From BRMS to Stan

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2025-05-07

Stan Development Team

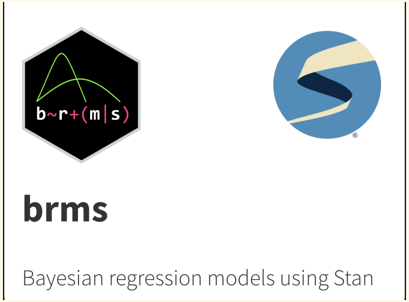
My Questions for You

- 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: github.com/mitzimorris/brms2stan/brms2stan.qmd

BRMS: Bayesian Regression and Multilevelmodeling in Stan



brms

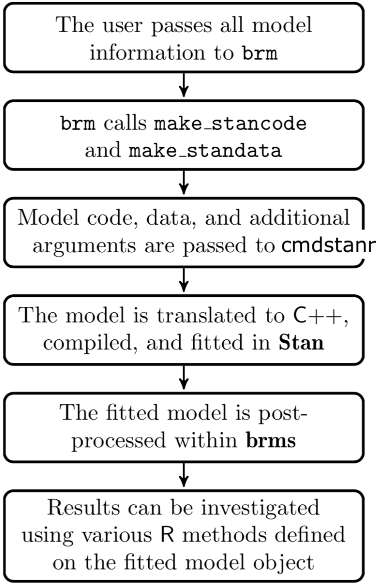
Bayesian regression models using Stan

- Fit Bayesian generalized linear / non-linear multivariate multilevel models using Stan.
- Specify model via `lme4`-like formula syntax.

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

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

BRMS Processing


The user passes all model information to brm
brm calls make_stancode and make_standata
Model code, data, and additional arguments are passed to cmdstanr
The model is translated to C++, compiled, and fitted in Stan
The fitted model is post-processed within brms
Results can be investigated using various R methods defined on the fitted model object

BRMS Processing

- Pass all information to BRMS

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

- Get results

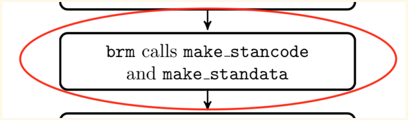
```
 Family: gaussian
  Links: mu = identity; sigma = identity
Formula: Reaction ~ Days + (Days | Subject)
   Data: sleepstudy (Number of observations: 180)

Multilevel Hyperparameters:                    Regression Coefficients:
~Subject (Number of levels: 18)                      Estimate Est.Error
                    Estimate Est.Error         Intercept   251.31      7.40
sd(Intercept)          27.27      7.03         Days         10.45      1.70
sd(Days)                6.60      1.51         sigma        25.87      1.52
cor(Intercept,Days)     0.07      0.30
```

Reasons to Use BRMS

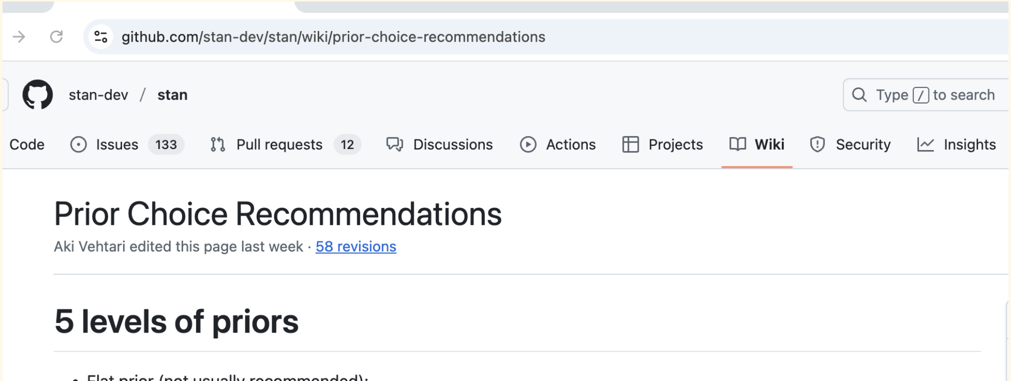
- Familiar syntax (for R users).
- Handles many common models: IRT, zero-inflated, additive distributional, phylogenetic, missing data imputation.
  - See Vignettes and Articles
- Sound and robust implementations, e.g.
  - Zero-centers predictors (like RStanARM).
  - Makes varying slope/ varying intercept 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



Prior Choice Recommendations

Aki Vehtari edited this page last week · 58 revisions

5 levels of priors

- Flat prior (not usually recommended);

BRMS Priors

Prior Definitions for brms Models

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

- 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

```
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)
```

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`

```stan
data {
  int<lower=0> N;
  vector[N] day;
  vector[N] y;  // 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

```
> stancode(sleep_simple_brmsfit)
// generated with brms 2.22.0
functions {
}
data {
  int<lower=1> N;  // total number of observations
  vector[N] Y;  // response variable
  int<lower=1> K;  // number of population-level effects
  matrix[N, K] X;  // population-level design matrix
  int<lower=1> Kc;  // number of population-level effects
  int prior_only;  // should the likelihood be ignored?
}
transformed data {
  matrix[N, Kc] Xc;  // centered version of X without an i
  vector[Kc] means_X;  // column means of X before centeri
  for (i in 2:K) {
    means_X[i - 1] = mean(X[, i]);
    Xc[, i - 1] = X[, i] - means_X[i - 1];
  }
}
```

```
parameters {
  vector[Kc] b;  // regression coefficients
  real Intercept;  // temporary intercept for centered pred
  real<lower=0> sigma;  // dispersion parameter
}
transformed parameters {
  real lprior = 0;  // prior contributions to the log poste
  lprior += normal_lpdf(b | 10, 10);
  lprior += normal_lpdf(Intercept | 250, 50);
  lprior += normal_lpdf(sigma | 0, 10)
    - 1 * normal_lccdf(0 | 0, 10);
}
model {
  if (!prior_only) {    // likelihood including constants
    target += normal_id_glm_lpdf(Y | Xc, Intercept, b, sigm
  }
  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 $\rightarrow$ Low hierarchical variance $\rightarrow$ 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

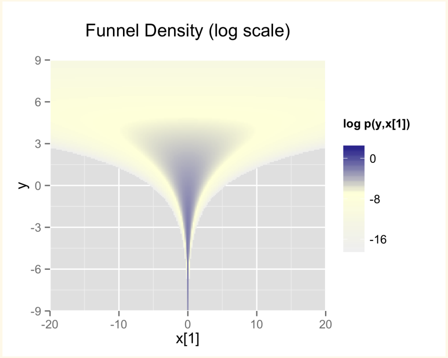
- Expand Stan model:
  - A per-subject parameter vector β (`b_subj`) is *multivariate normal*
  - `b_subj ~ multi_normal(mu_subj, sigma_subj)`
  - `mu_subj` is vector, of length number of subjects,
    `sigma_subj` is covariance matrix.

- *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

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



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.

Prior distribution; no data.

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

- 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(y/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

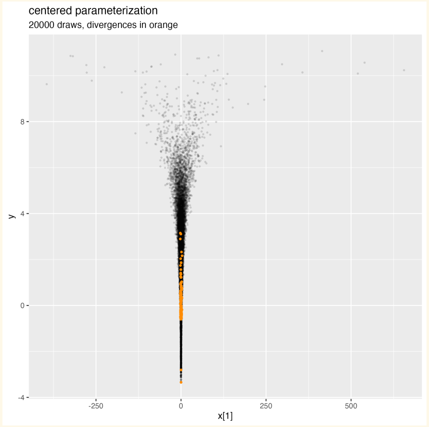
Stan's Affinely Transformed Scalar can be applied element-wise to vector `x` to facilitate the non-centered parameterization

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

Compare Funnel Fits

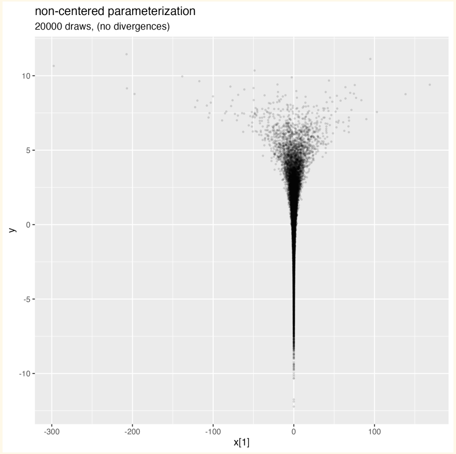
Centered parameterization

- 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

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);
```

Multi-variate reparameterization

Centered parameterization

```
data {
  int K; // num predictors + intercept
  int J; // num groups
}
parameters {
  vector[K, J] beta;  // group covariates
  vector[K] mu;     // location
  cov_matrix[K] Sigma;  // scale
  // ...
}
model {
  // hierarchical prior
  for (j in 1:J) {
    beta[ , j] ~ multi_normal(mu, Sigma);
  }
  // ...
}
```

Non-centered parameterization

```
data {
  int K; int J;
}
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 {
  // non-centered priors
  tau ~ exponential(1);
  L_Omega ~ lkj_corr_cholesky(K);
  to_vector(beta_std) ~ std_normal();
```

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

- github.com/mitzimorris/brms2stan/brms2stan.qmd
- Let’s run this in RStudio

References

Stan User's Guide:

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

Andrew Gelman's Blog

- Gelman blogpost varying-slope/varying-intercept models
- Bob Carpenter's response Varying slopes and intercepts in Stan: still painful in 2024

Many Thanks!

Questions???