Generalized Linear Models with the rstanarm R Package

Ben Goodrich April 20, 2020

Important Maximimum Entropy Distributions

- · If Θ is some convex set, the maximum entropy distribution is the uniform distribution over Θ . For example, if $\Theta=[0,1]$, it is the standard uniform distribution with PDF $f(\theta|a=0,b=1)=1$
- · If $\Theta=\mathbb{R}$, the maximum entropy distribution given an expectation and variance is the normal distribution. This extends to bivariate and multivariate distributions if you have given covariances.
- · If $\Theta=\mathbb{R}_+$, then the maximum entropy distribution for a given expectation is the exponential distribution with expectation $\mu=\frac{1}{\lambda}$. You can utilize the fact that the median is $F^{-1}\left(0.5\right)=\mu\ln 2$ to go from the median to μ .
- · The binomial and Poisson distributions are maximum entropy distributions given μ for their respective Ω
- Additional examples (often with weird constraints) are given at the bottom of https://en.wikipedia.org/wiki/Maximum_entropy_probability_distribution

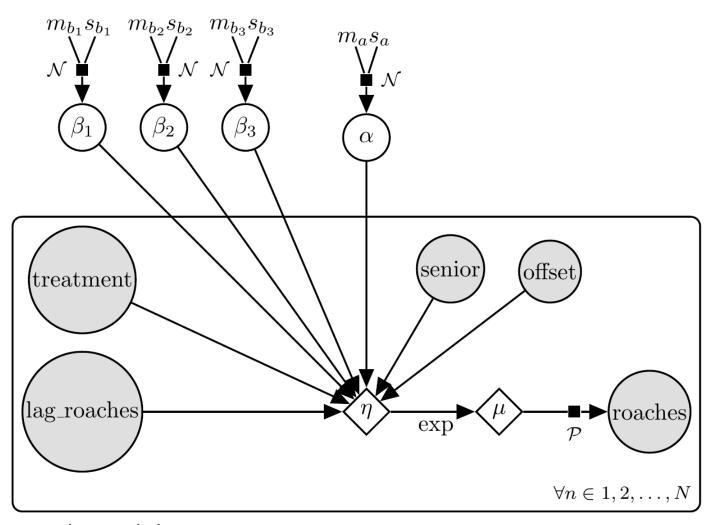
Do This Once on Each Computer You Use

- R comes with a terrible default coding for ordered factors in regressions known as "Helmert" contrasts
- Execute this once to change them to "treatment" contrasts, which is the conventional coding in the social sciences with dummy variables relative to a baseline category

```
cat('options(contrasts = c(unordered = "contr.treatment", ordered = "contr.treatment"))',
    file = "~/.Rprofile", sep = "\n", append = TRUE)
```

- Without this, you will get a weird rotation of the coefficients on dummy variables derived from ordered factors
- "contr.sum" is another reasonable (but rare) choice

Prior Predictive Distribution for Roach Study



Roach Model

Prior Predictive Distribution in Symbols

$$egin{aligned} lpha &\sim \mathcal{N}\left(m_{lpha}, s_{lpha}
ight) \ eta_{1} &\sim \mathcal{N}\left(m_{eta_{1}}, s_{eta_{1}}
ight) \ eta_{2} &\sim \mathcal{N}\left(m_{eta_{2}}, s_{eta_{2}}
ight) \ eta_{3} &\sim \mathcal{N}\left(m_{eta_{3}}, s_{eta_{3}}
ight) \ orall n : \eta_{n} = lpha + OFFSET_{n} + eta_{1} imes \log LAG_{n} + eta_{2} imes SENIOR_{n} + eta_{3} imes T_{n} \ orall n : \mu_{n} = e^{\eta_{n}} \ orall n : \mu_{n} &\sim \mathcal{P}oisson\left(\mu_{n}
ight) \end{aligned}$$

Breakout Rooms

Draw S=1000 times (using replicate) from a prior predictive distribution

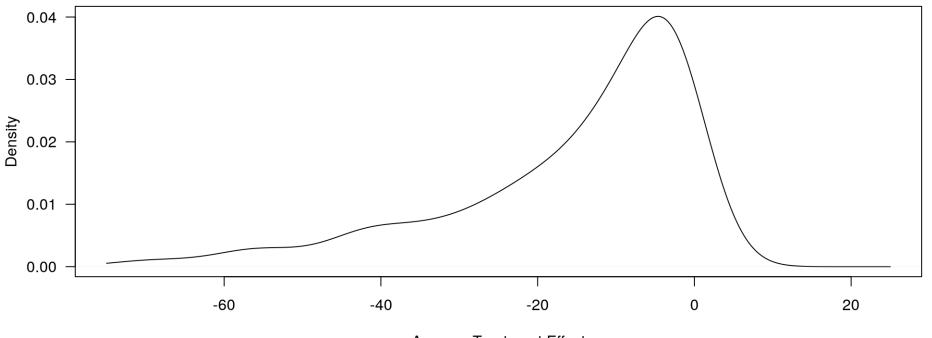
- The average number of pre-treatment roaches (roaches\$roach1) in a building was about 42 with a standard deviation of 75
- Use log(roach1) as the predictor
- The offset is log(roaches\$exposure2)
- · Remember to center the predictors, including the offset, when predicting

Posterior Distribution

```
post <- stan glm(y ~ senior + log(roach1) + treatment, data = roaches,</pre>
                family = poisson, offset = log(exposure2), QR = TRUE,
                 prior intercept = normal(location = log(42), scale = 4, autoscale = FALSE),
                prior = normal(location = 0, scale = c(5, 5, 1), autoscale = FALSE))
print(post, digits = 2)
##
              Median MAD SD
## (Intercept) 1.57 0.05
## senior -0.46 0.04
## log(roach1) 0.62 0.01
## treatment -0.49 0.03
##
## Sample avg. posterior predictive distribution of y:
           Median MAD SD
##
## mean PPD 31.54 0.55
##
## ----
## * For help interpreting the printed output see ?print.stanreg
## * For info on the priors used see ?prior summary.stanreg
. . .
```

Estimating Treatment Effects

```
df <- roaches; df$treatment <- 0
Y_0 <- posterior_linpred(post, newdata = df, offset = log(df$exposure2), transform = TRUE)
df$treatment <- 1
Y_1 <- posterior_linpred(post, newdata = df, offset = log(df$exposure2), transform = TRUE)
plot(density(colMeans(Y_1 - Y_0), from = -75, to = 25), xlab = "Average Treatment Effect", mai</pre>
```



Average Treatment Effect

Why NUTS Is Better than Other MCMC Samplers

- · With Stan, it is almost always the case that things either go well or you get warning messages saying things did not go well
- · Because Stan uses gradients, it scales well as models get more complex
- The first-order autocorrelation tends to be negative so you can get greater effective sample sizes (for mean estimates) than nominal sample size

0.68

```
round(bayesplot::neff_ratio(post), digits = 2)
## (Intercept) senior log(roach1) treatment
```

0.67

0.62

##

0.84

Divergent Transitions

- NUTS only uses first derivatives
- First order approximations to Hamiltonian physiscs are fine for if either the second derivatives are constant or the discrete step size is sufficiently small
- When the second derviatives are very not constant across Θ , Stan can (easily) mis-tune to a step size that is not sufficiently small and θ_k gets pushed to $\pm\infty$
- When this happens there will be a warning message, suggesting to increase adapt_delta
- When adapt_delta is closer to 1, Stan will tend to take smaller steps
- Unfortunately, even as $adapt_delta \lim 1$, there may be no sufficiently small step size and you need to try to reparameterize your model

Exceeding Maximum Treedepth

- · When the step size is small, NUTS needs many (small) steps to cross the "typical" subset of Θ and hit the U-turn point
- Sometimes, NUTS has not U-turned when it reaches its limit of 10 steps (by default)
- When this happens there will be a warning message, suggesting to increase max_treedepth
- There is always a sufficiently high value of $\max_{treedepth}$ to allow NUTS to reach the U-turn point, but increasing $\max_{treedepth}$ by 1 approximately doubles the wall time to obtain S draws

Low Bayesian Fraction of Missing Information

- · When the tails of the posterior PDF are very light, NUTS can have difficulty moving through Θ efficiently
- · This will manifest itself in a low (and possibly unreliable) estimate of n_{eff}
- · When this happens there will be a warning message, saying that the Bayesian Fraction of Missing Information (BFMI) is low
- $^{\circ}$ In this situation, there is not much you can do except increase S or preferably reparameterize your model to make it easier for NUTS

Runtime Exceptions

- Sometimes you will get a "informational" (not error, not warning) message saying that some parameter that should be positive is zero or some parameter that should be finite is infinite
- This means that a 64bit computer could not represent the number accurately
- If it only happens a few times and only during the warmup phase, do not worry
- Otherwise, you might try to use functions that are more numerically stable, which is discussed throughout the Stan User Manual

Initial Values

- Sometimes a Markov Chain will not get started because the log-kernel evaluates to $-\infty$ or NaN at the initial values (which are randomly generated)
- You can provide you own initial values
- But it is usually easier to specify init_r to be some value between 0 and 2 (the default) which governs the range at which the initial values are drawn from on the unconstrained scale

Tail / Bulk ESS

- Sometimes you will get a message about the tail or bulk ESS being low
- Call monitor on an object produced by Stan to see the estimates
- I do not worry too much about it if ONLY the lp__ margin is too low
- · Otherwise, you can increase the number of iterations and / or chains
- But it does suggest that there is something in the parameterization of your model that would make it difficult for Stan to sample from the implied posterior distribution

ShinyStan

· ShinyStan can be launched on an object produced by rstanarm via

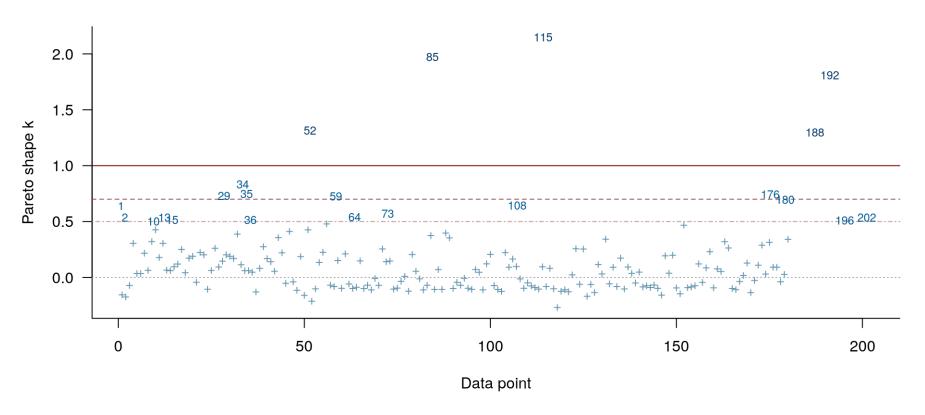
launch_shinystan(post)

· A webapp will open in your default web browser that helps you visualize the posterior distribution and diagnose problems

Sensitivity to Individual Observations

plot(loo(post), label_points = TRUE)

PSIS diagnostic plot



Numerical Assessment of Calibration

```
PPD <- posterior_predict(post); dim(PPD)

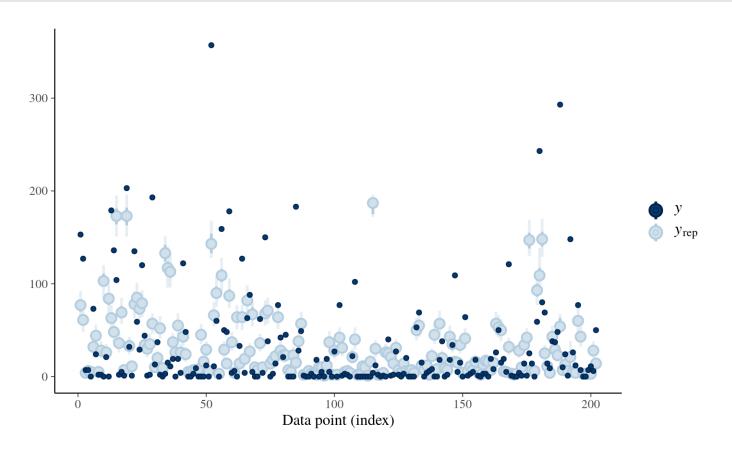
## [1] 4000 202

lower <- apply(PPD, MARGIN = 2, FUN = quantile, probs = 0.25)
upper <- apply(PPD, MARGIN = 2, FUN = quantile, probs = 0.75)
mean(roaches$y > lower & roaches$y < upper) # bad fit</pre>
```

- ## [1] 0.04950495
- Overal, the model is fitting the data poorly
- You will often overfit when you lazily use all predictors that are available in the dataset

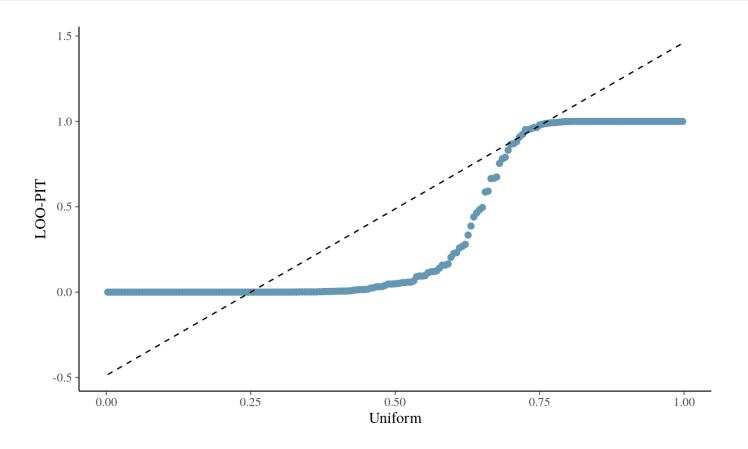
Leave-One-Out Based Intervals

```
library(bayesplot)
pp_check(post, plotfun = "loo_intervals")
```



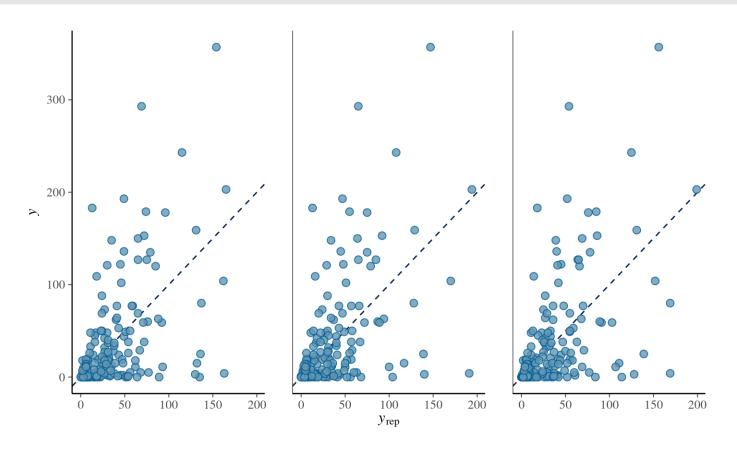
Leave-One-Out Probability Integral Transform

```
pp_check(post, plotfun = "loo_pit_qq")
```



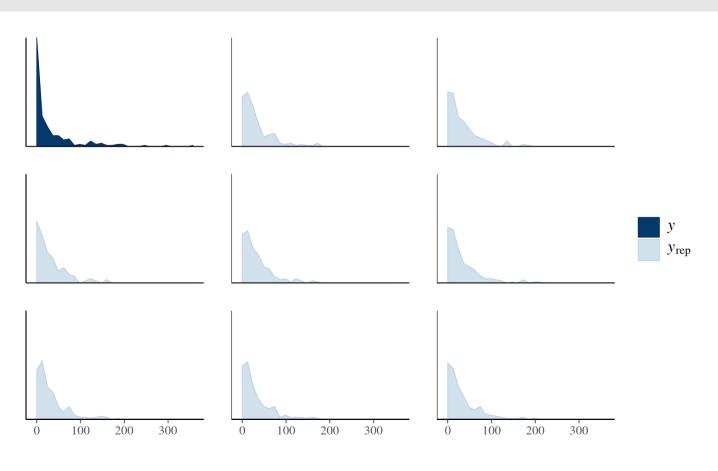
Scatterplots

pp_check(post, plotfun = "scatter")



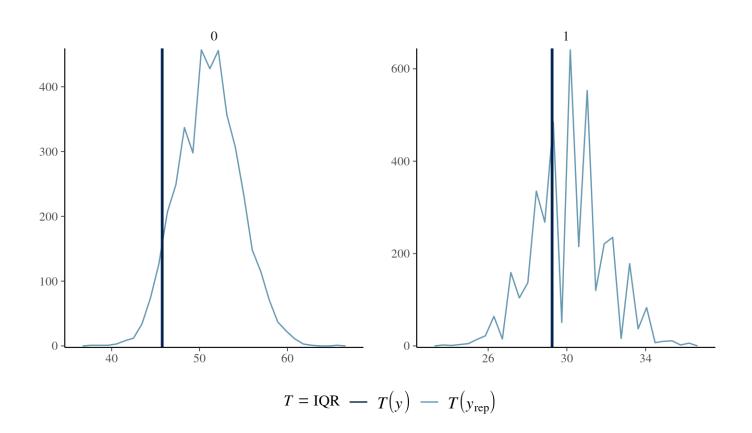
Frequency Polygons

pp_check(post, plotfun = "freqpoly")



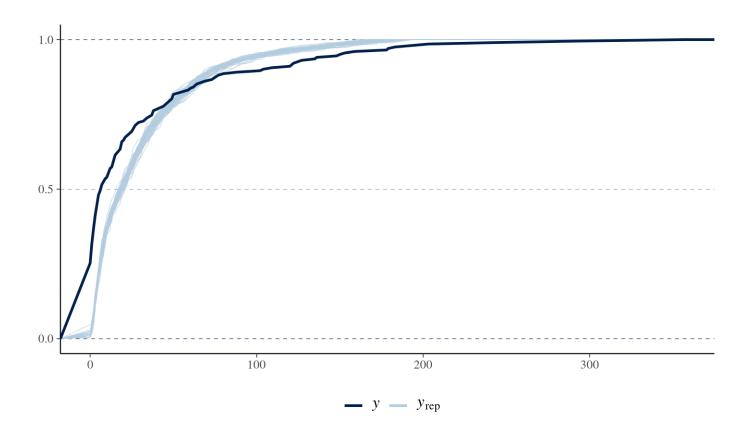
Frequency Polygons with Grouping

pp_check(post, plotfun = "stat_freqpoly_grouped", group = roaches\$treatment, stat = "IQR") +
 legend_move("bottom")



Empirical CDF

```
pp_check(post, plotfun = "ecdf_overlay") + legend_move("bottom")
```



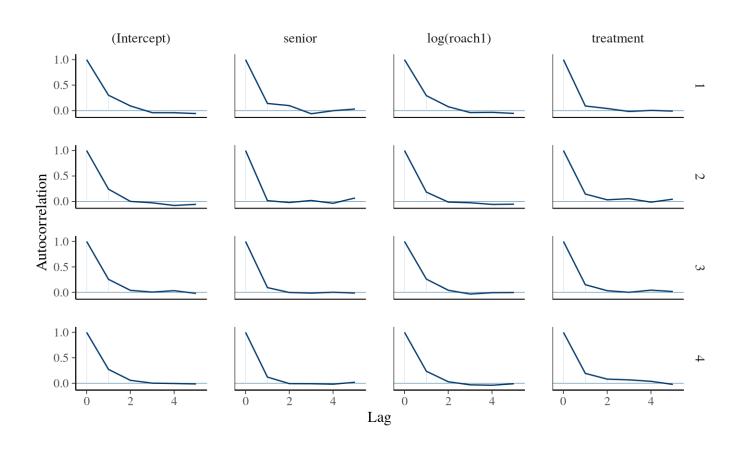
MCMC Performance Plots

```
format(available_mcmc(pattern = "data$", invert = TRUE))
```

```
[1] "mcmc acf
                                " "mcmc acf bar
                                                         " "mcmc areas
##
        "mcmc areas ridges
                                " "mcmc combo
                                                         " "mcmc dens
   [4]
        "mcmc_dens_chains
                                " "mcmc dens overlay
                                                         " "mcmc hex
                                " "mcmc_hist_by_chain
        "mcmc hist
                                                         " "mcmc intervals
   [10]
                                " "mcmc neff hist
                                                         " "mcmc nuts acceptance
## [13] "mcmc neff
                                                         " "mcmc nuts stepsize
                                " "mcmc nuts energy
        "mcmc nuts divergence
## [16]
                                " "mcmc pairs
                                                         " "mcmc parcoord
        "mcmc nuts treedepth
                                                         " "mcmc recover hist
        "mcmc rank hist
                                " "mcmc rank overlay
   [22]
   [25] "mcmc recover intervals" "mcmc recover scatter
                                                         " "mcmc rhat
                                                                                   Ш
                                                         " "mcmc trace
        "mcmc rhat hist
                                " "mcmc scatter
   [28]
   [31] "mcmc trace highlight
                                " "mcmc violin
```

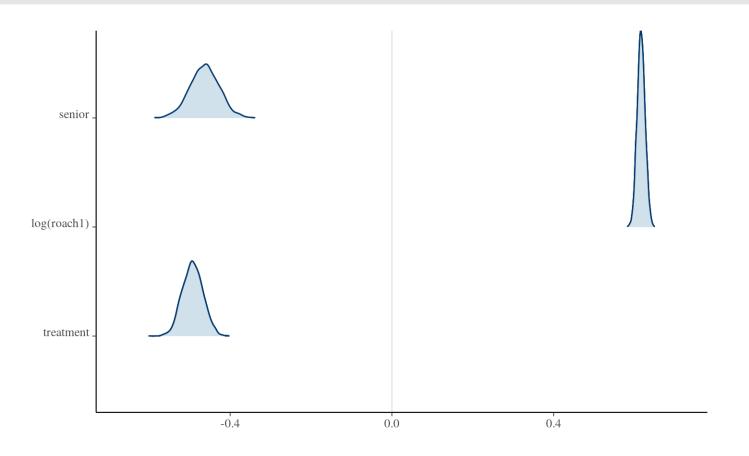
Autocorrelation Function

 $mcmc_acf(post, lags = 5)$



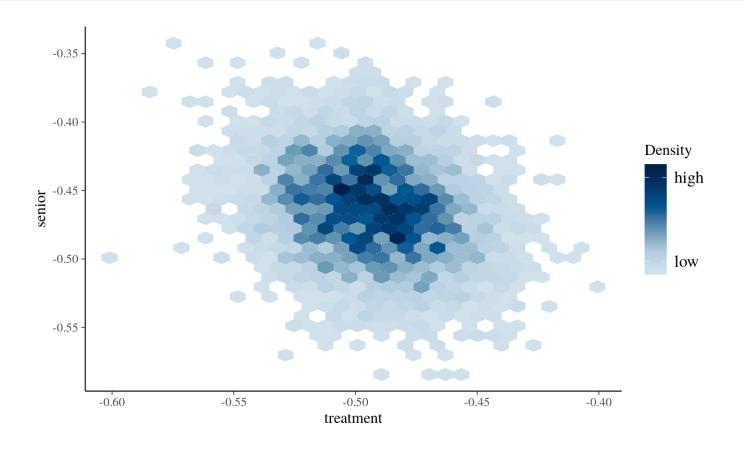
Ridges

mcmc_areas_ridges(post, regex_pars = "^[^(]") # exclude (Intercept)



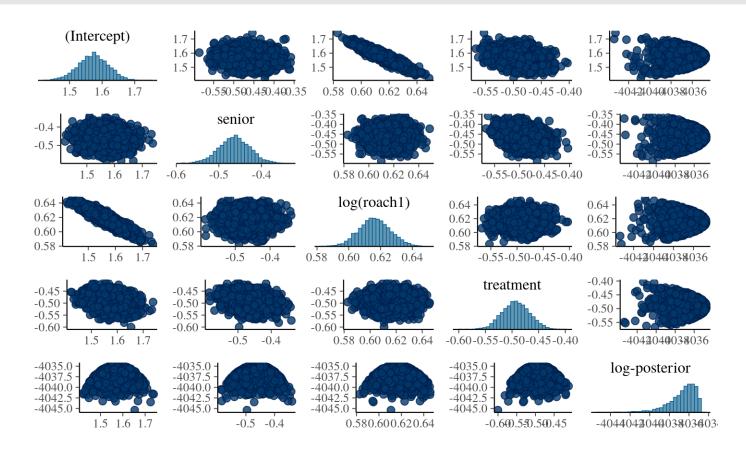
Hexograms

```
mcmc_hex(post, pars = c("treatment", "senior"))
```

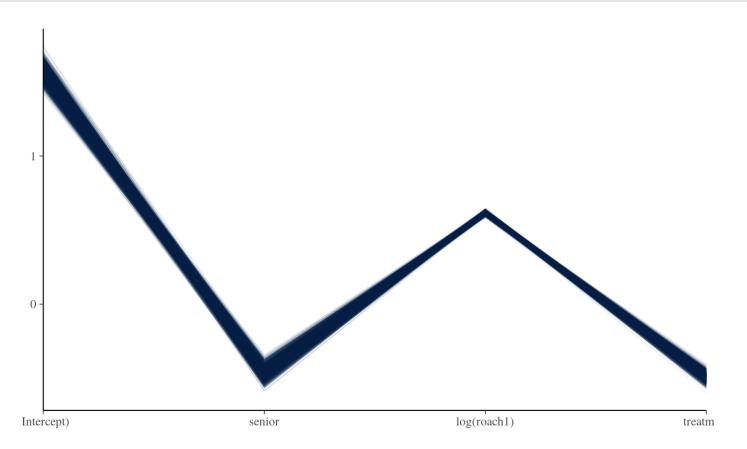


Pairs

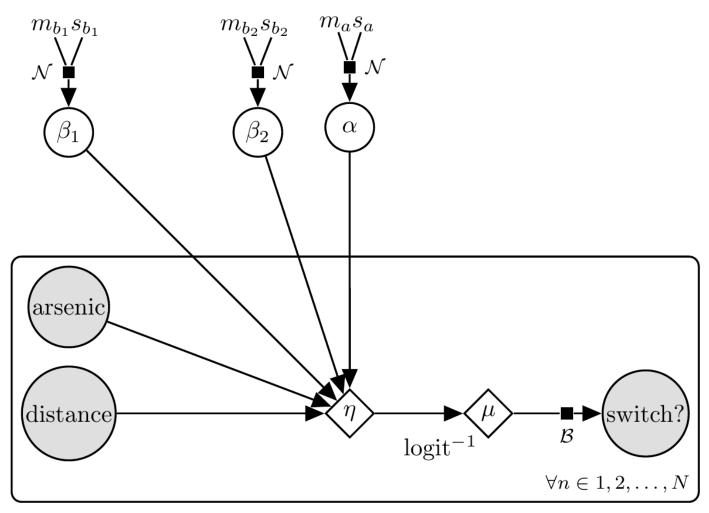
pairs(post)



Parallel Coordinates



Prior Predictive Distribution for Well Switching

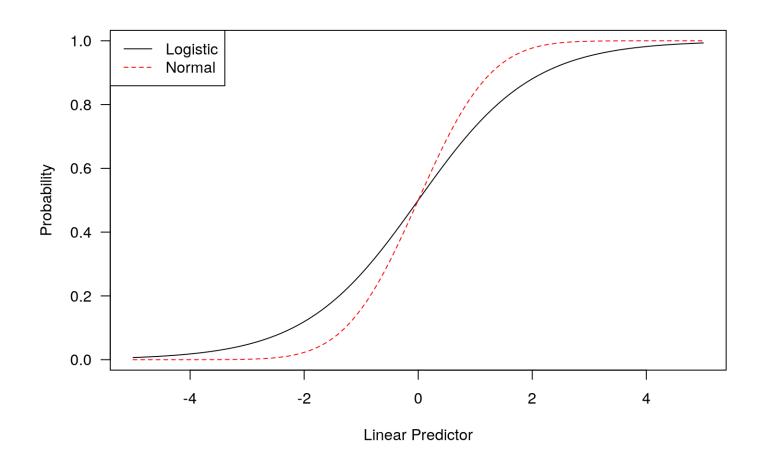


Well Switching Model

Prior Predictive Distribution in Symbols

$$egin{aligned} lpha &\sim \mathcal{N}\left(m_{lpha}, s_{lpha}
ight) \ eta_1 &\sim \mathcal{N}\left(m_{eta_1}, s_{eta_1}
ight) \ eta_2 &\sim \mathcal{N}\left(m_{eta_2}, s_{eta_2}
ight) \ orall n : \eta_n = lpha + eta_1 imes ARSENIC_n + eta_2 imes DISTANCE_n \ orall n : \epsilon_n &\sim \mathcal{L}ogistic\left(0, 1
ight) \ orall n : u_n = \eta_n + \epsilon_n \ orall n : Y_n = u_n > 0 \end{aligned}$$

Inverse Link Functions



Breakout Rooms

Draw S=1000 times (using replicate) from a prior predictive distribution

str(wells)

```
## 'data.frame': 3020 obs. of 5 variables:
## $ switch : int 1 1 0 1 1 1 1 1 1 1 1 ...
## $ arsenic: num 2.36 0.71 2.07 1.15 1.1 3.9 2.97 3.24 3.28 2.52 ...
## $ dist : num 16.8 47.3 21 21.5 40.9 ...
## $ assoc : int 0 0 0 0 1 1 1 0 1 1 ...
## $ educ : int 0 0 10 12 14 9 4 10 0 0 ...
```

- · You do not have to use assoc or educ
- To draw from the logistic distribution use rlogis
- · Remember to center the predictors when predicting

Posterior Distribution

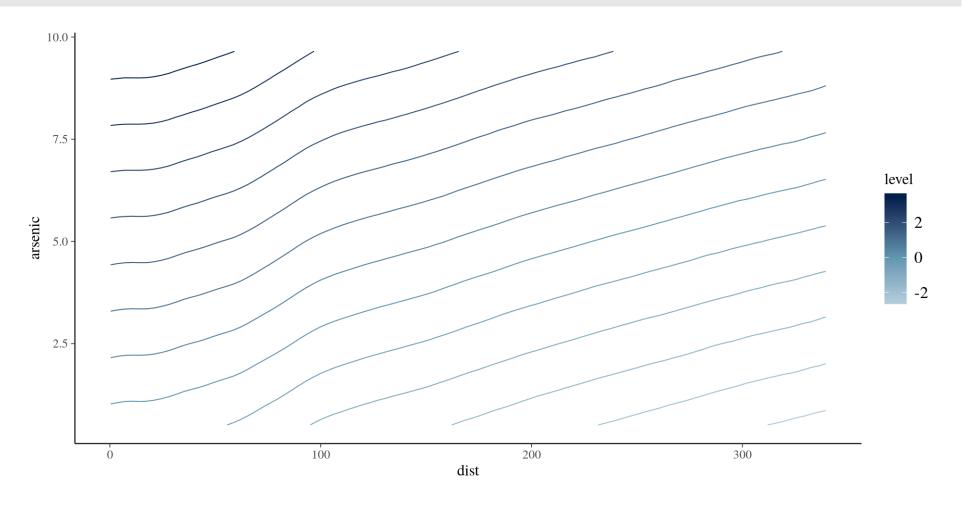
```
post <- stan_gamm4(switch ~ s(dist, arsenic), data = wells, family = binomial)</pre>
```

```
print(post, digits = 2)
                             0.04
## (Intercept)
                     0.33
## s(dist,arsenic).1
                             0.56
                     -0.03
## s(dist,arsenic).2 0.00
                             0.55
## s(dist,arsenic).3 0.00
                             0.55
## s(dist,arsenic).4 0.00
                             0.53
## s(dist,arsenic).5 -0.06
                             0.53
                             0.52
## s(dist,arsenic).6 -0.02
## s(dist,arsenic).7 0.00
                             0.52
                             0.55
## s(dist,arsenic).8 -0.04
                                            ##
                             0.55
## s(dist,arsenic).9 -0.08
## s(dist,arsenic).10 -0.04
                             0.53
                                            ##
                             0.57
## s(dist,arsenic).11 0.05
## s(dist,arsenic).12 0.09
                             0.55
## s(dist,arsenic).13 -0.31
                             0.62
                                            ##
## s(dist,arsenic).14 -0.23
                             0.59
## s(dist, arsenic).15 0.04
                             0.55
## s(dist, arsenic).16 0.02
                             0.55
## s(dist,arsenic).17 -0.03
                             0.53
                                            ##
```

```
## s(dist,arsenic).18 -0.11
                              0.54
## s(dist, arsenic).19 0.08
                              0.53
## s(dist,arsenic).20 0.02
                              0.45
## s(dist,arsenic).21 -0.04
                              0.47
## s(dist,arsenic).22 -0.02
                              0.53
## s(dist,arsenic).23 -0.64
                              0.50
## s(dist,arsenic).24 -0.20
                              0.41
                              0.56
## s(dist,arsenic).25 -0.17
## s(dist,arsenic).26 0.08
                              0.54
## s(dist,arsenic).27 -0.02
                              0.42
## s(dist, arsenic).28 7.97
                              1.06
## s(dist,arsenic).29 6.80
                              2.11
  Smoothing terms:
                               Median MAD SD
## smooth sd[s(dist,arsenic)1] 0.65
                                      0.45
## smooth sd[s(dist,arsenic)2] 4.62
                                      1.19
## Sample avg. posterior predictive distribution
            Median MAD SD
## mean PPD 0.58
                   0.01
```

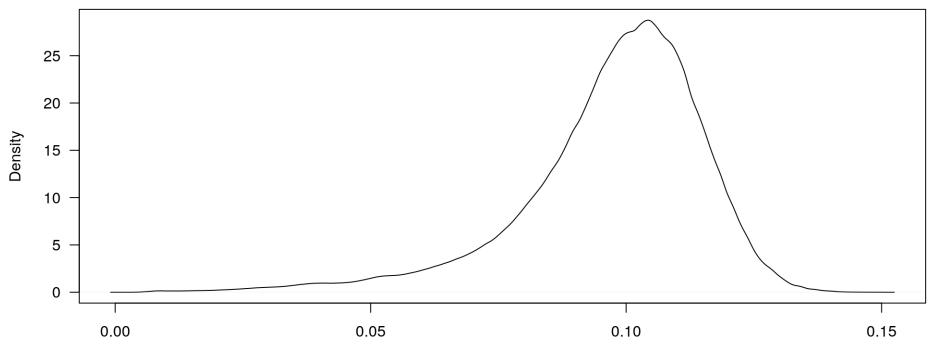
Nonlinear Plot

plot_nonlinear(post)



Plotting the Effect of an Increase in Arsenic

```
mu_0 <- posterior_linpred(post, transform = TRUE)
df <- wells; df$arsenic <- df$arsenic + 1
mu_1 <- posterior_linpred(post, newdata = df, transform = TRUE)
plot(density(mu_1 - mu_0), main = "", xlab = "Change in Probabilty of Switching")</pre>
```



Change in Probabilty of Switching

Effective Number of Parameters

loo(post) # nominal number of estimated parameters is 32

```
##
## Computed from 4000 by 3020 log-likelihood matrix
##
          Estimate SE
##
## elpd loo -1967.7 15.3
## p loo 6.7 0.2
## looic 3935.4 30.6
## ----
## Monte Carlo SE of elpd loo is 0.0.
##
## Pareto k diagnostic values:
                        Count Pct.
                                    Min. n eff
##
## (-Inf, 0.5] (good) 3018 99.9%
                                    2220
## (0.5, 0.7] (ok) 2 0.1%
                                    3759
   (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).
## See help('pareto-k-diagnostic') for details.
```

A Binomial Model for Romney vs Obama in 2012

```
poll <- readRDS("GooglePoll.rds") # WantToWin is coded as 1 for Romney and 0 for Obama
library(dplyr)
collapsed <- filter(poll, !is.na(WantToWin)) %>%
             group by (Region, Gender, Urban Density, Age, Income) %>%
             summarize(Romney = sum(grepl("Romney", WantToWin)), Obama = n() - Romney) %>%
             na.omit
post <- stan glm(cbind(Romney, Obama) ~ ., data = collapsed, family = binomial(link = "probit"), QR = TRUE)</pre>
## Warning in .local(object, ...): some chains had errors; consider specifying chains = 1 to
## debug
## here are whatever error messages were returned
                                                          ## [1] 5
print(post, digits = 2)
                                                          ## $link
                                                          ## [1] 2
                                                          ##
## $xbar
## [1] 0.57 0.85 1.48 0.98 0.82 1.77 0.44 0.44 ## $has_weights
## [1] FALSE -1.58 -0.99 -1.41 1.16
## [15] -1.02 -0.34
##
                                                          ## $has offset
## $dense X
                                                          ## [1] FALSE
## [1] TRUE
##
## $family
```

Same Linear Predictor, Logistic Link, ${\mathbb R}^2$ Prior

```
print(post, digits = 2)
## (Intercept)
                         -0.52
                                 0.14
## RegionNORTHEAST
                                0.09
                         -0.14
## RegionSOUTH
                        0.30
                                0.07
                                0.08
## RegionWEST
                         -0.14
## GenderMale
                         0.37
                                0.06
## Urban DensitySuburban -0.20
                                0.09
## Urban DensityUrban
                         -0.50
                               0.09
## Age25-34
                         0.10
                                0.10
                          0.52
                                 0.10
## Age35-44
```

```
## Age45-54
                         0.82
                                0.09
## Age55-64
                                0.09
                         0.83
## Age65+
                         1.30
                                0.11
                                0.08
## Income25,000-49,999
                         -0.11
## Income50,000-74,999
                         -0.07
                                0.09
## Income75,000-99,999
                                0.14
                         -0.09
## Income100,000-149,999
                                0.28
                         0.17
## Income150,000+
                         0.82
                                1.01
##
```

What Does QR = TRUE Do?

- · Let the vector of linear predictions in a GLM be $oldsymbol{\eta} = \mathbf{X}oldsymbol{eta}$
- · If we apply the QR decomposition to the linear predictor,

$$oldsymbol{\eta} = \widehat{\mathbf{Q}} \widehat{\mathbf{R}} oldsymbol{eta} = \widehat{\mathbf{Q}} \widehat{oldsymbol{ heta}}$$

- · When you specify QR = TRUE in stan_glm (or use stan_lm or stan_polr), rstanarm internally does a GLM using ${\bf Q}$ as the matrix of predictors instead of ${\bf X}$ to get the posterior distribution of ${\boldsymbol \theta}$ and then pre-multiplies each posterior draw of ${\boldsymbol \theta}$ by ${\bf R}^{-1}$ to get a posterior draw of ${\boldsymbol \beta} = {\bf R}^{-1}{\boldsymbol \theta}$
- Doing so makes it easier for NUTS to sample from the posterior distribution (of $m{ heta}$) efficiently because the columns of ${f Q}$ are orthogonal, whereas the columns of ${f X}$ are not