Stan Tutorial

Module 4: Hierarchical Nested Multinomial Logit

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Module Objectives

In this module we illustrate how Stan can be used to fit a non-standard model. This flexibility to fit almost any model you can imagine is a key advantage of Stan.

Acknowledgments



Based on work done for the Modellers along with Michael Smith. Stan code $\ \odot$ 2015, The Modellers, licensed under GPL v2.

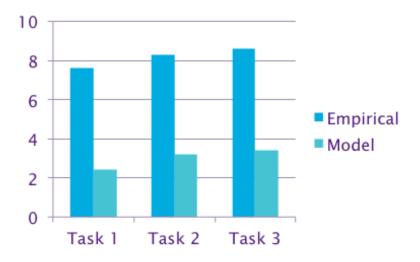


Thanks to Kevin's employer Adobe Systems for their support.

The Problem: Failed Validation Tasks

Choice-based conjoint survey; dual-response DCM.

Validation tasks: one product shown, asked if they would buy.



Posterior Predictive Probabilities

Weighted average of choice probabilities.

Weight by posterior probability of parameter vector ψ .

$$Pr(c \mid s, i, D) = \int Pr(c \mid s, i, \psi) p(\psi \mid D) d\psi$$

Choice c, scenario s, individual i.

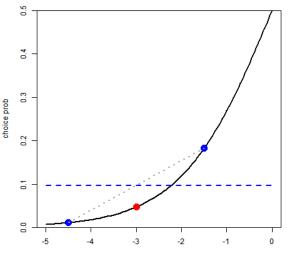
Survey data D, model parameters ψ .

Implemented by averaging predictions over posterior draws.

$$\Pr(c \mid s, i, D) \approx \frac{1}{n} \sum_{i=1}^{n} \Pr(c \mid s, i, \psi^{(j)})$$

Jensen's Inequality

For any convex function f, $E[f(\eta)] > f(E[\eta])$.



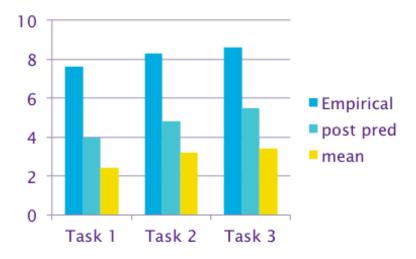
Example: $\frac{1}{2}f(-4.5) + \frac{1}{2}f(-1.5) > f(-3)$

Jensen's Inequality (continued)

Pr(buy) = $f(\eta)$ where f is inverse logit, $\eta = \sum_i \beta_i x_i$ $E[f(\eta)]$ is posterior predictive choice probability. $f(E[\eta])$ is choice probability using point estimate of β . $f(\eta)$ is convex for $\eta < 0$.

If $\eta < 0$ and using point estimate of β computed choice prob $f(E[\eta])$ is biased downward.

Results: Using Posterior Predictive Probabilities



One of These Things Is Not Like the Others









Clashes with MNL property: Independence of Irrelevant Alternatives

The Problem with Multinomial Logit

I Can Make You Buy If I Give You Enough Options Even if they're all similar.



The Math

Let η_i be linear predictor for product i.

Linear predictor for none is 0.

$$Pr(none) = \frac{1}{1 + \sum_{i=1}^{C} exp(\eta_i)}$$

So Pr(none) \rightarrow 0 as $C \rightarrow \infty$.

Tasks used for estimation: 5 product alternatives and none.

Tasks used for validation: 1 product and none.

Nested Multinomial Logit ("none" vs. all else)

$$Pr(\text{choose product } i) = \frac{1}{1 + \exp(-\alpha - \lambda I)} \cdot \frac{\exp(\beta' \mathbf{x}_i)}{\sum_j \exp(\beta' \mathbf{x}_j)}$$

$$Pr(choose none) = \frac{1}{1 + exp(\alpha + \lambda I)}$$

$$I = \log \sum_{j} \exp(\beta' \mathbf{x}_{j})$$

 $0 \le \lambda \le 1$; if $\lambda = 1$ then MNL.

Hierarchical Nested MNL

r indexes respondents.

$$\mathsf{Pr}(\mathsf{choose}\;\mathsf{product}\;i) = \frac{1}{1 + \mathsf{exp}(-\alpha_r - \lambda I_r)} \cdot \frac{\mathsf{exp}(\beta_r' \boldsymbol{x}_i)}{\sum_j \mathsf{exp}(\beta_r' \boldsymbol{x}_j)}$$

$$Pr(\text{choose none}) = \frac{1}{1 + \exp(\alpha_r + \lambda I_r)}$$

$$I_r = \log \sum_j \exp(\beta'_r \mathbf{x}_j)$$

$$\begin{array}{lcl} \beta_{rk} & \sim & \operatorname{Normal}\left(\boldsymbol{\theta}_{k}^{\prime}\boldsymbol{z}_{r},\,\sigma_{k}\right) \\ \alpha_{r} & \sim & \operatorname{Normal}\left(\boldsymbol{\varphi}^{\prime}\boldsymbol{z}_{r},\,\sigma_{\alpha}\right) \end{array}$$

$$\lambda \sim \text{Uniform}(0,1)$$
 $\theta_{kg} \sim \text{Normal}(0,10)$
 $\sigma_k \sim \text{HalfNormal}(5)$

Initial Stan Model (1)

```
data {
  int<lower=1> R; // # respondents
  int<lower=1> K; // # product covariates; no intercept
  int<lower=1> G; // # respondent covariates
  int<lower=1> S; // # scenarios per respondent
  int<lower=2> C; // # alts (choices) per scenario
  matrix[C, K] X[R, S];
   // X[r,s] is cov mat of scen s for resp r.
 matrix[G, R] Z;
   // Z[,r] is vector of covariates for resp r
  int<lower=1,upper=C> Y1[R,S]; // forced choice
  int<lower=0,upper=1> Y2[R,S]; // dual response
```

Initial Stan Model (2)

```
parameters {
  real<lower=0, upper=1> lambda;
  vector<lower=0>[K+1] sigma;
  matrix[K+1, G] Theta;
  matrix[K+1, R] Beta;
model {
  lambda ~ uniform(0, 1);
  sigma ~ normal(0, 5);
  to_vector(Theta) ~ normal(0, 10);
  to vector(Beta) ~
    normal(to_vector(Theta * Z),
           to_vector(rep_matrix(sigma, R)));
```

Vectorization

```
to_vector(Theta) ~ normal(0, 10);
  to vector(Beta) ~
    normal(to vector(Theta * Z),
           to vector(rep matrix(sigma, R)));
is equivalent to
  for (k in 1:(K+1))
    for (g in 1:G)
      Theta[k,g] ~ normal(0, 10);
  for (k in 1:(K+1))
    for (r in 1:R)
      Beta[k, r] ~ normal((Theta * Z)[k, r], sigma[k]);
```

Initial Stan Model (3)

```
model {
  for (r in 1:R) {
    vector[K] b = Beta[2:(K+1), r];
    real alpha = Beta[1,r];
    for (s in 1:S) {
      vector[C] u = X[r,s] * b;
      real u_buy = alpha + lambda * log_sum_exp(u);
      Y1[r,s] ~ categorical_logit(u);
      Y2[r,s] ~ bernoulli logit(u buy);
```

Some Stan Details

 $log_sum_exp(u)$ is numerically robust form of

$$\log\left(\sum_{i}\exp\left(u_{i}\right)\right)$$

y ~ categorical_logit(u) means

$$Pr(y = i) = \frac{\exp(u_i)}{\sum_{i} \exp(u_i)}$$

y ~ bernoulli_logit(u) means

$$\Pr(y=1) = \frac{\exp(u)}{1 + \exp(u)}$$

And When We Run It...

See

```
## There were 11 divergent transitions after warmup.
## Increasing adapt_delta above 0.8 may help.
## See http://mc-stan.org/misc/warnings.html#divergent-tran
## There were 4 chains where the estimated
## Bayesian Fraction of Missing Information was low.
```

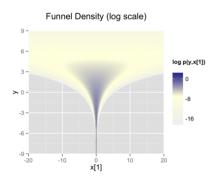
http://mc-stan.org/misc/warnings.html#bfmi-low

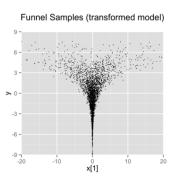
An Extreme Form of the Problem: Neal's Funnel

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

Variance for x strongly varies with y!

Distribution for Neal's Funnel





Why Neal's Funnel Is a Problem

Hamiltonian MC simulates trajectory of system whose potential energy is

$$V(x) = -\log(\text{prob density at } x)$$

To efficiently explore distribution, need

- ▶ large step size when curvature of V(x) is small;
- ightharpoonup small step size when curvature of V(x) is large.

But have to use a single step size globally.

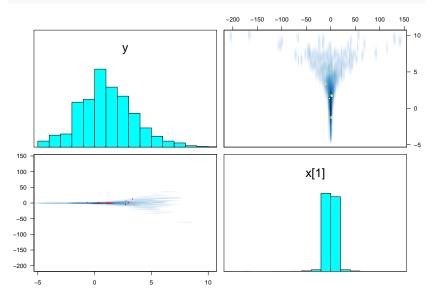
- Normal distribution: constant curvature.
- Neal's Funnel: extreme variation in curvature.

HMC has trouble entering the narrow neck of the funnel.

Warning / error message: "divergent transitions after warmup."

Run the Funnel Model

```
fit <- stan_demo('funnel', seed=928374)
pairs(fit, pars=c('y','x[1]'), las=1)</pre>
```



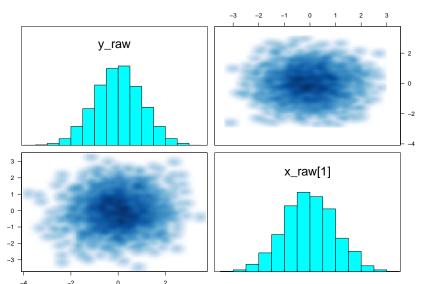
Reparameterized Model

Non-Centered Parameterization

```
parameters {
  real y raw;
  vector[9] x raw;
transformed parameters {
  real y = 3.0 * y_raw;
  vector[9] x = exp(y/2) * x_raw;
model {
  y_raw ~ normal(0,1);
  x_raw \sim normal(0,1);
```

Run the Reparameterized Model

```
fit <- stan_demo('funnel_reparam', seed=928374)
pairs(fit, pars=c('y_raw','x_raw[1]'), las=1)</pre>
```



Reparameterized Stan Model (2a)

```
parameters {
   real<lower=0, upper=1> lambda;
   // vector<lower=0>[K+1] sigma;
   vector<lower=0>[K+1] sigma_raw;
   // matrix[K+1, G] Theta;
   matrix[K+1, G] Theta_raw;
   // matrix[K+1, R] Beta;
   matrix[K+1, R] Epsilon;
}
```

Reparameterized Stan Model (2b)

```
transformed parameters {
  vector<lower=0>[K+1] sigma = 5 * sigma_raw;
  matrix[K+1, G] Theta = 10 * Theta raw;
  matrix[K+1, R] Beta =
    Theta * Z + diag pre multiply(sigma, Epsilon);
model {
  lambda ~ uniform(0, 1);
  // sigma ~ normal(0, 5);
  sigma_raw ~ normal(0, 1);
  // to_vector(Theta) ~ normal(0, 10);
  to_vector(Theta_raw) ~ normal(0, 1);
  // to_vector(Beta) ~ normal(to_vector(Theta * Z),
  //
                         to vector(rep matrix(sigma, R)));
  to vector(Epsilon) ~ normal(0, 1);
  . . .
```

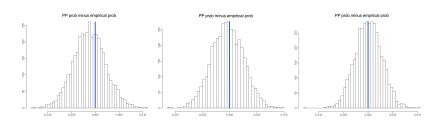
Results: Hnestedmnl + Posterior Predictive Probs

Histograms of $p^{(j)}$ with j running over posterior draws.

$$p^{(j)} = \frac{1}{R} \sum_{r=1}^{R} \Pr\left(\mathsf{buy} \mid r, \psi^{(j)}\right)$$

Each of three validation tasks.

Blue lines are empirical probs on holdout data.





In this module we have:

- Discussed posterior predictive probabilities
 - ▶ How to compute them
 - When predictions from point estimates are biased
- Created a custom model to solve a specific problem
 - A common case where MNL goes wrong: none vs actual product
 - Solution using restricted form of nested multinomial logit
 - Converting equations into Stan code
- Discussed computational issues
 - Vectorization
 - Problem of highly variable posterior curvature
 - Non-centered parameterization