# Shape Constrained Regression for Excel

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## 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 wiggliness 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)
plan(multisession, workers = 6) # set to 2 for most PCs
set.seed(2001)
nobs <- 100000
x1 <- rnorm(nobs)</pre>
x2 <- rnorm(nobs)
# Population log odds is a function of sigmoid features
z \leftarrow -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)</pre>
summary(full_data)
##
                                                 x2
                             x1
         :0.00000
                            :-4.469540
                                                  :-4.349958
                     Min.
                                           Min.
## 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)</pre>
train_data <- full_data[train_index,] # small</pre>
test_data <- full_data[!train_index,] # large</pre>
```

#### **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

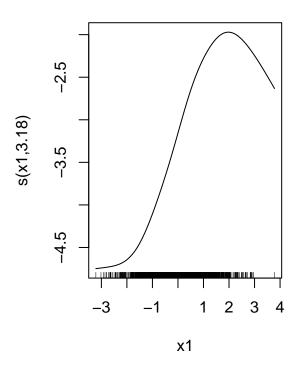
mod_gam <- gam(y ~ s(x1) + s(x2), data = train_data, family = binomial)</pre>
```

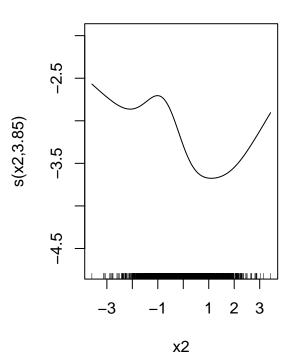
#### summary(mod\_gam)

```
##
## Family: binomial
## Link function: logit
##
## Formula:
## y \sim 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
plot(mod_gam, pages=1, se=FALSE, main="Unconstrained GAM",
shift=coef(mod_gam)[1])
```

### **Unconstrained GAM**

## **Unconstrained GAM**





#### **SCAM**

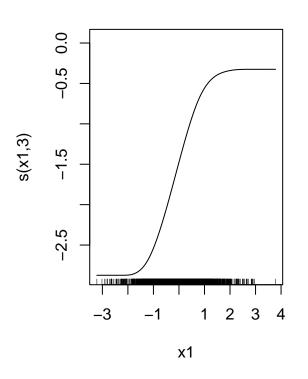
Shape constraints on each predictor reduce variance (wiggliness). Out-of-sample performance is similar between gam and scam.

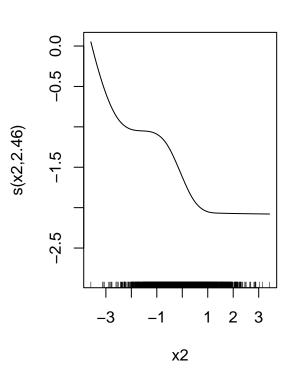
```
##
## Family: binomial
## Link function: logit
##
## Formula:
## y ~ s(x1, bs = "mpi") + s(x2, bs = "mpd")
##
```

```
## Parametric coefficients:
              Estimate Std. Error z value Pr(>|z|)
##
  (Intercept)
                -1.467
                           19.323 -0.076
##
##
## 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
## BFGS termination condition:
## 0.002513042
plot(mod_mono_gam, pages=1, se=FALSE, main="Constrained GAM",
     shift=coef(mod_mono_gam)[1])
```

### **Constrained GAM**

#### **Constrained GAM**





```
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

C-AUC
7097935 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 mono_gam	$\begin{array}{c} 0.1908626 \\ 0.1909576 \end{array}$

# 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)</pre>
```

```
## 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

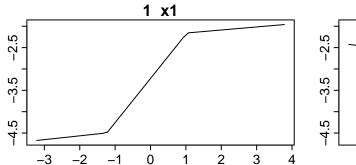
## 3rd Qu.:-2.5328 3rd Qu.: 0.639760 3rd Qu.: 0.65565

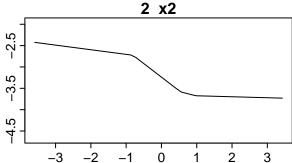
## Max. :-0.9548 Max. : 3.783016 Max. : 3.42584
```

### 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)</pre>
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
##
           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=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	0.7091226

```
map_dfr(list(gam=preds_gam, mono_gam=preds_mono_gam, pseudo=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	0.1910508

### **Excel-friendly Equation**

The equation below predicts the log odds or logit.

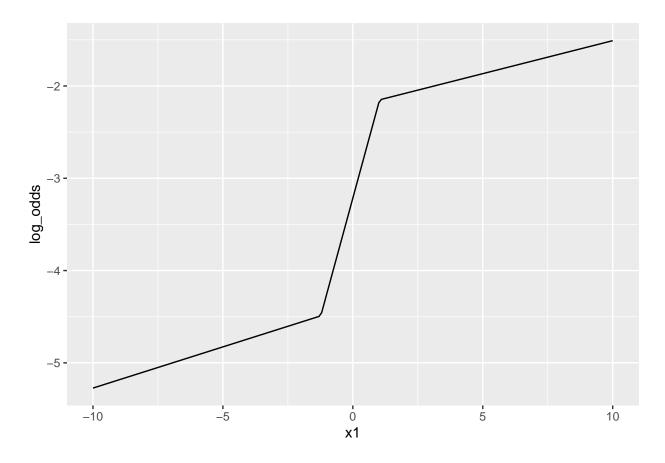
```
cat(format(mod logit pseudo, style="pmax", use.names=TRUE))
##
     -3.994732
##
     + 0.9448377 * pmax(0,
                                     x1 - -1.233707
     -0.08924666 * pmax(0,
                              1.029901 -
##
     - 0.8733752 * pmax(0,
                                     x1 -
                                          1.029901)
##
     - 0.5263907 * pmax(0,
                                     x2 - -0.8074673)
     + 0.4177184 * pmax(0,
##
                                     x2 - 0.5422403)
    + 0.1083663 * pmax(0, 0.9636977 -
                                     x2 - 0.9636977)
     + 0.08567365 * pmax(0,
## 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 \leftarrow 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)</pre>
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)</pre>
score_preds <- score_function(compare_df)</pre>
max(abs(earth_preds - score_preds))
```

## [1] 1.776357e-15

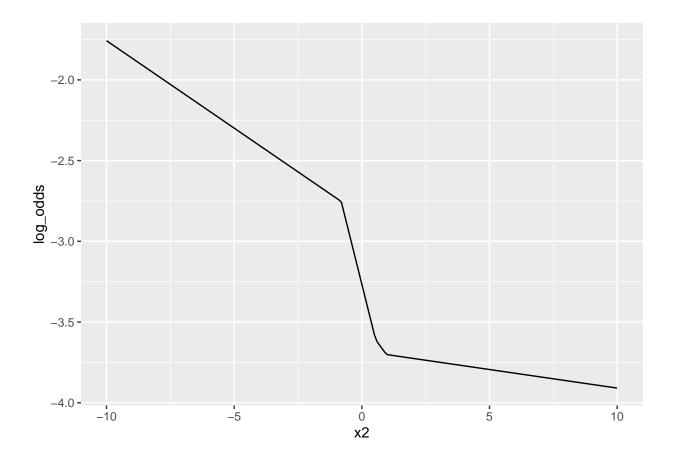
# Testing monotonicity

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){</pre>
  if(increasing==TRUE){
    out \leftarrow all(x == cummax(x))
    out <- all(x==cummin(x))</pre>
 return(out)
}
df_x1 \leftarrow data.frame(x1 = seq(-10,10, 0.1),
                      x2 = mean(train_data$x2))
df_x2 \leftarrow data.frame(x1 = mean(train_data$x1),
                     x2 = seq(-10, 10, 0.1)
df_x1$log_odds <- score_function(df_x1)</pre>
df_x2$log_odds <- score_function(df_x2)</pre>
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 * SSfpl(x1, -2, 2, 0, 0.5) - 5 * SSfpl(x2, -1, 1, 0, 0.1) + rnorm(nobs, 0, 20)</pre>
```

```
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)</pre>
  train_index <- sample.split(full_data$y, SplitRatio = 2/100)</pre>
  train_data <- full_data[train_index,] # small</pre>
  test_data <- full_data[!train_index,] # large</pre>
  # SCAM
  my_mod_mono_gam \leftarrow scam(y \sim s(x1, bs="mpi") + s(x2, bs="mpd"),
                         data = train_data, family = binomial)
  # Pseudo data
  pseudo_train_data <- train_data
  pseudo_train_data$y <- as.numeric(predict(my_mod_mono_gam, newdata=train_data))</pre>
  summary(pseudo_train_data)
  # MARS
  my_mod_pseudo_mars <- earth(y ~ x1 + x2, data=pseudo_train_data)</pre>
  # Check shape constraints
  df_x1 \leftarrow data.frame(x1 = seq(-10,10, 0.1),
                       x2 = mean(train_data$x2))
  df_x2 <- data.frame(x1 = mean(train_data$x1),</pre>
                       x2 = seq(-10, 10, 0.1)
  df_x1$log_odds <- predict(my_mod_pseudo_mars, newdata=df_x1)</pre>
  df_x2$log_odds <- predict(my_mod_pseudo_mars, newdata=df_x2)</pre>
  success <- mono_check(df_x1$log_odds) & mono_check(df_x2$log_odds, FALSE)</pre>
  return(success)
mono_success <- future_map_int(1:60, simulate_one,</pre>
                           .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.

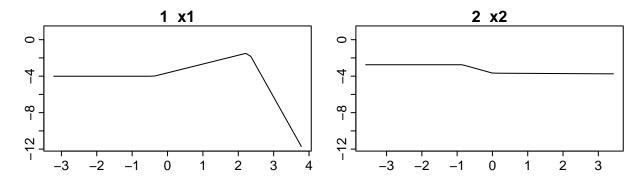
## Why Pseudo Data?

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))</pre>
summary(mod_earth)
## Call: earth(formula=y~x1+x2, data=train_data, glm=list(family=binomial))
##
## GLM coefficients
##
## (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
##
                                                        6
## 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
##
           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.

```
fmla <- object$formula

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

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

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

return(preds)
}</pre>
```

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())</pre>
```

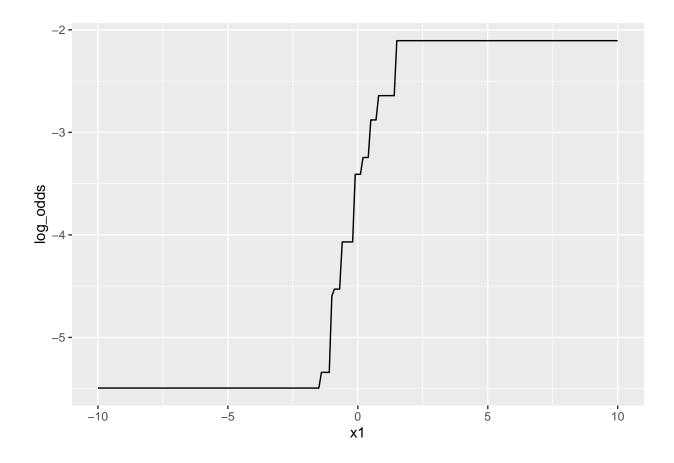
Inside mod\_scar is an object called componentfit. It contains partial fitted values by predictor (column) and observation (row). Each observation in the training set corresponds to a row in componentfit. The fitted value for a single observation is the row sum of the partial fitted values.

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).

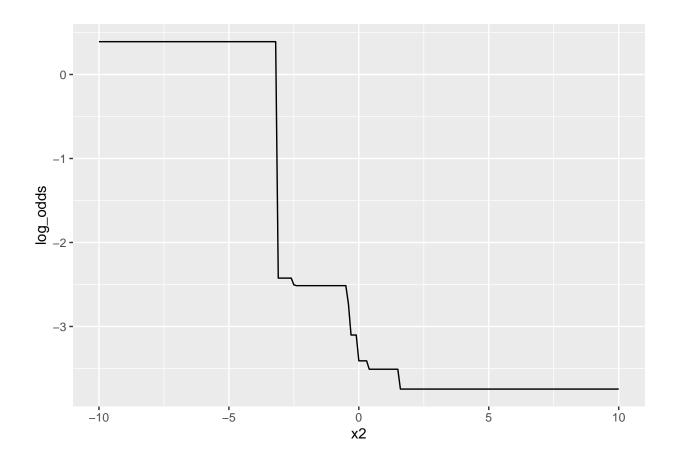
The interpolation of partial fitted values causes the relationship between a response and a predictor to appear "step-like".

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()</pre>
```



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=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	0.7091226
scar	0.7063029

```
map_dfr(list(gam=preds_gam, mono_gam=preds_mono_gam, pseudo=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	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)</pre>
```

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

```
est <- coef(mod_pseudo_scar)

est_df <- data.frame(Estimate=est)

knitr::kable(est_df)</pre>
```

	Estimate
constant	0.1050215
a	2.2854845
b	0.4915371

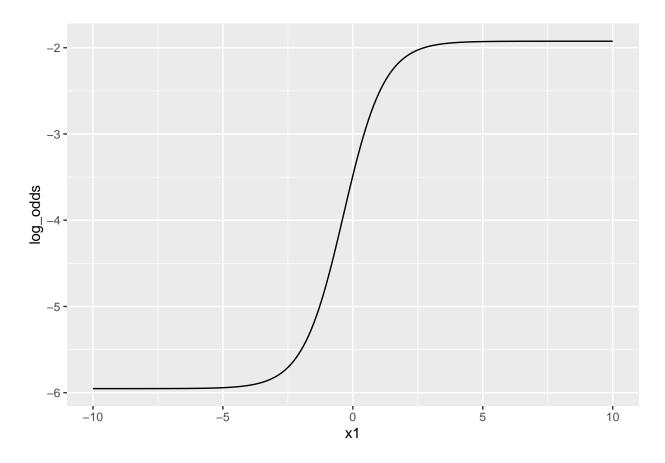
	Estimate
A1	-2.3602224
B1	-0.5978491
xmid1	-0.3596639
scal1	0.7826701
A2	0.3961789
B2	-1.7651710
xmid2	-0.2375986
scal2	0.1368247

Some plots.

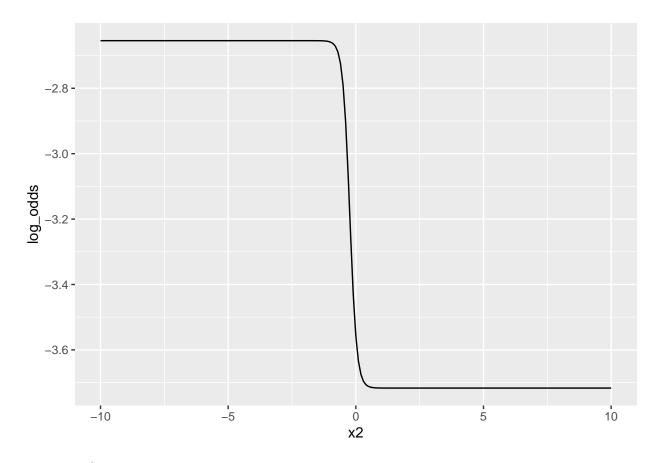
```
df_x1$log_odds <- predict(mod_pseudo_scar, newdata=df_x1)

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

ggplot(df_x1, aes(x=x1, y=log_odds)) + geom_line()</pre>
```



ggplot(df\_x2, aes(x=x2, y=log\_odds)) + geom\_line()



Test set performance

model	ROC-AUC
gam	0.7097935
$mono\_gam$	0.7098818
pseudo	0.7091226
scar	0.7063029
$pseudo\_scar$	0.7090304

model	Log Loss
gam	0.1908626
mono_gam	0.1909576
pseudo	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 (wiggliness). 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 (?SSfpl for equation) and implement in an Excel formula.