated quantities {
 real b intercept = alpha - b day * day mean; // recover intercept
```

BRMS stancode for Reaction ~ Days

for (i in 2:K) {

means X[i - 1] = mean(X[, i]):

Xc[, i-1] = X[, i] - means X[i-1]:

```
> stancode(sleep_simple_brmsfit)
                                                          parameters {
// generated with brms 2.22.0
                                                            vector[Kc] b; // regression coefficients
functions {
                                                            real Intercept; // temporary intercept for centered pred
                                                            real<lower=0> sigma; // dispersion parameter
data {
  int<lower=1> N; // total number of observations
                                                          transformed parameters {
  vector[N] Y: // response variable
                                                            real lprior = 0; // prior contributions to the log poste
  int<lower=1> K; // number of population-level effects
                                                            lprior += normal lpdf(b | 10, 10);
  matrix[N, K] X; // population-level design matrix
                                                            lprior += normal_lpdf(Intercept | 250, 50);
  int<lower=1> Kc: // number of population-level effects
                                                            lprior += normal lpdf(sigma | 0, 10)
  int prior only: // should the likelihood be ignored?
                                                              -1 * normal lccdf(0 | 0, 10):
transformed data {
                                                          model {
  matrix[N, Kc] Xc: // centered version of X without an i if (!prior only) { // likelihood including constants
  vector[Kc] means_X; // column means of X before centeri
                                                             target += normal_id_glm_lpdf(Y | Xc, Intercept, b, sign
```

target += lprior: // priors including constants

generated quantities { // actual population-level intercep real b Intercept = Intercept - dot product(means X, b):

Multilevel Models

- Account for the structure in the data.
 - Individual observations are drawn from one or more common populations.
 - Estimate population-level mean, variance as well as individual-level mean, variance.
 - Population level parameters inform priors for individual level parameters.
- Provide partial pooling of information.
 - The hierarchical prior controls the pooling between levels.
 - Similar data across levels \to Low hierarchical variance \to strong pooling. When hierarchical variance approaches 0, complete pooling.
 - Dissimilar data across levels \rightarrow High hierarchical variance \rightarrow weak pooling. When hierarchical variance approaches ∞ , no pooling.

Multilevel models

- Expand Stan model:
 - A per-subject parameter vector β (b_subj) is multivariate normal
 - b_subj ~ multi_normal(mu_subj, sigma_subj)
 - mu_subj is vector, of length number of subjects, sigma_subj is covariance matrix.

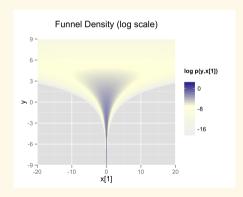
Problems

- Stan distribution multi_normal requires inverting covariance matrix at every evaluation - computationally expensive.
- Two sources of variance: sigma and hierarchical variance sigma_subj difficult to estimate from small number of observations per group.
 - Without sufficient data \rightarrow funnel distribution
- **Solution**: Reparameterization, following code example in Stan User's Guide section Hierarchical models and the non-centered parameterization

Multilevel models and the Funnel

Neal's Funnel: extreme example of a challenging hierarchical prior

$$p(y,x) = \operatorname{normal}(y \mid 0,3) \times \prod_{n=1}^{9} \operatorname{normal}(x_n \mid 0, \exp(y/2)).$$



Prior distribution; no data.

To explore neck of the funnel:

small steps on x-axis, large steps on y-axis.

To explore mouth of the funnel:

large steps on x-axis, small steps on y-axis.

But stepsize is same for all axes; cannot adequately sample either.

Funnel Example: Stan Implementations

Centered parameterization

"Natural" parameterization.

```
parameters {
    real y;
    vector[9] x;
}
model {
    y ~ normal(0, 3);
    x ~ normal(0, exp(y/2));
}
```

Note: minimal model, no predictors

- ullet variable y== hierarchical variance
- variable x == group-level covariate

Non-centered parameterization

- Parameters block: declare standardized parameters.
- Transformed parameters: declare variables add offset (location), multiply by scale.

```
parameters {
 real y_raw;
 vector[9] x raw;
transformed parameters {
  // offset is 0. just multiply by scale
 real y = 3.0 * y_raw;
  vector[9] x = exp(v/2) * x raw:
model {
  y_raw ~ std_normal(); // y ~ normal(0, 3)
 x_raw ~ std_normal(); // x ~ normal(0, exp(y/2))
```

Stan's Affine Transform

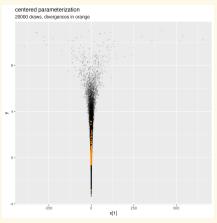
Stan's Affinely Transformed Scalar can be applied element-wise to vector \mathbf{x} to facilitate the non-centered parameterization

```
parameters {
  real<multiplier = 3.0> y;
  vector<multiplier = \exp(v/2) > [9] x;
model {
  y \sim \text{std normal}(); // y \sim normal(0, 3)
  x ~ std normal(); // x ~ normal(0, exp(y/2))
```

Compare Funnel Fits

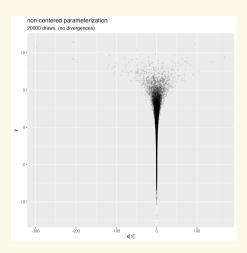
Centered parameterization

 Cannot explore neck of funnel many divergences (in orange)



Non-centered parameterization

Explores further; no divergences



BRMS to Stan

- "Hello, World!" model formula Reaction ~ 1 + Days
 - coded as distribution statement:

```
y ~ normal(alpha + day_centered * b_day, sigma);
```

- Target model formula Reaction ~ 1 + Days + (1 + Days | Subject)
 - Global intercept and slope for Days
 - Subject-specific random intercepts and slopes
- Correlation between random effects: prior on subject effect is a multivariate normal with mean vector μ (mu) and covariance matrix Σ (Sigma).
- See Gelman & Hill 2007, chapter 11, 12, 13 or this blogpost
- Multivariate reparameterization

Multi-variate reparameterization

Centered parameterization

```
data {
data {
                                              int K; int J;
  int K; // num predictors + intercept
  int J: // num groups
                                            parameters {
                                              vector<lower=0>[K] tau;
parameters {
                                              cholesky_factor_corr[K] L_Omega;
  vector[K, J] beta; // group covariates
                                              matrix[K, J] beta_std;
  vector[K] mu; // location
  cov_matrix[K] Sigma; // scale
                                            transformed parameters {
 // ...
                                              matrix[J, K] beta =
                                                (diag_pre_multiply(tau, L_Omega) * beta_std)';
model {
 // hierarchical prior
                                            model {
  for (j in 1:J) {
                                              // non-centered priors
    beta[ , j] ~ multi_normal(mu, Sigma);
                                              tau ~ exponential(1);
                                              L_Omega ~ lkj_corr_cholesky(K);
  // ...
                                              to vector(beta std) ~ std normal();
```

Non-centered parameterization

Specifying the Likelihood

- Reaction ~ 1 + Day + (1 + Subject | Day)
- Create design matrix x with column 1 for group-level intercept term

```
transformed data {
  matrix[N, 2] x;
  x[ , 1] = rep_vector(1, N);
  x[ , 2] = day;
}
```

Add group-level term to regression formula.

```
vector[N] eta = b_intercept + b_day * day + rows_dot_product(x, beta[ subj, ]);
y ~ normal(eta, sigma);
```

Parameters, transformed parameters, model blocks

```
parameters {
  real b_intercept; real b_day; real<lower=0> sigma;
  vector<lower=0>[2] tau; cholesky_factor_corr[2] L_Omega;
  matrix[2, J] beta std:
transformed parameters {
  // random effects matrix scaled, transposed (centered at 0)
 matrix[J, 2] beta = (diag pre multiply(tau, L Omega) * beta std)';
model {
  vector[N] eta = b intercept + b day * day + rows dot product(x, beta[ subj. ]);
  v ~ normal(eta, sigma);
  b_intercept ~ normal(250, 50); b_day ~ normal(10, 10); sigma ~ exponential(1);
  tau ~ exponential(1); L_Omega ~ lkj_corr_cholesky(2);
  to vector(beta std) ~ std normal();
```

Recovering the Quantities of Interest

```
generated quantities {
 // match BRMS outputs
 real sd intercept = tau[1];
 real sd_day = tau[2];
 // Reconstruct correlation matrix
 matrix[2, 2] Omega;
  Omega = multiplv lower tri self transpose(L Omega);
 real cor_intercept_day = Omega[1, 2];
  // Posterior likelihood and posterior predictive y-replicates
  vector[N] v rep: vector[N] log lik;
  { // don't save to output
    vector[N] eta = b_intercept + b_day * day + rows_dot_product(x, beta[ subj, ]);
    y_rep = to_vector(normal_rng(eta, sigma));
    for (n in 1:N) {
     log_lik[n] = normal_lpdf(y[n] | eta[n], sigma);
```

Notebook

Run notebook brms2stan.qmd in RStudio

References

Stan User's Guide:

- Efficiency Tuning, Hierarchical models and the non-centered parameterization
- Efficiency Tuning, Multivariate reparameterization
- Regression, Multivariate regression example

Many Thanks!

Questions???