From BRMS to Stan

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BRMS: Bayesian Regression and Multilevelmodeling in Stan

Recap from last week * BRMS extended formula syntax for multi-level regressions

```
response ~ pterms + (gterms | group)
```

- *pterms* define *population-level* effects; same for all observations.
- *gterms* define *group-level* effects; vary across *group* variable.
- The intercept term is 1 or 0 for no intercept; if unspecified, default is 1.

```
fit1 <- brm(Reaction ~ Days + (Days | Subject), data = sleepstudy)
```

equivalent to

```
fit1 <- brm(Reaction ~ 1 + Days + (1 + Days | Subject), data = sleepstudy)
```

Stan Program File (review)

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 Blocks - Execution During Sampling (review)

- `data`, `transformed data` blocks - executed once on startup
- `parameters` -
  - on startup: initialize parameters
  - at every step of inference algorithm: validate constraints
- `transformed parameters`, `model` blocks - executed every *step* of the sampler
- `generated quantities` - executed every *iteration* of the sampler
- After every sampler iteration, program outputs current values of all variables in parameters, transformed parameters, and generated quantities blocks.

From BRMS to Stan

- BRMS: specify arguments to the `brm` function: formula, data, family, prior.
  - BRMS generates Stan model code.
  - BRMS code is not quite human-readable, but efficiently coded.

- *Goal: write efficient, robust Stan program*
  - map regression formula to Stan program's sampling distribution statement.
  - `data` block defines all data inputs - outcomes and predictors, plus dimensions.
  - `transformed data` block mean-centers predictor variables.
  - `parameters` block defines all distributional parameters.
  - `model` block specifies the likelihood and priors.

- When should you do this?
  - When model specification in BRMS is long / complicated / not quite possible.

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 - complete pooling across subjects
  `Reaction ~ Days`
  (`Reaction ~ 1 + Days` - by default, model includes global intercept.)
- Carry over BRMS efficiencies to Stan model

Stan Model `sleep_simple.stan`

```
data {
  int<lower=0> N;   vector[N] day;   vector[N] y;  // reaction time
}
transformed data {
  real day_mean = mean(day);
  vector[N] day_centered = day - day_mean;
}
parameters {
  real alpha;  real b_day;  // intercept, slope
  real<lower=0> sigma; // residual standard deviation
}
model {
  y ~ normal(alpha + day_centered * 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
}
generated quantities {
  real b_intercept = alpha - b_day * day_mean;
  array[N] real y_rep = normal_rng(alpha + day_centered * b_day, sigma);
}
```

Notebook - Stan, BRMS complete pooling model

```r
sleep_data = list(
    N = nrow(sleepstudy), J = length(unique(sleepstudy$Subject)),
    subj = as.integer(sleepstudy$Subject), day = sleepstudy$Days,
    y = as.double(sleepstudy$Reaction)
)

sleep_simple = cmdstan_model("stan/sleep_simple.stan")
sleep_simple_stanfit = sleep_simple$sample(data = sleep_data)
as.data.frame(sleep_simple_stanfit$summary(variables = c('b_intercept', 'b_day', 'sigma'))

priors <- c(set_prior("normal(250, 50)", class = "Intercept"),
set_prior("normal(10, 10)", class = "b"),
set_prior("normal(0, 10)", class = "sigma"))

sleep_simple_brmsfit = brm(Reaction ~ Days, data = sleepstudy, prior = priors)
sleep_simple_brmsfit
```

Multilevel models

- Specify model in terms of the inherent structure of the data
- Sleep study: reaction time varies by subject
  - BRMS formula: `Reaction ~ 1 + Days + (1 + Days|Subject)`
- Expand Stan model:
  - Predictor vector β is *multivariate normal*
  - `b_subj ~ multi_normal(mu_subj, sigma_subj)`
  - `mu_subj` is vector, `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.

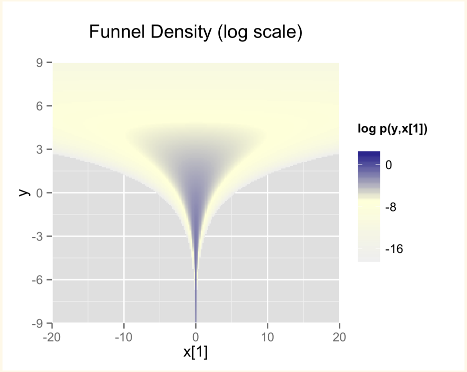
Multilevel models

- **Partial Pooling**: The hierarchical prior controls the pooling between levels:
  - Similar data across levels $\rightarrow$ Low hierarchical variance $\rightarrow$ Strong pooling
  - Dissimilar data across levels $\rightarrow$ High hierarchical variance $\rightarrow$ Weak pooling
- **Problem**: For low numbers of observations, MCMC sampler cannot resolve residual variance `sigma` and variance of hierarchical prior `sigma_subj`; many divergences
- **Solution**: Reparameterization, following code example in Stan User's Guide section Hierarchical models and the non-centered parameterization

Multilevel models and Neal's Funnel

- Neal's Funnel: extreme example of a challenging hierarchical model

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



Explore neck: need small stepsize on x-axis, large stepsize on y-axis.

Explore mouth: need large stepsize on x-axis, small stepsize on y-axis.

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

Funnel Example: Hierarchical Logistic Regression

Centered parameterization

- "Natural" parameterization.

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

Non-centered parameterization

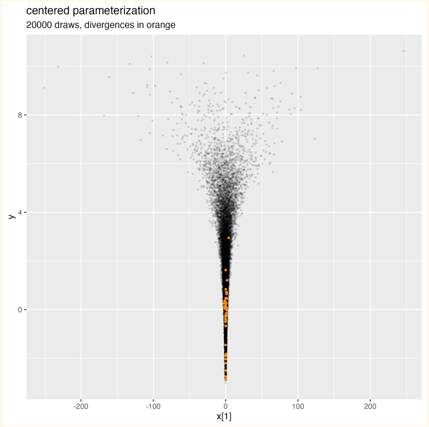
- Parameters block: declare standardized parameters.
- Transformed parameters: declare *variables* add offset (location), multiply by scale.

```
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(y/2) * x_raw;
}
model {
  y_raw ~ std_normal(); // y ~ normal(0, 3)
  x_raw ~ std_normal(); // x ~ normal(0, exp(y/2))
}
```

Compare Funnel Fits

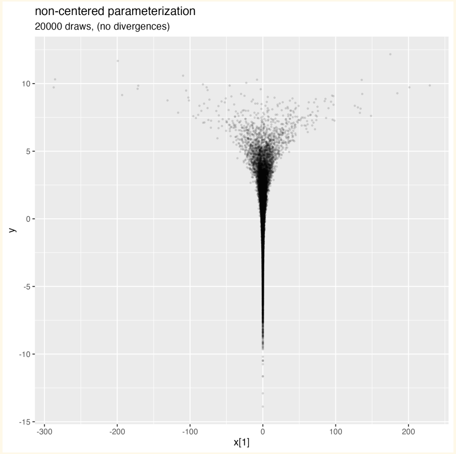
Centered parameterization

- Cannot explore neck of funnel
  many divergences (in orange)



Non-centered parameterization

- Explores further; no divergences



BRMS to Stan

- Recap: formula `Reaction ~ 1 + Days` becomes distribution statement:

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

- Coding `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 and covariance matrix Σ.
- Multivariate reparameterization

Multi-variate reparameterization

Following blogpost Varying slopes and intercepts in Stan: still painful in 2024

Centered parameterization

```
parameters {
  vector[K] beta;
  vector[K] mu;
  cov_matrix[K] Sigma;
  // ...
}
model {
  beta ~ multi_normal(mu, Sigma);
  // ...
}
```

Non-centered parameterization

```
parameters {
  vector<lower=0>[K] tau;
  cholesky_factor_corr[K] L_Omega;
  matrix[K, J] beta_std;
}
transformed parameters {
  matrix[J, K] beta =
    (diag_pre_multiply(tau, L_Omega) * beta_std)';
}
model {
  tau ~ exponential(1);
  L_Omega ~ lkj_corr_cholesky(K);
  to_vector(beta_std) ~ std_normal();
```

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, ]);
  y ~ 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 = multiply_lower_tri_self_transpose(L_Omega);
  real cor_intercept_day = Omega[1, 2];

  // Posterior likelihood and posterior predictive y-replicates
  vector[N] y_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 Demo

```r
# Stan multilevel model
sleep_mlm = cmdstan_model(stan_file = "stan/sleep_mlm.stan")
sleep_mlm_stanfit = sleep_mlm$sample(data = sleep_data, ... )
as.data.frame(sleep_mlm_stanfit$summary(
  variables = c('b_intercept', 'b_day', 'sigma',
  'sd_intercept', 'sd_day', 'cor_intercept_day')))
```

```r
# BRMS multilevel model
priors <- c(
set_prior("normal(250, 50)", class = "Intercept"),
set_prior("normal(10, 10)", class = "b"),
set_prior("exponential(1)", class = "sigma"),
set_prior("exponential(1)", class = "sd"),
set_prior("lkj_corr_cholesky(2)", class = "cor"),
)
sleep_mlm_brmsfit <- brm(Reaction ~ Days + (Days|Subject),
                         data = sleepstudy,
                         prior = priors)
sleep_mlm_brmsfit
```

Discussion

- BRMS formula syntax provides concise description of the regression.
  - function `brm` generates Stan code given both the formula and the data
  - default is a simple linear model.
- There is a point beyond which writing a model in Stan becomes easier than coding up the equivalent statements using BRMS.
- An efficient Stan program makes it easy for the sampler to converge and sample from the posterior.
  - zero-center predictors, make sure they are on the same scale.
  - the choice of the centered vs. non-centered parameterization depends on the amount of observations per group-level predictor.
  - use the non-centered parameterization for low-data regimes.

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???