

Shape Constrained Regression for Excel

William Chiu

2022-10-21

Summary

Generalized Additive Models (gam) estimate non-linear but additive relationships between a response and a set of predictors. However, when the training data has a high noise to signal ratio, gam could estimate wiggly (non-monotonic) relationships that are difficult to explain. Shape Constrained Additive Models (scam) impose user-defined monotonic relationships that can be explained by the user.

The `mgcv` and `scam` packages are highly effective tools for developing gam and scam models. Both packages use the p-spline basis to construct non-linear features. Although p-splines have desirable properties, they are difficult to implement in other software tools like Excel. There is no closed-form equation that I could export from gam/scam and into Excel for an end-user.

Multivariate Adaptive Regression Splines (mars), from the `earth` package, allow us to approximate the scam model with linear basis functions – which are Excel-friendly.

Through a data simulation, I demonstrate how to fit gam and scam models using the `mgcv` and `scam` packages. Then I approximate the scam model and provide an Excel-friendly regression equation. Reader should be aware that MARS does *not guarantee* monotonicity. Therefore, after fitting an approximation of the scam model, reader should test the predictions by feeding extreme values of the predictors into the final model.

We also explore the `scar` package which uses monotonic binning. Then I approximate the scar model with non-linear least squares and sigmoid functions. Sigmoid functions guarantee monotonicity. However, sigmoid functions assume that the response tapers off on the tails (i.e., the relationship is S-shaped).

Approximations are achieved by turning the logistic regression problem into a least squares problem. The trick is to use a pseudo response that is continuous (rather than binary).

Data Generating Process (DGP)

The chunk generates 3 data frames: full data, training data, and test data. To demonstrate the wiggleness associated with gam, the sample size of the training data is limited to only 2000 observations.

Each data frame contains a binary response and two predictors. The first predictor has a monotonically increasing relationship with the response, while the second predictor has a monotonically decreasing relationship with the response. Both relationships are sigmoidal and hence highly non-linear.

In addition, the event rate of the response is rare.

```
library(mgcv)
library(scam)
library(tidyverse)
library(caTools)
library(MLmetrics)
```

```

library(earth)
library(plotmo)
library(furrr)
library(scar)
library(minpack.lm)
library(car)

plan(multisession, workers = 6) # set to 2 for most PCs

set.seed(2001)

nobs <- 100000

x1 <- rnorm(nobs)
x2 <- rnorm(nobs)

# Population log odds is a function of sigmoid features

z <- -35 + 5 * SSfpl(x1, -2, 2, 0, 0.5) - 5 * SSfpl(x2, -1, 1, 0, 0.1) +
  rnorm(nobs, 0, 20)

y <- rbinom(nobs, 1, prob=boot::inv.logit(z))

full_data <- data.frame(y=y, x1=x1, x2=x2)

summary(full_data)

##           y           x1           x2
## Min.      :0.00000   Min.      :-4.469540   Min.      :-4.349958
## 1st Qu.:0.00000   1st Qu.: -0.672327   1st Qu.: -0.667040
## Median :0.00000   Median : 0.006574   Median : 0.002566
## Mean    :0.05212   Mean    : 0.004819   Mean    : 0.000159
## 3rd Qu.:0.00000   3rd Qu.: 0.681828   3rd Qu.: 0.676167
## Max.    :1.00000   Max.    : 4.071722   Max.    : 4.590295

train_index <- sample.split(full_data$y, SplitRatio = 2/100)

train_data <- full_data[train_index,] # small
test_data <- full_data[!train_index,] # large

```

GAM

Due to the high noise to signal ratio in the training data, gam estimates very wiggly relationships between the binary response and the predictors. The y-axis is on the log-odds (or logit) scale.

```

## fit a gam

## when population error is high, gam returns non-monotonic relationships
## even when the population relationships are monotonic

mod_gam <- gam(y ~ s(x1) + s(x2), data = train_data, family = binomial)

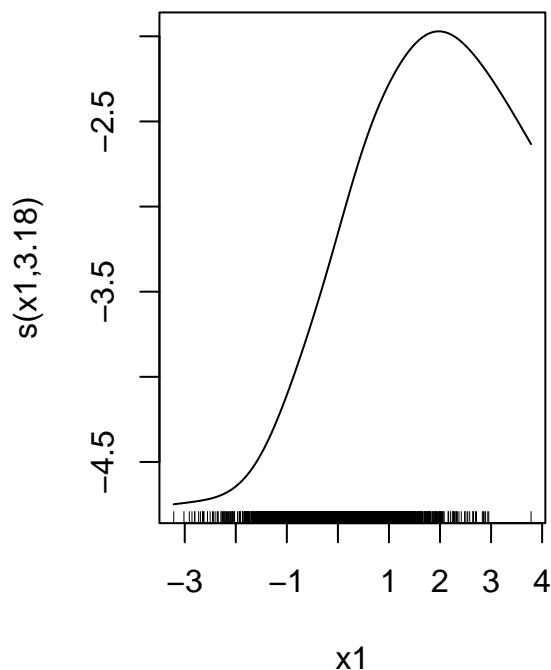
```

```
summary(mod_gam)
```

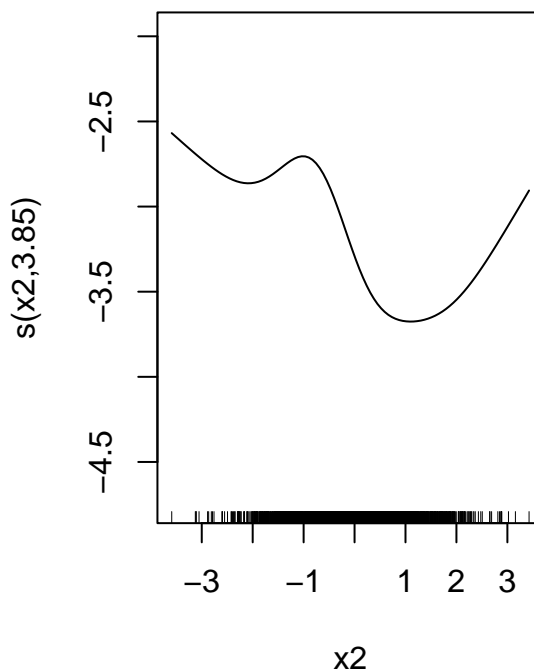
```
##
## Family: binomial
## Link function: logit
##
## Formula:
## y ~ s(x1) + s(x2)
##
## Parametric coefficients:
##           Estimate Std. Error z value Pr(>|z|)
## (Intercept) -3.2119      0.1329  -24.17  <2e-16 ***
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Approximate significance of smooth terms:
##           edf Ref.df Chi.sq p-value
## s(x1)  3.180  4.051  41.96  <2e-16 ***
## s(x2)  3.846  4.845  13.73   0.015 *
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## R-sq.(adj) =  0.0351   Deviance explained = 8.26%
## UBRE = -0.61702   Scale est. = 1           n = 2000
```

```
plot(mod_gam, pages=1, se=FALSE, main="Unconstrained GAM",
      shift=coef(mod_gam)[1])
```

Unconstrained GAM



Unconstrained GAM



SCAM

Shape constraints on each predictor reduce variance (wiggliness). Out-of-sample performance is similar between `gam` and `scam`.

```
## gam with monotonic constraints

## scam imposes monotonic relationships between each
## feature and the binary response
## mpi = monotonic p-spline increasing
## mpd = monotonic p-spline decreasing

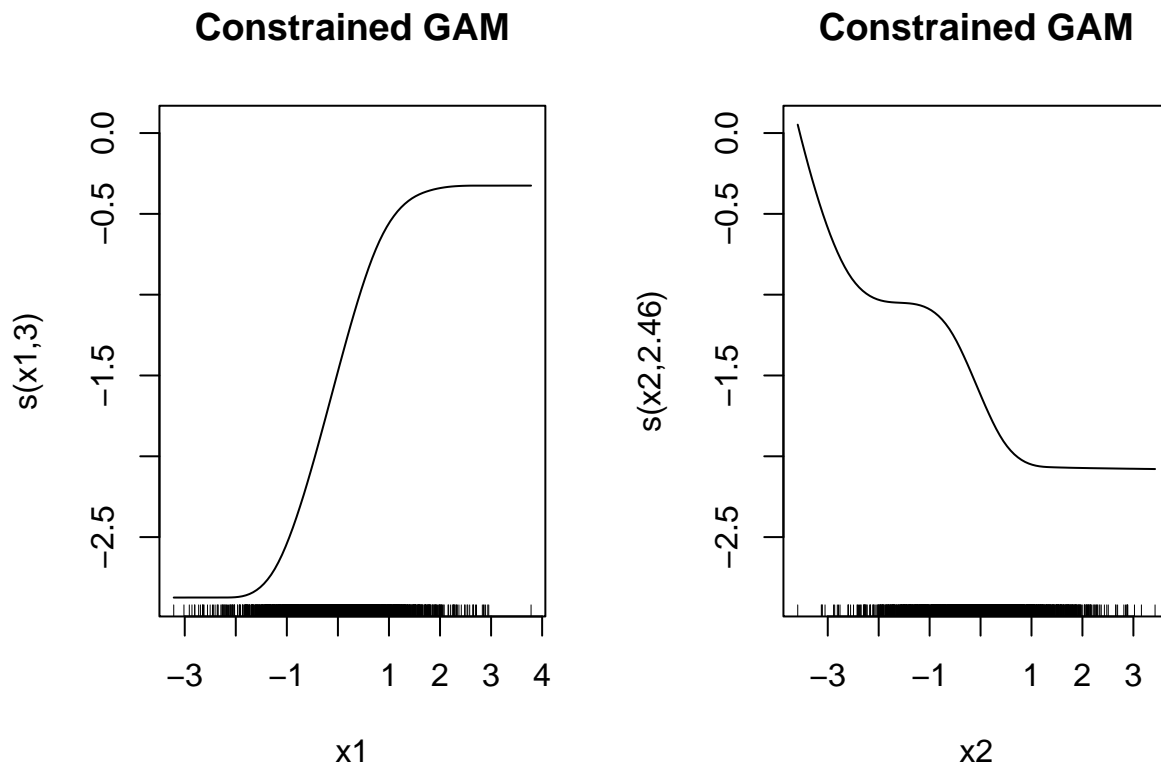
mod_mono_gam <- scam(y ~ s(x1, bs="mpi") + s(x2, bs="mpd"),
                    data = train_data, family = binomial)

summary(mod_mono_gam)
```

```
##
## Family: binomial
## Link function: logit
##
## Formula:
## y ~ s(x1, bs = "mpi") + s(x2, bs = "mpd")
##
```

```
## Parametric coefficients:
##           Estimate Std. Error z value Pr(>|z|)
## (Intercept)  -1.467      19.323  -0.076   0.939
##
## Approximate significance of smooth terms:
##           edf Ref.df Chi.sq  p-value
## s(x1)  3.003   3.005  42.10 3.89e-09 ***
## s(x2)  2.463   2.632  16.07 0.00088 ***
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## R-sq.(adj) =  0.0328   Deviance explained = 7.93%
## UBRE score = -0.61724   Scale est. = 1         n = 2000
##
## BFGS termination condition:
## 0.002513042
```

```
plot(mod_mono_gam, pages=1, se=FALSE, main="Constrained GAM",
     shift=coef(mod_mono_gam)[1])
```



```
map_dfr(list(mod_gam=mod_gam, mod_mono_gam=mod_mono_gam), AIC) %>%
  pivot_longer(everything(), names_to="model", values_to="AIC") %>%
  knitr::kable()
```

model	AIC
mod_gam	765.9699
mod_mono_gam	765.5259

```
## test set performance

preds_gam <- predict(mod_gam, newdata=test_data, type="response")
preds_mono_gam <- predict(mod_mono_gam, newdata=test_data,
                           type="response")

map_dfr(list(gam=preds_gam, mono_gam=preds_mono_gam), function(x){
  caTools::colAUC(x, test_data$y)
}) %>%
  pivot_longer(everything(), names_to="model", values_to="ROC-AUC") %>%
  knitr::kable()
```

model	ROC-AUC
gam	0.7097935
mono_gam	0.7098818

```
map_dfr(list(gam=preds_gam, mono_gam=preds_mono_gam), function(x){
  MLmetrics::LogLoss(x, test_data$y) }) %>%
  pivot_longer(everything(), names_to="model", values_to="Log Loss") %>%
  knitr::kable()
```

model	Log Loss
gam	0.1908626
mono_gam	0.1909576

Generate Pseudo-Training Data

The next step is controversial. I pretend that the scam model is the data generating process. In the actual training data, we observe binary outcomes rather than the log odds. In the pseudo data, I ignore the binary outcomes and “observe” the log odds from the scam model.

The reader should be aware that in the actual training data, y is a binary response. In the pseudo data, y is log odds from the scam model, which is analogous to z in the true data generating process.

```
## generate pseudo-data using Mono GAM

## suppose the scam model is the data generating process (dgp).
## append the log odds for each observation in the training
## data

pseudo_train_data <- train_data

pseudo_train_data$y <- as.numeric(predict(mod_mono_gam, newdata=train_data))

summary(pseudo_train_data)
```

```
##           y           x1           x2
## Min.      :-5.0697   Min.      :-3.215527   Min.      :-3.58923
## 1st Qu.   :-3.9582   1st Qu.   :-0.712003   1st Qu.   :-0.73931
## Median    :-3.1844   Median    : 0.003207   Median    :-0.03104
## Mean      :-3.2400   Mean      :-0.023366   Mean      :-0.04149
## 3rd Qu.   :-2.5328   3rd Qu.   : 0.639760   3rd Qu.   : 0.65565
## Max.      :-0.9548   Max.      : 3.783016   Max.      : 3.42584
```

Approximate SCAM with MARS

```
## approximate the Mono GAM model with MARS
```

```
## unfortunately, both gam and scam models are very difficult to
## implement outside of R due to how the basis functions are defined.
## an alternative is to approximate the scam relationships
## with simpler basis functions like the linear basis (which can be
## easily implemented in Excel) -- the linear basis is also called the
## reLU (rectified linear unit)
```

```
mod_logit_pseudo <- earth(y ~ x1 + x2, data=pseudo_train_data)
```

```
summary(mod_logit_pseudo)
```

```
## Call: earth(formula=y~x1+x2, data=pseudo_train_data)
```

```
##
```

```
##           coefficients
```

```
## (Intercept)      -3.9947320
```

```
## h(x1- -1.23371)    0.9448377
```

```
## h(1.0299-x1)      -0.0892467
```

```
## h(x1-1.0299)      -0.8733752
```

```
## h(x2- -0.807467)  -0.5263907
```

```
## h(x2-0.54224)     0.4177184
```

```
## h(0.963698-x2)    0.1083663
```

```
## h(x2-0.963698)    0.0856736
```

```
##
```

```
## Selected 8 of 8 terms, and 2 of 2 predictors
```

```
## Termination condition: RSq changed by less than 0.001 at 8 terms
```

```
## Importance: x1, x2
```

```
## Number of terms at each degree of interaction: 1 7 (additive model)
```

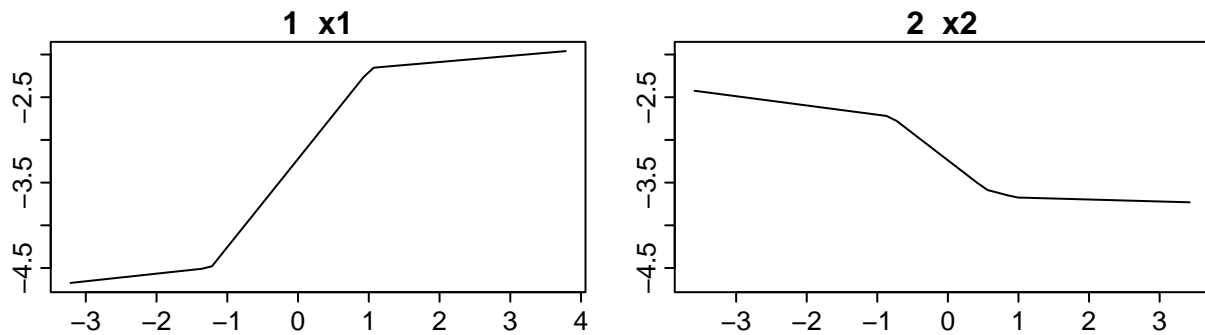
```
## GCV 0.002690246    RSS 5.300087    GRSq 0.9967042    RSq 0.9967502
```

```
plotmo(mod_logit_pseudo, caption="MARS with Pseudo Data")
```

```
## plotmo grid:      x1           x2
```

```
##           0.003206692 -0.03104272
```

MARS with Pseudo Data



Since the pseudo model is in the log-odds scale, I need to convert the predictions into probabilities to compare against the probability predictions from gam and scam.

test set performance

```
preds_pseudo <- boot::inv.logit(predict(mod_logit_pseudo, newdata=test_data))

map_dfr(list(gam=preds_gam, mono_gam=preds_mono_gam, pseudo_mono=preds_pseudo), function(x){
  caTools::colAUC(x, test_data$y)
}) %>%
  pivot_longer(everything(), names_to="model", values_to="ROC-AUC") %>%
  knitr::kable()
```

model	ROC-AUC
gam	0.7097935
mono_gam	0.7098818
pseudo_mono	0.7091226

```
map_dfr(list(gam=preds_gam, mono_gam=preds_mono_gam, pseudo_mono=preds_pseudo), function(x){
  MLmetrics::LogLoss(x, test_data$y)
}) %>%
  pivot_longer(everything(), names_to="model", values_to="Log Loss") %>%
  knitr::kable()
```


model	Log Loss
gam	0.1908626
mono_gam	0.1909576
pseudo_mono	0.1910508

Excel-friendly Equation

The equation below predicts the log odds or logit.

```
cat(format(mod_logit_pseudo, style="pmax", use.names=TRUE))
```

```
## -3.994732
## + 0.9448377 * pmax(0, x1 - -1.233707)
## - 0.08924666 * pmax(0, 1.029901 - x1)
## - 0.8733752 * pmax(0, x1 - 1.029901)
## - 0.5263907 * pmax(0, x2 - -0.8074673)
## + 0.4177184 * pmax(0, x2 - 0.5422403)
## + 0.1083663 * pmax(0, 0.9636977 - x2)
## + 0.08567365 * pmax(0, x2 - 0.9636977)
```

```
## Compare predict() against score_function
```

```
as.func <- function(object, digits = 20, use.names = TRUE, ...)
  eval(parse(text=paste(
    "function(x){\n",
    "if(is.vector(x))\n",
    "  x <- matrix(x, nrow = 1, ncol = length(x))\n",
    "with(as.data.frame(x),\n",
    format(object, digits = digits, use.names = use.names, style = "pmax", ...),
    ")\n",
    "}\n", sep = "")))

score_function <- as.func(mod_logit_pseudo)

compare_df <- expand.grid(x1 = seq(-10, 10, 0.1),
  x2 = seq(-10, 10, 0.1))

earth_preds <- predict(mod_logit_pseudo, newdata=compare_df)

score_preds <- score_function(compare_df)

max(abs(earth_preds - score_preds))
```

```
## [1] 1.776357e-15
```

Testing monotonicity

MARS does not guarantee monotonic relationships. Reader should always test the model for violations of monotonicity by feeding extreme predictor values into the model.

```

mono_check <- function(x, increasing=TRUE){
  if(increasing==TRUE){
    out <- all(x == cummax(x))
  } else {
    out <- all(x==cummin(x))
  }

  return(out)
}

df_x1 <- data.frame(x1 = seq(-10,10, 0.1),
                   x2 = mean(train_data$x2))

df_x2 <- data.frame(x1 = mean(train_data$x1),
                   x2 = seq(-10,10, 0.1))

df_x1$log_odds <- score_function(df_x1)

df_x2$log_odds <- score_function(df_x2)

mono_check(df_x1$log_odds)

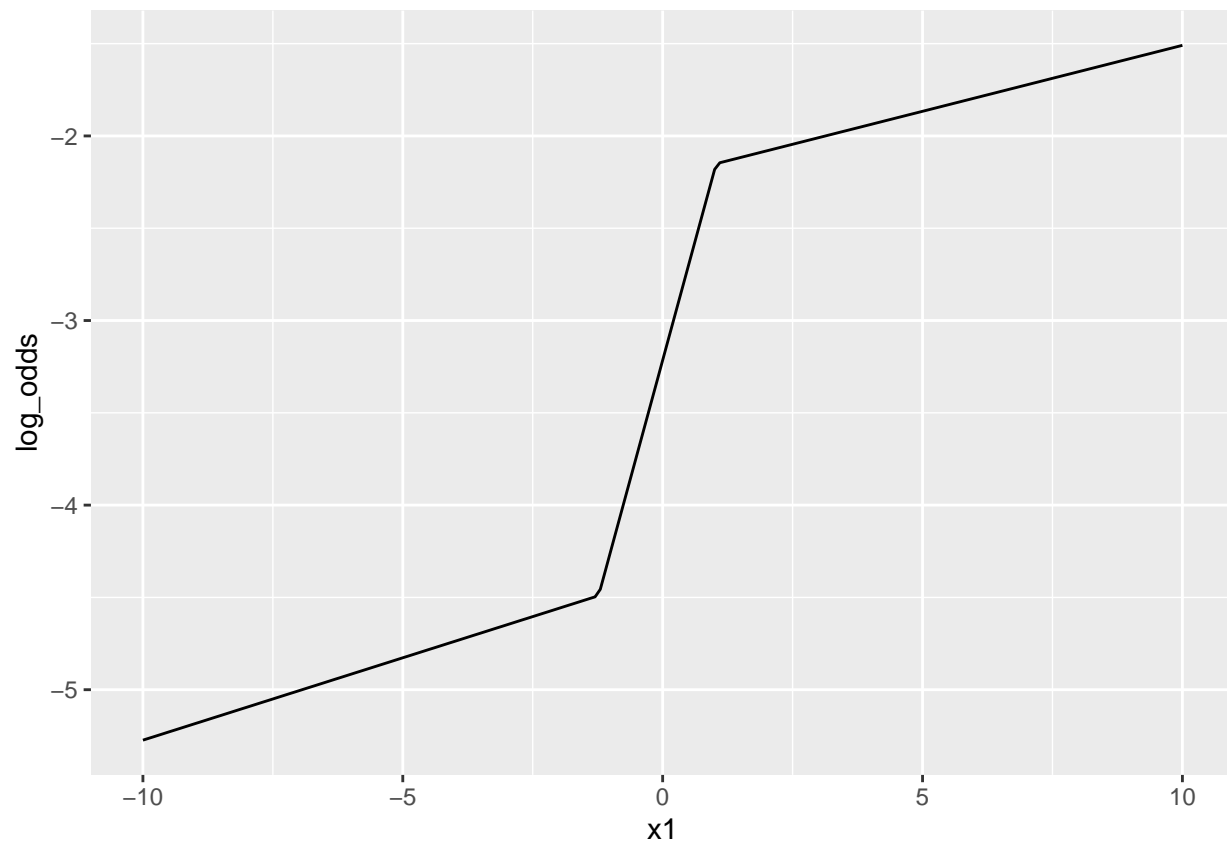
## [1] TRUE

mono_check(df_x2$log_odds, FALSE)

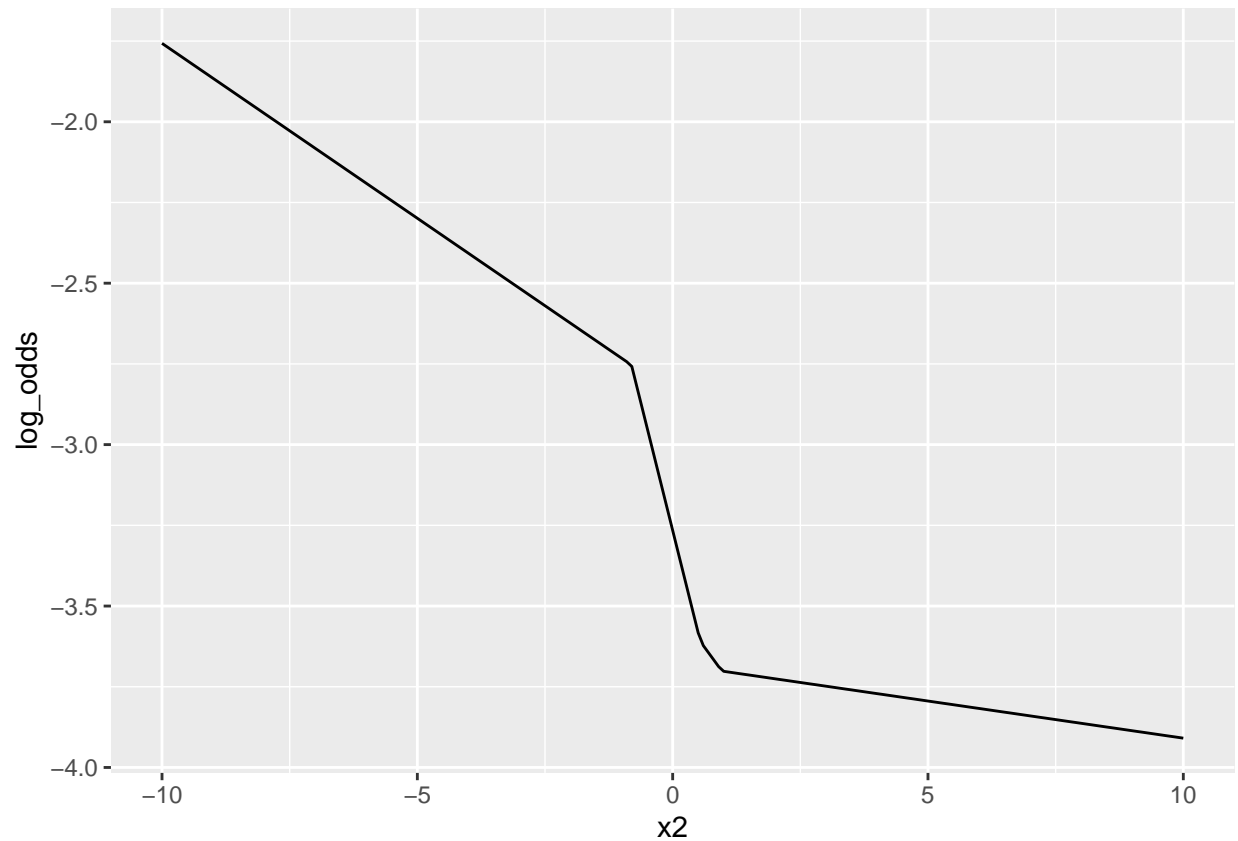
## [1] TRUE

ggplot(df_x1, aes(x=x1, y=log_odds)) + geom_line()

```



```
ggplot(df_x2, aes(x=x2, y=log_odds)) + geom_line()
```



How often does monotonicity fail?

Since MARS does not guarantee monotonicity. I repeated, 60 times, the following steps:

1. Set a new seed value
2. Generate full, train, and test sets
3. Fit a scam model to the training data
4. Generate pseudo data
5. Fit a MARS model to the pseudo data
6. Check shape constraints (x1 should increase with y and x2 should decrease with y)

```
simulate_one <- function(myseed){
  # Set a new seed value
  set.seed(myseed)

  nobs <- 100000

  x1 <- rnorm(nobs)
  x2 <- rnorm(nobs)

  z <- -35 + 5 * SSfp1(x1, -2, 2, 0, 0.5) - 5 * SSfp1(x2, -1, 1, 0, 0.1) +
    rnorm(nobs, 0, 20)
```

```

y <- rbinom(nobs, 1, prob=boot::inv.logit(z))

# Generate full, train, and test sets
full_data <- data.frame(y=y, x1=x1, x2=x2)

train_index <- sample.split(full_data$y, SplitRatio = 2/100)
train_data <- full_data[train_index,] # small
test_data <- full_data[!train_index,] # large

# SCAM
my_mod_mono_gam <- scam(y ~ s(x1, bs="mpi") + s(x2, bs="mpd"),
                        data = train_data, family = binomial)

# Pseudo data
pseudo_train_data <- train_data

pseudo_train_data$y <- as.numeric(predict(my_mod_mono_gam, newdata=train_data))

summary(pseudo_train_data)

# MARS
my_mod_pseudo_mars <- earth(y ~ x1 + x2, data=pseudo_train_data)

# Check shape constraints
df_x1 <- data.frame(x1 = seq(-10,10, 0.1),
                    x2 = mean(train_data$x2))

df_x2 <- data.frame(x1 = mean(train_data$x1),
                    x2 = seq(-10,10, 0.1))

df_x1$log_odds <- predict(my_mod_pseudo_mars, newdata=df_x1)
df_x2$log_odds <- predict(my_mod_pseudo_mars, newdata=df_x2)

success <- mono_check(df_x1$log_odds) & mono_check(df_x2$log_odds, FALSE)

return(success)
}

mono_success <- future_map_int(1:60, simulate_one,
                              .options=furrr_options(seed=NULL,
                                                       packages=c('earth', 'scam')
                              )

future:::ClusterRegistry("stop")

```

```
mean(mono_success)
```

```
## [1] 0.7
```

MARS successfully approximated the scam model about 70% of the time.

Why Pseudo Data?

The pseudo data filters out the noise in the latent response (z), which drives the binary response (y). Although we could directly pass the actual training data into MARS, the noise in the data generating process could cause **earth** to return non-monotonic relationships.

Reader should notice that y in the actual training data is a binary outcome.

```
mod_earth <- earth(y ~ x1 + x2, data=train_data, glm=list(family=binomial))

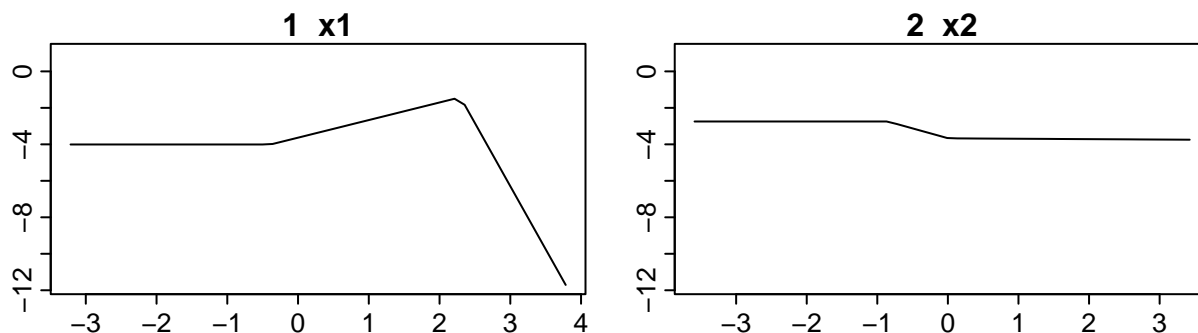
summary(mod_earth)
```

```
## Call: earth(formula=y~x1+x2, data=train_data, glm=list(family=binomial))
##
## GLM coefficients
##
##              y
## (Intercept)  -3.1240890
## h(x1- -0.387815)  0.9645083
## h(x1-2.2952)    -7.8781852
## h(x2- -0.852946) -1.0756331
## h(x2-0.00710431) 1.0539147
##
## GLM (family binomial, link logit):
## nulldev  df      dev  df  devratio    AIC iters converged
##   817.45 1999   754.646 1995    0.0768   764.6     6           1
##
## Earth selected 5 of 8 terms, and 2 of 2 predictors
## Termination condition: RSq changed by less than 0.001 at 8 terms
## Importance: x1, x2
## Number of terms at each degree of interaction: 1 4 (additive model)
## Earth GCV 0.04804009   RSS 95.2174   GRSq 0.0264512   RSq 0.0342279
```

```
plotmo(mod_earth, type="link", caption="MARS with Training Data")
```

```
## plotmo grid:    x1          x2
##              0.003206692 -0.03104272
```

MARS with Training Data



Alternative to SCAM: SCAR

Models developed in `scam` return smooth relationships between a response and each predictor. However, the smoothness (and monotonicity) is achieved through the p-spline basis, which is difficult to implement. If smoothness is not required, an alternative approach is to use monotonic step functions to approximate the relationships. The `scar` package achieves this goal.

Unfortunately, the `scar` package does not take data frames. I wrote two helper functions to convert a data frame into a matrix, which is then passed to the `scar` function.

```
fit_scar <- function(formula, shape=rep("l", d), data, family=gaussian(),
                     weights=rep(1, length(y)), epsilon = 1e-08){

  x <- model.matrix(formula, data)[,-1]

  y <- data[,all.vars(formula)[1]]

  mod <- scar(x, y, shape, family, weights, epsilon)

  mod$formula <- formula

  return(mod)
}

predict_scar <- function(object, newdata, type = c("link", "response"),
```

```

      rule=1, ...){

  fmla <- object$formula

  pred_names <- all.vars(fmla)[-1]

  x <- as.matrix(newdata[,pred_names])

  preds <- predict(object, x, type, rule, ...)

  return(preds)
}

```

Now we can fit a scar model with monotonic binning.

```

mod_scar <- fit_scar(y ~ x1 + x2, shape=c("in", "de"),
                    data=train_data, family=binomial())

```

Inside `mod_scar` is an object called `componentfit`. It contains partial fitted values by predictor (column) and observation (row). Each observation in the training set corresponds to a row in `componentfit`. The fitted value for a single observation is the row sum of the partial fitted values.

Given a pair of new predictor values (that are not in the training data), the `predict` function interpolates the partial fitted values from `componentfit`. This may be problematic if `componentfit` is very big. A similar problem arises with generating predictions from k-nearest-neighbors (knn).

The interpolation of partial fitted values causes the relationship between a response and a predictor to appear “step-like”.

Check the partial plots.

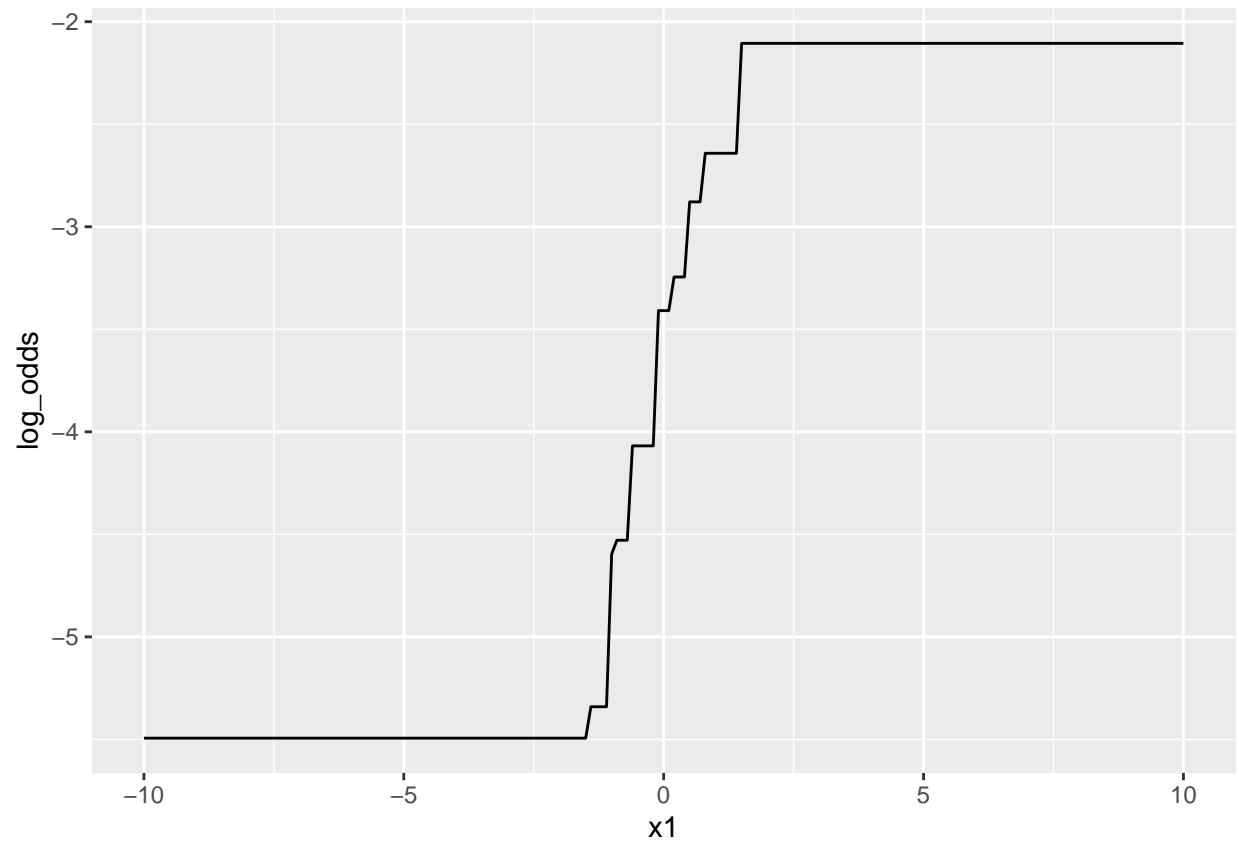
```

df_x1$log_odds <- predict_scar(mod_scar, newdata=df_x1)

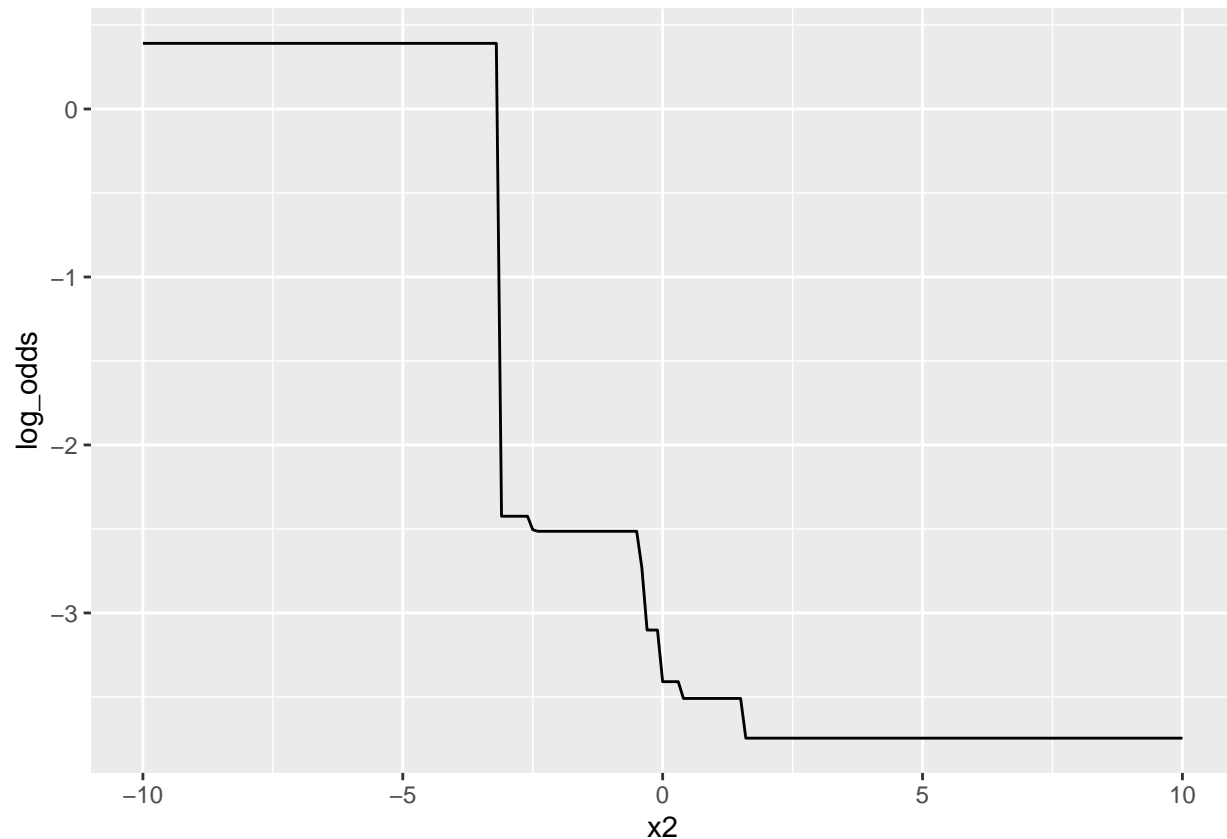
df_x2$log_odds <- predict_scar(mod_scar, newdata=df_x2)

ggplot(df_x1, aes(x=x1, y=log_odds)) + geom_line()

```

```
ggplot(df_x2, aes(x=x2, y=log_odds)) + geom_line()
```



Check test set performance

```
preds_scar <- predict_scar(mod_scar, newdata=test_data, type="response")

map_dfr(list(gam=preds_gam, mono_gam=preds_mono_gam, pseudo_mono=preds_pseudo,
             scar=preds_scar), function(x){
  caTools::colAUC(x, test_data$y)
}) %>%
  pivot_longer(everything(), names_to="model", values_to="ROC-AUC") %>%
  knitr::kable()
```

model	ROC-AUC
gam	0.7097935
mono_gam	0.7098818
pseudo_mono	0.7091226
scar	0.7063029

```
map_dfr(list(gam=preds_gam, mono_gam=preds_mono_gam, pseudo_mono=preds_pseudo,
             scar=preds_scar), function(x){
  MLmetrics::LogLoss(x, test_data$y)
}) %>%
```

```
pivot_longer(everything(), names_to="model", values_to="Log Loss") %>%
knitr::kable()
```

model	Log Loss
gam	0.1908626
mono_gam	0.1909576
pseudo_mono	0.1910508
scar	0.1931901

Approximating SCAR

Similar to the MARS approximation of scam, we could approximate scar with another method (with the help of pseudo data). The pseudo response would be the log-odds from the scar model. The features would be sigmoid functions that are fed into non-linear least squares. Sigmoid functions guarantee monotonicity.

First, some pseudo data!

```
pseudo_train_data_nls <- train_data

pseudo_train_data_nls$y <- predict_scar(mod_scar, newdata=train_data
                                     , type="link")

summary(pseudo_train_data_nls)
```

```
##           y           x1           x2
##  Min.    :-5.830   Min.    :-3.215527   Min.    :-3.58923
##  1st Qu. :-4.168   1st Qu. :-0.712003   1st Qu. :-0.73931
##  Median :-3.245   Median  : 0.003207   Median  :-0.03104
##  Mean   :-3.367   Mean    :-0.023366   Mean    :-0.04149
##  3rd Qu. :-2.514   3rd Qu. : 0.639760   3rd Qu. : 0.65565
##  Max.    : 1.694   Max.     : 3.783016   Max.     : 3.42584
```

Second, non-linear least squares and sigmoid features. The classical `nls` function is very sensitive to initial parameter guesses. I have never been successful in using it. I suggest using `nlsLM` from the `minpack.lm` package.

```
mod_pseudo_scar <- nlsLM(y ~ constant + a * SSfpl(x1, A1, B1, xmid1, scal1) +
                        b * SSfpl(x2, A2, B2, xmid2, scal2),
                        data=pseudo_train_data_nls,
                        start=list(constant=0, a=1, b=1,
                                  A1=-1, B1=1, xmid1=0.5, scal1=0.5,
                                  A2=-1, B2=1, xmid2=0.5, scal2=0.5))
```

```
est <- coef(mod_pseudo_scar)

est_df <- data.frame(Estimate=est)

knitr::kable(est_df)
```

	Estimate
constant	0.1050215
a	2.2854845
b	0.4915371
A1	-2.3602224
B1	-0.5978491
xmid1	-0.3596639
scal1	0.7826701
A2	0.3961789
B2	-1.7651710
xmid2	-0.2375986
scal2	0.1368247

We could also bootstrap 95% confidence intervals for each estimate.

```
boot_psuedo <- Boot(mod_pseudo_scar, R=1000)

CI_nls <- data.frame(confint(boot_psuedo, type="perc"))

names(CI_nls) <- c("p2.5", "p97.5")

CI_nls$signif <- (CI_nls$p2.5 * CI_nls$p97.5) > 0

knitr::kable(CI_nls)
```

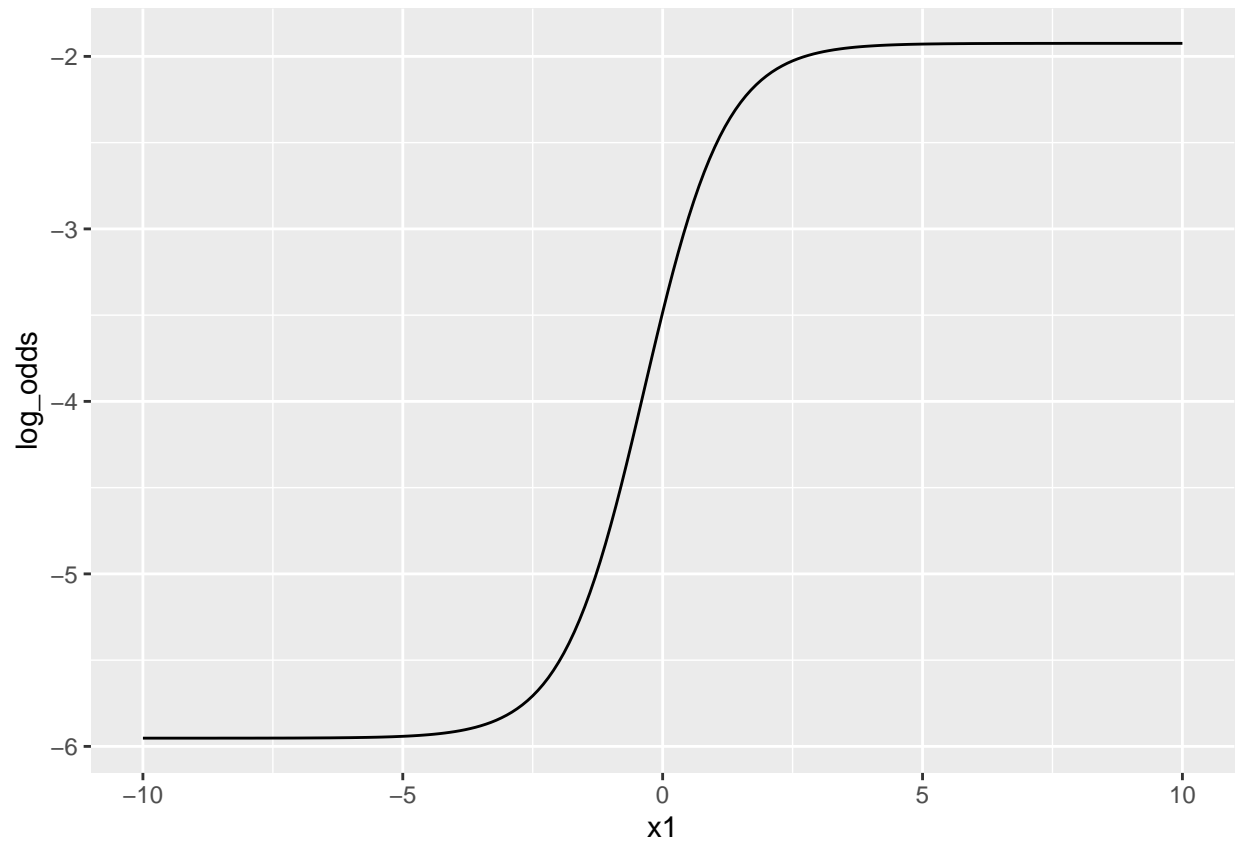
	p2.5	p97.5	signif
constant	0.0880270	0.5475834	TRUE
a	2.2691678	2.3693818	TRUE
b	0.4858069	0.5517686	TRUE
A1	-2.4498165	-2.3423218	TRUE
B1	-0.7245286	-0.5713068	TRUE
xmid1	-0.4066790	-0.3146518	TRUE
scal1	0.7405104	0.8291195	TRUE
A2	-0.1608590	0.4342162	FALSE
B2	-2.1004007	-1.7291594	TRUE
xmid2	-0.2539679	-0.2200998	TRUE
scal2	0.1208838	0.1543505	TRUE

Some plots.

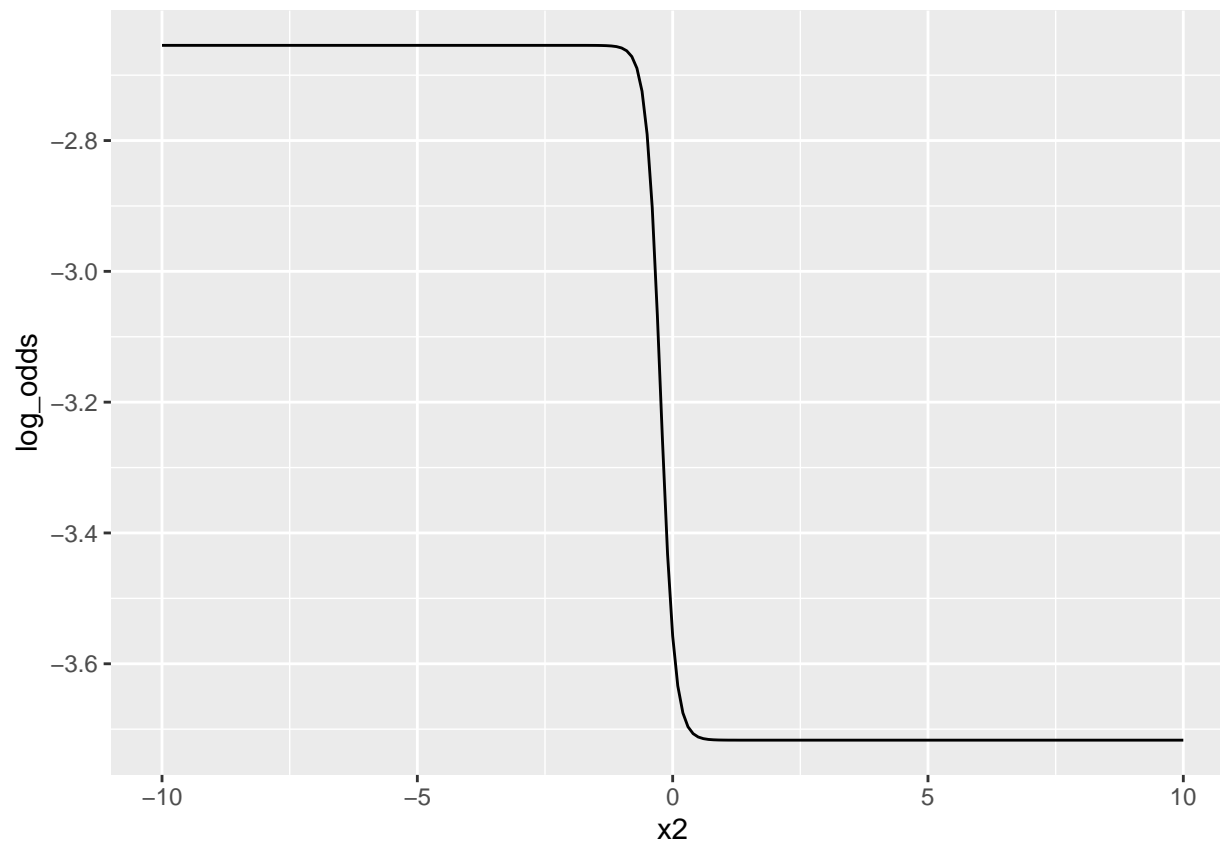
```
df_x1$log_odds <- predict(mod_pseudo_scar, newdata=df_x1)

df_x2$log_odds <- predict(mod_pseudo_scar, newdata=df_x2)

ggplot(df_x1, aes(x=x1, y=log_odds)) + geom_line()
```



```
ggplot(df_x2, aes(x=x2, y=log_odds)) + geom_line()
```



Test set performance

```
preds_pseudo_scar <- boot::inv.logit(predict(mod_pseudo_scar, newdata=test_data))

map_dfr(list(gam=preds_gam, mono_gam=preds_mono_gam, pseudo_mono=preds_pseudo,
             scar=preds_scar, pseudo_scar=preds_pseudo_scar), function(x){
  caTools::colAUC(x, test_data$y)
}) %>%
  pivot_longer(everything(), names_to="model", values_to="ROC-AUC") %>%
  knitr::kable()
```

model	ROC-AUC
gam	0.7097935
mono_gam	0.7098818
pseudo_mono	0.7091226
scar	0.7063029
pseudo_scar	0.7090304

```
map_dfr(list(gam=preds_gam, mono_gam=preds_mono_gam, pseudo_mono=preds_pseudo,
             scar=preds_scar, pseudo_scar=preds_pseudo_scar), function(x){
  MLmetrics::LogLoss(x, test_data$y)
}) %>%
  pivot_longer(everything(), names_to="model", values_to="Log Loss") %>%
  knitr::kable()
```

model	Log Loss
gam	0.1908626
mono_gam	0.1909576
pseudo_mono	0.1910508
scar	0.1931901
pseudo_scar	0.1919524

The approximation of scar actually outperforms the original scar model because the approximation extrapolates using the sigmoid functions that were estimated by non-linear least squares.

Sigmoid functions guarantee monotonicity.

Conclusion

Imposing shape constraints on data with high noise to signal ratios could greatly reduce variance (wiggleness). The **scam** package is highly effective in developing models with user-defined monotonicity constraints for each predictor. MARS can approximate the scam model with linear basis functions, which are easy to write down on paper and implement in an Excel formula.

The **scar** package also develops models with user-defined monotonicity constraints for each predictor. Non-linear least squares can approximate the scar model with sigmoid functions, which are easy to write down on paper (see Appendix A for equation) and implement in an Excel formula.