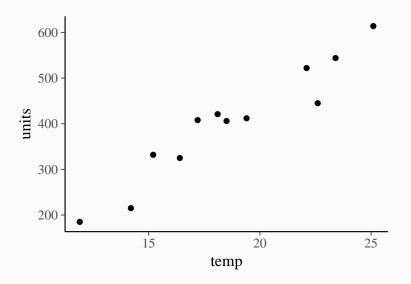
Bayesian Data Analysis Using Stan

Paul Bürkner

Workshop Material

 $https://github.com/paul-buerkner/2019_DAGStat_Stan_Tutorial$

Example: Icecream Sold at Different Temperatures



Linear Models with Stan

Simple Linear Regression

We assume the following generative model (likelihood)

$$y_n = \alpha + \beta x_n + \varepsilon_n$$

$$\varepsilon_n \sim \text{Normal}(0, \sigma)$$

or equivalently

$$y_n \sim \text{Normal}(\alpha + \beta x_n, \sigma)$$

Let's vectorize the model

$$y \sim \text{Normal}(\alpha + \beta x, \sigma)$$

Stan Syntax: Simple Linear Regression

```
data {
  int<lower=1> N; // total number of observations
  vector[N] y; // response variable
  vector[N] x; // predictor variable
parameters {
  real alpha; // intercept
  real beta; // slope
  real<lower=0> sigma; // residual SD
model {
  // likelihood
  for (n in 1:N) {
    y[n] ~ normal(alpha + beta * x[n], sigma);
  }
```

Stan Syntax: Simple Linear Regression (Vectorized)

```
data {
  int<lower=1> N; // total number of observations
  vector[N] y; // response variable
 vector[N] x; // predictor variable
parameters {
  real alpha; // intercept
  real beta; // slope
  real<lower=0> sigma; // residual SD
model {
 // likelihood
  y ~ normal(alpha + beta * x, sigma);
```

The Posterior Distribution

$$p(\theta|y) = \frac{p(y|\theta)p(\theta)}{p(y)} \propto p(y|\theta)p(\theta) = p(y,\theta)$$

What's the matter with all the p functions?

- Likelihood: $p(y|\theta)$
- Prior: $p(\theta)$
- Marginal likelihood: p(y)
- Posterior: $p(\theta|y)$
- Joint Model: $p(y, \theta)$

Priors in Stan

```
data {
parameters {
  real alpha; // intercept
  real beta; // slope
  real<lower=0> sigma; // residual SD
model {
  // likelihood
  y ~ normal(alpha + beta * x, sigma);
  // priors
  alpha ~ normal(0, 100);
  beta \sim normal(0, 50);
  sigma \sim cauchy(0, 50);
```

How to obtain the Posterior Distribution?

Problem: Computing the marginal likelihood

$$p(y) = \int p(y|\theta)p(\theta)d\theta$$

Analytically?

• Only possible for specific models

Numerically?

Only possible for model with few parameters

Solution: Do not compute p(y) at all

Using Samples to Approximate Expectations

Every quantity of interest is an expectation over $p(\theta|y)$:

$$\mathbb{E}[h(\theta)] = \int h(\theta) p(\theta|y) d\theta$$

Approximate expectations using random samples θ_s from $p(\theta|y)$:

$$\mathbb{E}[h(\theta)] \approx \frac{1}{S} \sum_{s=1}^{S} h(\theta_s)$$

Moreover

$$\frac{1}{S}\sum_{s=1}^{S}h(\theta_s)\xrightarrow{S\to\infty}\mathbb{E}(h(\theta))$$

Markov-Chain Monte-Carlo (MCMC) Sampling

We can't simply draw independent samples from the posterior!

A Markov Chain is a sequence of values where the value at position t is based only on the former value at position t-1:

$$heta_1 o heta_2 o heta_3 o \ldots o heta_S$$
 $p(heta_t | heta_{t-1}, heta_{t-2}, \ldots, heta_1) = p(heta_t | heta_{t-1})$

If done correctly, the distribution of the values will converge to the target distribution:

$$p(\theta) = \int p(\theta^*) \, p(\theta|\theta^*) \, d\,\theta^*$$

Icecream Sold: Specification in (R)Stan

Prepare the data:

```
sdata <- list(
  y = icecream$units,
  x = icecream$temp,
  N = nrow(icecream)
)</pre>
```

Load rstan:

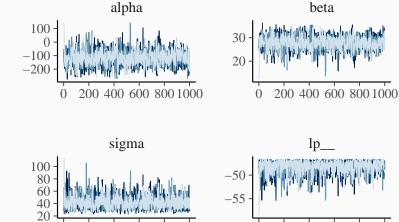
```
library(rstan)
```

Fit the model:

```
linreg_model <- stan(file = "linreg.stan", data = sdata)</pre>
```

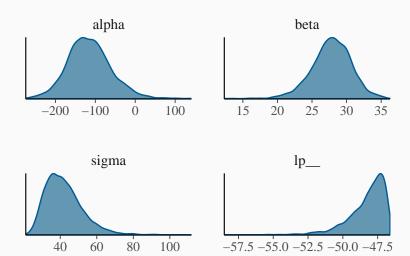
Icecream Sold: Visualize the Chains

200 400 600 800 1000



200 400 600 800 1000

Icecream Sold: Visualize the Posterior



Icecream Sold: Summarize the Parameters

print(linreg_model)

Inference for Stan model: linreg.

```
## 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% 50% 97.5% n eff Rhat
## beta 27.80 0.08 2.87 21.64 27.93 33.16 1163 1.00
## sigma 42.04 0.28 10.12 27.18 40.62 65.74 1298 1.00
## lp -48.25 0.04 1.30 -51.69 -47.91 -46.75 1025 1.01
##
## Samples were drawn using NUTS(diag e) at Mon Mar 18 10:40:40 2019.
## 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).
```

Stan: A Probabilistic Programming Language



Stan overview

- Probabilistic programming language written in C++ . . .
- ... to fit open-ended Bayesian models
- Algorithm: (Adaptive) Hamiltonian Monte-Carlo (HMC)
- Automatic differentiation (Stan-Math) library
- Runs on all major platforms (Windows, OS X, Linux)
- Can be called from R, Python, Julia, Stata, and Matlab

Explicitely Constructing the Log-Posterior in Stan

```
data {
parameters {
  real alpha; // intercept
  real beta; // slope
  real<lower=0> sigma; // residual SD
model {
  // likelihood
  target += normal lpdf(y | alpha + beta * x, sigma);
  // priors
  target += normal lpdf(alpha | 0, 100);
  target += normal lpdf(beta | 0, 50);
  target += cauchy_lpdf(sigma | 0, 50);
```

Stan Syntax: Model Blocks

```
functions
 // user defined Stan functions
data
  // data passed by the user
transformed data
  // variables depending on the data block
  // computed only once before fitting the model
parameters
  // unkown variables to be sampled
transformed parameters
  // variables depending on data and parameter blocks
model
  // specification of the log-posterior density
  // defined variables are local
generated quantities
  // variables to be computed after the model fitting
  // not included in the actual sampling process
```

Why Using Stan?

- Expressive language for probabilistic programming
- Efficient and numerically stable computations
- Powerful MCMC samplers scaling well to high dimensional Bayesian models where other samplers fail
- Continuously developed and improved
- Ecosystem of Stan-related R packages
- Large and friendly community

Learn more about Stan

- Website: http://mc-stan.org/
- Manual: http://mc-stan.org/users/documentation/index.html
- Forums: http://discourse.mc-stan.org/

Selected Publications:

- Carpenter B., Gelman A., Hoffman M. D., Lee D., Goodrich B., Betancourt M., Brubaker M., Guo J., Li P., and Riddell A. (2017). Stan: A probabilistic programming language. *Journal of Statistical Software*. 76(1). 10.18637/jss.v076.i01
- Gelman A., Lee D., and Guo J. (2015). Stan: A probabilistic programming language for Bayesian inference and optimization.
 Journal of Education and Behavioral Statistics. 40(5):530–543.

The Posterior Predictive Distribution

Distribution of model implied responses \tilde{y} conditional on the existing responses y:

$$p(\tilde{y}|y) = \int p(\tilde{y}|y,\theta)p(\theta|y) d\theta$$

For conditionally independent responses:

$$p(\tilde{y}|y) = \int p(\tilde{y}|\theta)p(\theta|y) d\theta$$

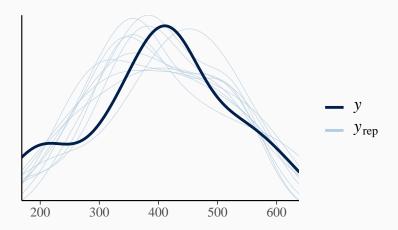
Posterior Predictions in Stan

Sample posterior predictions after model fitting:

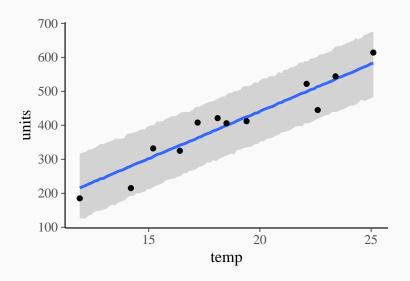
```
generated quantites {
  vector[N] yrep; // posterior predictions
  for (n in 1:N) {
    yrep[n] = normal_rng(alpha + beta * x[n], sigma);
  }
}
```

Icecream Sold: Posterior Predictive Checks

```
library(bayesplot)
yrep <- as.matrix(linreg_model, pars = "yrep")
yrep <- yrep[sample(1:nrow(yrep), 10), ]
ppc_dens_overlay(y = icecream$units, yrep = yrep)</pre>
```



Icecream Sold: Visualize Predictions



Time for exercise 'stan_linear_regression.R'

What's wrong with our modeling assumptions?

Generalized Linear Models with Stan

Binomial Regression Models

Suppose the icecream market size M is limited

We assume y_n to be binomial distributed with probability θ_n :

$$y_n \sim \text{Binomial}(\theta_n, M)$$

The probability θ_n is predicted via:

$$\theta_n = g(\alpha + \beta x_n)$$

g(.) is a response function for instance

$$g(\eta) = \mathsf{logistic}(\eta) = \frac{\mathsf{exp}(\eta)}{1 + \mathsf{exp}(\eta)}$$

Binomial Model in Stan

```
data {
  int<lower=1> N; // total number of observations
  int<lower=1> M; // market size
  int y[N]; // response variable
  vector[N] x; // predictor variable
parameters {
  real alpha; // intercept
  real beta; // slope
model {
  // likelihood
  for (n in 1:N) {
    real theta = inv logit(alpha + beta * x[n]);
    y[n] ~ binomial(M, theta);
  }
```

Binomial Model in Stan (Optimized)

```
data {
  int<lower=1> N; // total number of observations
  int<lower=1> M; // market size
  int y[N]; // response variable
  vector[N] x; // predictor variable
}
parameters {
  real alpha; // intercept
 real beta; // slope
model {
 // likelihood
  y ~ binomial logit(M, alpha + beta * x);;
```

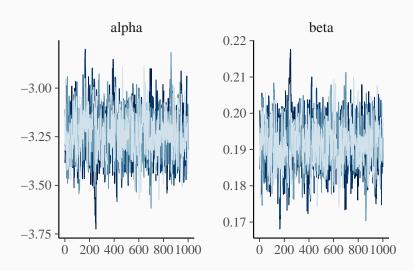
Fitting Binomial Models in (R)Stan

Prepare the data:

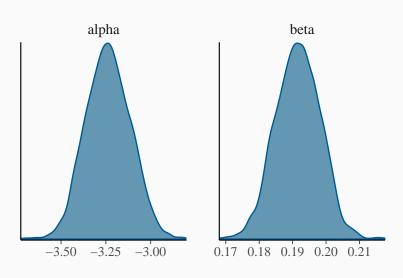
```
sdata <- list(
  y = icecream$units,
  x = icecream$temp,
  N = nrow(icecream),
  M = 700
)</pre>
```

Fit the model:

Binomial Model: Visualize the Chains



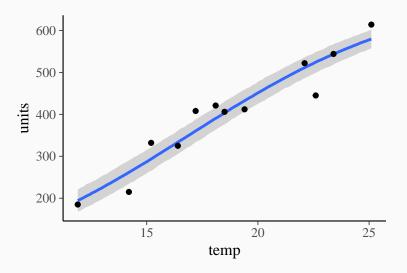
Binomial Model: Visualize the Posterior



Binomial Model: Summarize the Parameters

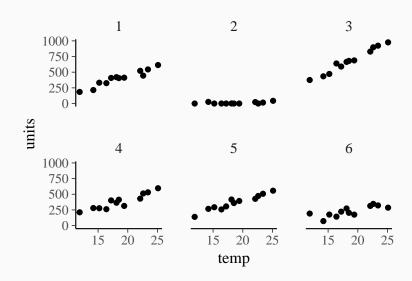
print(binom_model)

Binomial: Visualize Predictions

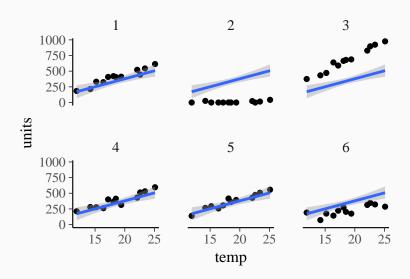


Linear Multilevel Models with Stan

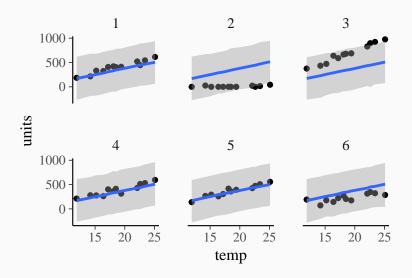
Selling Icecream at Multiple Locations



Simple Linear Model: Visualize Expectations



Simple Linear Model: Visualize Predictions



Varying Intercept Models

We assume the following generative model:

$$y_n \sim \mathsf{Normal}(\alpha_{j_n} + \beta x_n, \sigma)$$

with

$$\alpha_j \sim \mathsf{Normal}(\mu_\alpha, \tau_\alpha)$$

or equivalently

$$\tilde{\alpha}_j \sim \mathsf{Normal}(0,1)$$

$$\alpha_j = \mu_\alpha + \tau_\alpha \times \tilde{\alpha}_j$$

Varying Intercept Model in Stan (Centered)

```
data {
  . . .
  int<lower=1> Nlocation; // number of locations
  int<lower=1> location[N]; // location index
parameters {
  vector[Nlocation] alpha; // intercepts
  real mu_alpha; // intercept mean
  real<lower=0> tau_alpha; // intercept SD
  . . .
model {
  vector[N] mu;
  for (n in 1:N) {
    mu[n] = alpha[location[n]] + beta * x[n];
  y ~ normal(mu, sigma);
  alpha ~ normal(mu_alpha, tau_alpha);
```

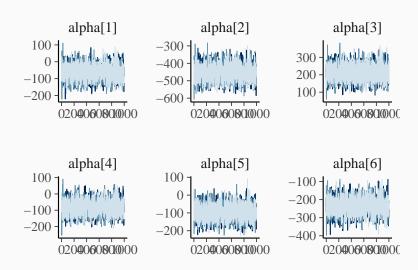
Varying Intercept Model in Stan (Non-Centered)

```
parameters {
  vector[Nlocation] z_alpha; // dummy intercepts
  real mu_alpha; // intercept mean
  real<lower=0> tau_alpha; // intercept SD
  . . .
transformed parameters {
  vector[Nlocation] alpha = mu_alpha + tau_alpha * z_alpha;
model {
  vector[N] mu;
  for (n in 1:N) {
    mu[n] = alpha[location[n]] + beta * x[n];
  y ~ normal(mu, sigma);
  z_alpha ~ normal(0, 1);
```

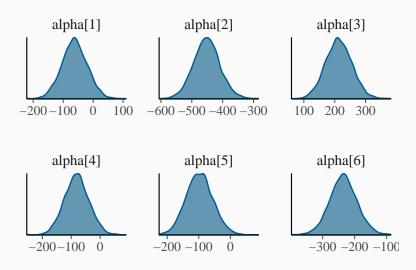
Fitting Varing Intercept Models in (R)Stan

```
sdata <- list(
  y = icecream2$units,
  x = icecream2$temp,
  location = icecream2$location,
  N = nrow(icecream2),
  Nlocation = length(unique(icecream2$location))
mlm2 <- stan(
  "stanmodels/multilevel intercept2.stan",
  data = sdata
```

Varying Intercepts: Visualize the Chains



Varying Intercepts: Visualize the Posterior

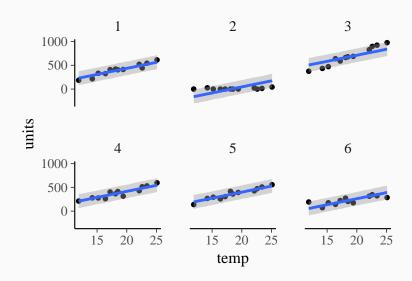


Varying Intercept Model: Summarize the Parameters

Inference for Stan model: multilevel intercept2.

```
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%
                                            50%
                                                  97.5% n eff Rhat
## alpha[1]
           -61.87
                      0.81 42.27 -143.98 -62.31
                                                  21.68
                                                         2730
## alpha[2]
            -451.74
                     0.81 42.72 -535.12 -451.99 -364.54 2749
                                                                 1
## alpha[3]
             213.32
                      0.76 42.40 130.52 212.45
                                                 295.75 3089
## alpha[4]
           -81.09
                     0.83 42.48 -163.88 -81.36
                                                   4.28
                                                         2603
                                                                 1
## alpha[5]
           -97.67
                      0.81 42.27 -178.43 -98.39
                                                 -12.67
                                                         2690
## alpha[6]
                      0.83 42.80 -319.03 -235.51 -149.72
                                                         2668
            -235.23
                                                                 1
## mu alpha
             -65.85
                      1.82 70.23 -192.87
                                         -68.37
                                                  83.86 1494
                      2.45 75.55 128.77 213.31 420.04
                                                        951
## tau alpha
             228.38
                                                                 1
## beta
              24.87
                      0.04 2.02 20.87 24.84
                                                  28.80 2592
## sigma
              68.78
                      0.12 6.10 57.93 68.45
                                                  82.07
                                                         2524
                                                                 1
##
## Samples were drawn using NUTS(diag_e) at Mon Mar 18 10:44:11 2019.
## 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).
```

Varying Intercept Model: Visualize Predictions



Varying Slope Models (Centered)

We assume the following generative model:

$$y_n \sim \mathsf{Normal}(\alpha_{j_n} + \beta_{j_n} x_n, \sigma)$$

with

$$(\alpha_j, \beta_j) \sim \mathsf{MultiNormal}((\mu_\alpha, \mu_\beta), \Sigma)$$

$$\Sigma = \begin{pmatrix} \tau_{\alpha}^2 & \tau_{\alpha}\tau_{\beta}\rho_{\alpha\beta} \\ \tau_{\alpha}\tau_{\beta}\rho_{\alpha\beta} & \tau_{\beta}^2 \end{pmatrix}$$

Varying Slope Models (Non-Centered)

We assume the following generative model:

$$y_n \sim \mathcal{N}(\alpha_{j_n} + \beta_{j_n} x_n, \sigma)$$

with

$$ilde{lpha}_j, ilde{eta}_j \sim \mathsf{Normal}(0,1)$$
 $(lpha_j, eta_j) = (\mu_lpha, \mu_eta) + L imes (ilde{lpha}_j, ilde{eta}_j)$

where L is the Cholesky factor of Σ :

$$\Sigma = LL^{\mathsf{T}}$$

We may also write L as:

$$L = \mathsf{Diag}(\tau_{\alpha}, \tau_{\beta}) L_{\rho}$$

Varing Slope Models in Stan (Non-Centered Part 1)

```
parameters {
 real mu_alpha; // intercept mean
 real mu_beta; // slope mean
 real<lower=0> tau_alpha; // intercept SD
 real<lower=0> tau_beta; // slope SD
  // cholesky factor of the correlation matrix
  cholesky_factor_corr[2] L_Cor;
  matrix[2, Nlocation] z_theta; // dummy varying effects
 real<lower=0> sigma; // residual SD
```

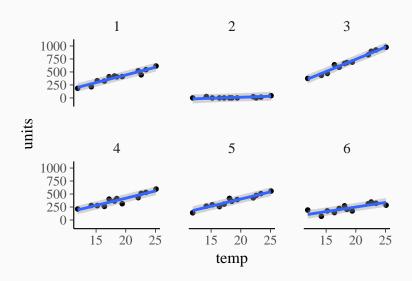
Varing Slope Models in Stan (Non-Centered Part 2)

```
transformed parameters {
  // cholesky factor of the covariance matrix
  matrix[2, 2] L_Sigma =
    diag_pre_multiply([tau_alpha, tau_beta]', L_Cor);
  matrix[2, Nlocation] theta; // actual varying effects
  for (j in 1:Nlocation) {
    theta[, j] = [mu_alpha, mu_beta]' + L_Sigma * z_theta[, j];
model {
  vector[N] mu;
  for (n in 1:N) {
    mu[n] = theta[1, location[n]] + theta[2, location[n]] * x[n];
  y ~ normal(mu, sigma);
  to_vector(z_theta) ~ normal(0, 1);
```

Fitting Varing Slope Models in (R)Stan

```
sdata <- list(
  v = icecream2$units,
  x = icecream2$temp,
  location = icecream2$location,
 N = nrow(icecream2),
 Nlocation = length(unique(icecream2$location))
mlm3 <- stan(
  "stanmodels/multilevel_slope.stan",
  data = sdata,
  control = list(adapt delta = 0.99)
```

Varying Slope Model: Visualize Predictions



Cross-Validation

Idea: Estimate the model based on one part of the data (training data) to predict the other part of the data (test data)

Special case: Leave-One-Out cross-validation (LOO-CV):

$$p(y_i|y_{-i}) = \int p(y_i|\theta)p(\theta|y_{-i}) d\theta \approx \frac{1}{S} \sum_{s=1}^{S} p(y_i|\theta_{-i,s})$$

Criterion for model comparison:

$$\mathsf{ELPD}_{\mathrm{loo}} = \sum_{n=1}^{N} \log p(y_i|y_{-i})$$

Disadvantage of CV: Requires fitting the model multiple times

Solution: Replace $p(\theta|y_{-i})$ by $p(\theta|y)$ and adjust the result via Pareto-Smoothed Importance Sampling (PSIS)

Icecream Sold: Compute Log-Likelihood Values

Compute log-likelihoods values after model fitting:

```
generated quantities {
  vector[N] 11; // log-likelihood values
  for (n in 1:N) {
    ll[n] = normal_lpdf(y[n] | alpha + beta * x[n], sigma);
  }
}
```

Approximate LOO-CV (Constant Intercept)

```
library(loo)
11 <- as.matrix(lm1, pars = "11")</pre>
(loo lm1 \leftarrow loo(ll))
##
## Computed from 4000 by 72 log-likelihood matrix
##
          Estimate SE
##
## elpd loo -490.6 6.4
## p_loo 2.5 0.5
## looic 981.1 12.8
## ----
## Monte Carlo SE of elpd loo is 0.0.
##
## All Pareto k estimates are good (k < 0.5).
## See help('pareto-k-diagnostic') for details.
```

Approximate LOO-CV (Varying Intercepts)

```
11 <- as.matrix(mlm2, pars = "11")
(loo mlm2 \leftarrow loo(ll))
##
## Computed from 4000 by 72 log-likelihood matrix
##
##
          Estimate SE
## elpd_loo -411.4 6.4
## p_loo 8.4 1.5
## looic 822.8 12.9
## ----
## Monte Carlo SE of elpd_loo is 0.1.
##
## All Pareto k estimates are good (k < 0.5).
## See help('pareto-k-diagnostic') for details.
```

Approximate LOO-CV (Varying Intercepts and Slopes)

```
11 <- as.matrix(mlm3, pars = "11")
(loo mlm3 <- loo(ll))
##
## Computed from 4000 by 72 log-likelihood matrix
##
##
         Estimate SE
## elpd_loo -370.4 5.8
## p_loo 9.1 1.5
## looic 740.7 11.6
## ----
## Monte Carlo SE of elpd_loo is 0.1.
##
## Pareto k diagnostic values:
##
                       Count Pct. Min. n eff
## (-Inf, 0.5] (good) 70 97.2% 941
## (0.5, 0.7] (ok) 2 2.8% 815
  (0.7, 1] (bad) 0 0.0% <NA>
##
## (1, Inf) (very bad) 0 0.0% <NA>
##
## All Pareto k estimates are ok (k < 0.7).
```

Comparing Models via Approximate LOO-CV

```
loo_compare(loo_lm1, loo_mlm2, loo_mlm3)
```

```
## model3 0.0 0.0
## model2 -41.0 7.6
## model1 -120.2 9.6
```

The R Universe around Stan

- rstan: Call Stan from R
- rstantools: Development Tools for Stan-Based Packages
- rstanarm: Bayesian Applied Regression Modeling via Stan
- bayesplot: Plotting for Bayesian models
- shinystan: Interactive Plotting for Bayesian Models
- loo: Approximation Cross-Validation
- projpred: Variable Selection via Projective Predictions
- brms: Bayesian Regression Models using Stan

The brms package

A unified framework for Bayesian regression modeling



Selling Icecream with brms

Linear Model:

```
brm(units ~ temp, data = icecream)
```

Binomial Model:

```
brm(units | trials(size) ~ temp, data = icecream,
    family = binomial("logit"))
```

Varying Intercept Model:

```
brm(units ~ temp + (1 | location), data = icecream)
```

Varying Slope Model:

```
brm(units ~ temp + (temp | location), data = icecream)
```

Learn more about brms

- Help within R: help("brms")
- Vignettes: vignette(package = "brms")
- List of all methods: methods(class = "brmsfit")
- Website: https://github.com/paul-buerkner/brms
- Forums: http://discourse.mc-stan.org/
- Contact me: paul.buerkner@gmail.com
- Twitter: @paulbuerkner

Publications

- Bürkner P. C. (2017). brms: An R Package for Bayesian Multilevel Models using Stan. *Journal of Statistical Software*. 80(1), 1-28. doi:10.18637/jss.v080.i01
- Bürkner P. C. (2018). Advanced Bayesian Multilevel Modeling with the R Package brms. The R Journal. 10(1), 395–411. doi:10.32614/RJ-2018-017

Questions?

Appendix

Stan syntax: Multiple Linear Regression

```
data {
  int<lower=1> N; // total number of observations
  vector[N] y; // response variable
  int<lower=1> K; // number of regression coefficients
 matrix[N, K] X; // predictor design matrix
parameters {
  vector[K] b; // regression coeffcients
  real<lower=0> sigma; // residual SD
model {
 vector[N] mu;
 mu = X * b;
  y ~ normal(mu, sigma); // likelihood
```

Importance Sampling

Suppose $f(\theta)$ is the target and $g(\theta)$ the approximating distribution:

$$\mathbb{E}[h(\theta)] = \int h(\theta)f(\theta) d\theta = \frac{\int [h(\theta)f(\theta)/g(\theta)]g(\theta) d\theta}{\int [f(\theta)/g(\theta)]g(\theta) d\theta}$$
$$= \frac{\int h(\theta)r(\theta)g(\theta) d\theta}{\int r(\theta)g(\theta) d\theta}$$

with importance ratios

$$r(\theta) = \frac{f(\theta)}{g(\theta)}$$

If $\theta^{(s)}$ are S random draws from $g(\theta)$:

$$\mathbb{E}[h(\theta)] \approx \frac{\sum_{s=1}^{S} h(\theta^{(s)}) r(\theta^{(s)})}{\sum_{s=1}^{S} r(\theta^{(s)})}$$

Some Helpful brms Functions (1)

Specify the model using R formulas:

```
brmsformula(formula, ...)
```

Generate the Stan code:

```
make_stancode(formula, ...)
stancode(fit)
```

Generate the data passed to Stan:

```
make_standata(formula, ...)
standata(fit)
```

Handle priors:

```
get_prior(formula, ...)
set_prior(prior, ...)
```

Some Helpful brms Functions (2)

Generate expected values and predictions:

```
fitted(fit, ...)
predict(fit, ...)
marginal_effects(fit, ...)
```

Model comparison:

```
loo(fit1, fit2, ...)
bayes_factor(fit1, fit2, ...)
model_weights(fit1, fit2, ...)
```

Hypothesis testing:

```
hypothesis(fit, hypothesis, ...)
```