GameRank Vignette

# Introduction

This vignette describes how to perform wrapper-based feature selection using the GameRank package. In a feature selection scenario likely the following individual steps will be performed:

1. Feature screening - Evaluating missing data, outliers and how much information each feature contains about the outcome
2. Feature construction - If the data doesn’t comprise good features, try to construct better ones
3. Feature selection - Apply variable selection methods to determine best combination, here: we’ll use wrapper algorithms
4. Model evaluation - Check performance of final model on hold-out data
5. Model exploitation - Using the model [not discussed here]

Within this vignette, we’ll use the following toy dataset:

summary( toy\_data )

## USUBJID dys srv resp pi reg the\_normal the\_squared the\_cubed   
## Length:360 Min. : 0.00 Min. : 0.000 Mode :logical Min. :0.0001832 Min. :-8.605 Min. :-1.6818 Min. :0.0000045 Min. :-0.0001198   
## Class :character 1st Qu.: 0.00 1st Qu.: 0.000 FALSE:298 1st Qu.:0.0137107 1st Qu.:-4.276 1st Qu.: 0.3713 1st Qu.:0.1268884 1st Qu.: 0.0419764   
## Mode :character Median : 30.25 Median : 1.000 TRUE :62 Median :0.0820357 Median :-2.415 Median : 1.0130 Median :0.2384235 Median : 0.1240778   
## Mean : 52.43 Mean : 1.733 Mean :0.1826005 Mean :-2.645 Mean : 1.0217 Mean :0.2781601 Mean : 0.1955912   
## 3rd Qu.: 60.50 3rd Qu.: 2.000 3rd Qu.:0.2520040 3rd Qu.:-1.088 3rd Qu.: 1.7131 3rd Qu.:0.3761562 3rd Qu.: 0.2839108   
## Max. :393.25 Max. :13.000 Max. :0.9944938 Max. : 5.196 Max. : 4.9241 Max. :1.1915268 Max. : 1.0272744   
## the\_exped the\_multi the\_power rnd01 rnd02 rnd03 rnd04 rnd05   
## Min. :0.4424 Min. :-0.03415 Min. :-8.485e-04 Min. :-0.895823 Min. :-0.89975 Min. :-0.93381 Min. :-0.87071 Min. :-1.01945   
## 1st Qu.:0.9308 1st Qu.: 0.18432 1st Qu.: 0.000e+00 1st Qu.:-0.245148 1st Qu.:-0.24803 1st Qu.:-0.22878 1st Qu.:-0.24089 1st Qu.:-0.21842   
## Median :1.0956 Median : 0.29742 Median : 1.045e-05 Median :-0.003956 Median : 0.01516 Median : 0.01009 Median : 0.01157 Median : 0.01399   
## Mean :1.1100 Mean : 0.39765 Mean : 1.086e-03 Mean : 0.000000 Mean : 0.00000 Mean : 0.00000 Mean : 0.00000 Mean : 0.00000   
## 3rd Qu.:1.2624 3rd Qu.: 0.62537 3rd Qu.: 3.346e-04 3rd Qu.: 0.222739 3rd Qu.: 0.23427 3rd Qu.: 0.23572 3rd Qu.: 0.21876 3rd Qu.: 0.21718   
## Max. :1.9547 Max. : 1.24000 Max. : 5.241e-02 Max. : 1.059025 Max. : 1.03332 Max. : 0.87338 Max. : 0.99214 Max. : 0.96611   
## rnd06 rnd07 rnd08 rnd09 rnd10 rnd11 rnd12 rnd13   
## Min. :-1.023543 Min. :-0.74406 Min. :-0.725357 Min. :-0.91298 Min. :-0.834911 Min. :-0.84161 Min. :-0.724573 Min. :-0.871357   
## 1st Qu.:-0.197988 1st Qu.:-0.21869 1st Qu.:-0.210077 1st Qu.:-0.18879 1st Qu.:-0.179982 1st Qu.:-0.18619 1st Qu.:-0.177177 1st Qu.:-0.180345   
## Median :-0.009801 Median :-0.01081 Median :-0.001269 Median : 0.03393 Median :-0.004205 Median : 0.01189 Median :-0.004727 Median : 0.003534   
## Mean : 0.000000 Mean : 0.00000 Mean : 0.000000 Mean : 0.00000 Mean : 0.000000 Mean : 0.00000 Mean : 0.000000 Mean : 0.000000   
## 3rd Qu.: 0.192261 3rd Qu.: 0.20511 3rd Qu.: 0.187060 3rd Qu.: 0.20128 3rd Qu.: 0.191714 3rd Qu.: 0.19780 3rd Qu.: 0.191943 3rd Qu.: 0.197726   
## Max. : 1.024342 Max. : 0.79706 Max. : 0.853221 Max. : 0.85610 Max. : 0.767039 Max. : 0.65062 Max. : 0.674054 Max. : 0.853855   
## rnd14 rnd15 rnd16 rnd17 rnd18 rnd19 rnd20   
## Min. :-0.725219 Min. :-0.778140 Min. :-0.66952 Min. :-0.58989 Min. :-0.741684 Min. :-0.60174 Min. :-0.6009688   
## 1st Qu.:-0.176727 1st Qu.:-0.172492 1st Qu.:-0.18740 1st Qu.:-0.18795 1st Qu.:-0.174414 1st Qu.:-0.15839 1st Qu.:-0.1639815   
## Median :-0.007533 Median : 0.006181 Median :-0.00934 Median :-0.01686 Median :-0.003821 Median :-0.01282 Median : 0.0005244   
## Mean : 0.000000 Mean : 0.000000 Mean : 0.00000 Mean : 0.00000 Mean : 0.000000 Mean : 0.00000 Mean : 0.0000000   
## 3rd Qu.: 0.185752 3rd Qu.: 0.185962 3rd Qu.: 0.19247 3rd Qu.: 0.16418 3rd Qu.: 0.176406 3rd Qu.: 0.14829 3rd Qu.: 0.1565510   
## Max. : 0.755752 Max. : 0.733144 Max. : 0.63413 Max. : 0.62369 Max. : 0.770763 Max. : 0.73547 Max. : 0.5820029

vars <- grep( "the\_|rnd", colnames(toy\_data), value=TRUE )  
resp <- "resp"

# 1. Feature screening

Let’s start with variable screening. The goal is to check for missing data, outliers and evaluate how much information each variable bears about the response variable.

GameRank provides a one-stop function for that: check\_variables function.

vck <- check\_variables( toy\_data, resp, vars )

## Evaluating variable resp   
## Evaluating variable the\_normal   
## Evaluating variable the\_squared   
## Evaluating variable the\_cubed   
## Evaluating variable the\_exped   
## Evaluating variable the\_multi   
## Evaluating variable the\_power

## Warning in KL.plugin(freqs2d, freqs.null, unit = unit): Vanishing value(s) in argument freqs2!

## Evaluating variable rnd01   
## Evaluating variable rnd02   
## Evaluating variable rnd03   
## Evaluating variable rnd04   
## Evaluating variable rnd05   
## Evaluating variable rnd06   
## Evaluating variable rnd07   
## Evaluating variable rnd08   
## Evaluating variable rnd09   
## Evaluating variable rnd10   
## Evaluating variable rnd11   
## Evaluating variable rnd12   
## Evaluating variable rnd13   
## Evaluating variable rnd14   
## Evaluating variable rnd15   
## Evaluating variable rnd16   
## Evaluating variable rnd17   
## Evaluating variable rnd18   
## Evaluating variable rnd19   
## Evaluating variable rnd20

vck %>% summary

## variable N n nmiss p check\_missing type entropy mutual\_information check\_entropy  
## Length:27 Min. :360 Min. :360 Min. :0 Min. :100 Drop : 0 Entropy not done: 0 Min. :0.5406 Min. :0.002429 Entropy too low: 0   
## Class :character 1st Qu.:360 1st Qu.:360 1st Qu.:0 1st Qu.:100 Bad : 0 real :26 1st Qu.:1.2203 1st Qu.:0.003472 Entropy ok :27   
## Mode :character Median :360 Median :360 Median :0 Median :100 Try : 0 integer : 0 Median :1.3699 Median :0.005137   
## Mean :360 Mean :360 Mean :0 Mean :100 Good : 0 categorical : 0 Mean :1.3168 Mean :0.015715   
## 3rd Qu.:360 3rd Qu.:360 3rd Qu.:0 3rd Qu.:100 Perfect:27 binary : 1 3rd Qu.:1.5352 3rd Qu.:0.008757   
## Max. :360 Max. :360 Max. :0 Max. :100 Max. :2.1482 Max. :0.216255   
## NA's :1   
## is\_response rot.nmin rot.nmax rot.p rng\_sd   
## Mode :logical Min. :0.0000 Min. : 0.000 Min. : 0.0000 Min. : 4.721   
## FALSE:26 1st Qu.:0.0000 1st Qu.: 0.000 1st Qu.: 0.2778 1st Qu.: 5.217   
## TRUE :1 Median :0.0000 Median : 1.000 Median : 0.5556 Median : 5.594   
## Mean :0.8077 Mean : 4.269 Mean : 1.4103 Mean : 5.789   
## 3rd Qu.:1.7500 3rd Qu.: 2.000 3rd Qu.: 1.0417 3rd Qu.: 6.126   
## Max. :3.0000 Max. :57.000 Max. :16.6667 Max. :10.842   
## NA's :1 NA's :1 NA's :1 NA's :1

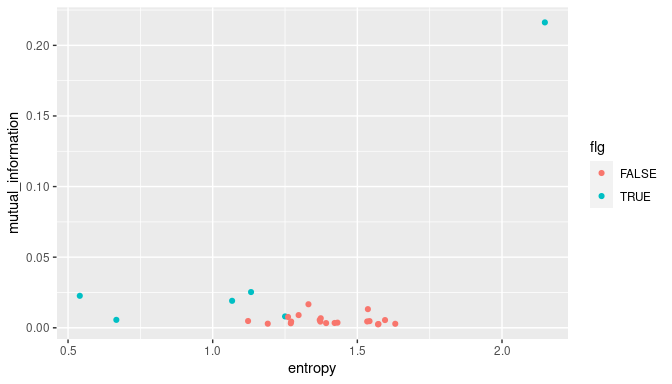
vck %>%   
 filter( !is\_response ) %>%   
 arrange( desc(entropy) )

## # A tibble: 26 × 15  
## variable N n nmiss p check\_missing type entropy mutual\_information check\_entropy is\_response rot.nmin rot.nmax rot.p rng\_sd  
## <chr> <int> <int> <int> <dbl> <fct> <fct> <dbl> <dbl> <fct> <lgl> <int> <int> <dbl> <dbl>  
## 1 the\_normal 360 360 0 100 Perfect real 2.15 0.216 Entropy ok FALSE 2 2 1.11 6.21  
## 2 rnd01 360 360 0 100 Perfect real 1.63 0.00284 Entropy ok FALSE 0 3 0.833 5.54  
## 3 rnd03 360 360 0 100 Perfect real 1.60 0.00547 Entropy ok FALSE 1 0 0.278 5.39  
## 4 rnd05 360 360 0 100 Perfect real 1.57 0.00267 Entropy ok FALSE 2 2 1.11 6.11  
## 5 rnd07 360 360 0 100 Perfect real 1.57 0.00243 Entropy ok FALSE 0 0 0 5.02  
## 6 rnd04 360 360 0 100 Perfect real 1.54 0.00473 Entropy ok FALSE 0 1 0.278 5.61  
## 7 rnd02 360 360 0 100 Perfect real 1.54 0.0132 Entropy ok FALSE 0 1 0.278 5.61  
## 8 rnd06 360 360 0 100 Perfect real 1.53 0.00448 Entropy ok FALSE 3 3 1.67 6.56  
## 9 rnd10 360 360 0 100 Perfect real 1.43 0.00364 Entropy ok FALSE 2 1 0.833 5.58  
## 10 rnd08 360 360 0 100 Perfect real 1.42 0.00342 Entropy ok FALSE 0 1 0.278 5.39  
## # … with 16 more rows

A look into the variable entropy and mutual information with respect to the response is a good idea to identify variables that are constant or contain low information

vck %>%   
 mutate( flg = grepl( "the\_", variable )) %>%  
 ggplot(aes(x=entropy, y=mutual\_information, color=flg ) ) +  
 geom\_point()

## Warning: Removed 1 rows containing missing values (geom\_point).



vck %>%   
 arrange( desc(mutual\_information), desc(entropy) )

## # A tibble: 27 × 15  
## variable N n nmiss p check\_missing type entropy mutual\_information check\_entropy is\_response rot.nmin rot.nmax rot.p rng\_sd  
## <chr> <int> <int> <int> <dbl> <fct> <fct> <dbl> <dbl> <fct> <lgl> <int> <int> <dbl> <dbl>  
## 1 the\_normal 360 360 0 100 Perfect real 2.15 0.216 Entropy ok FALSE 2 2 1.11 6.21  
## 2 the\_power 360 360 0 100 Perfect real 1.13 0.0253 Entropy ok FALSE 3 57 16.7 10.8   
## 3 the\_cubed 360 360 0 100 Perfect real 0.541 0.0227 Entropy ok FALSE 0 17 4.72 5.09  
## 4 the\_multi 360 360 0 100 Perfect real 1.07 0.0191 Entropy ok FALSE 0 0 0 4.72  
## 5 rnd14 360 360 0 100 Perfect real 1.33 0.0167 Entropy ok FALSE 1 3 1.11 5.51  
## 6 rnd02 360 360 0 100 Perfect real 1.54 0.0132 Entropy ok FALSE 0 1 0.278 5.61  
## 7 rnd15 360 360 0 100 Perfect real 1.30 0.00899 Entropy ok FALSE 2 1 0.833 5.72  
## 8 the\_exped 360 360 0 100 Perfect real 1.25 0.00805 Entropy ok FALSE 0 2 0.556 6.20  
## 9 rnd16 360 360 0 100 Perfect real 1.26 0.00766 Entropy ok FALSE 0 0 0 5.00  
## 10 rnd12 360 360 0 100 Perfect real 1.37 0.00675 Entropy ok FALSE 0 0 0 5.11  
## # … with 17 more rows

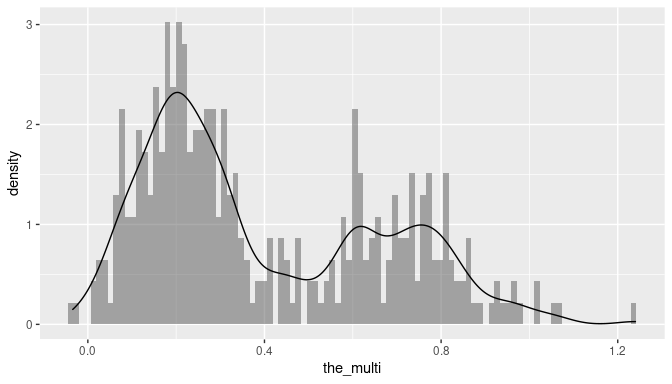
Sometimes variable distributions may be multi-modal. GameRank provides a function for this task: check\_multimodality.

GameRank determines multi-modal variables as follows: Let k be the number of mixture components ranging from 1 to kmax. The algorithm fits first m\_fits GMM models with k components using flexmix. Only models that converge are retained. For each k the minimum AIC is determined together with the number of converging models. All k with less than min\_fits\_converged models are removed. The k for which the minimum AIC is attained is then chosen. In case of ties for this AIC the minimum number of components are chosen. The first model obtaining these k and AIC is then used to determine cut-points if it has more than one component.

Cut-points are determined by the standard root finding algorithm, determining the points where the adjacent component distributions, scaled by their priors, are equal.

The chance for detecting multi-modal distributions depends on the available data and hence distributions reported may not be multi-modal or multi-modal distributions may go undetected. Thus a additional visual review of distributions is certainly a good idea, and the results from multi\_modal may be used as a starting point.

toy\_data %>%  
 ggplot( aes( x=the\_multi, y=..density.. ) ) +  
 geom\_histogram( bins = 100, alpha=0.5 ) +  
 geom\_density( bw = "ucv" )



mumo <- check\_multimodality( dat = toy\_data, resp = resp, vars = vars[1:9],n\_comp = 3, m\_fits = 25, min\_fits\_converged = 20 )

## Processing the\_normal   
## Processing the\_squared   
## Variable the\_squared is multi-modal with 3 Normal components. Determining cut-points.   
## Processing the\_cubed   
## Variable the\_cubed is multi-modal with 3 Normal components. Determining cut-points.   
## Processing the\_exped   
## Processing the\_multi   
## Variable the\_multi is multi-modal with 2 Normal components. Determining cut-points.   
## Processing the\_power   
## Variable the\_power is multi-modal with 3 Normal components. Determining cut-points.   
## Processing rnd01   
## Processing rnd02   
## Processing rnd03

mumo\_vars <- mumo$transforms %>% keep( function(x) !is.null( pluck( x, "transformed\_var" ) ) ) %>% map( "transformed\_var" ) %>% as.character  
mumo$data[,mumo\_vars]

## # A tibble: 360 × 4  
## the\_squared\_grp the\_cubed\_grp the\_multi\_grp the\_power\_grp  
## <chr> <chr> <chr> <chr>   
## 1 group[2] group[2] group[1] group[1]   
## 2 group[1] group[2] group[2] group[1]   
## 3 group[1] group[1] group[2] group[2]   
## 4 group[2] group[3] group[2] group[2]   
## 5 group[2] group[3] group[1] group[1]   
## 6 group[1] group[3] group[2] group[1]   
## 7 group[1] group[3] group[1] group[1]   
## 8 group[2] group[3] group[1] group[1]   
## 9 group[1] group[2] group[1] group[2]   
## 10 group[2] group[2] group[1] group[1]   
## # … with 350 more rows

mumo$transforms$the\_multi$aic\_aggregate

## # A tibble: 2 × 3  
## k min\_aic sum\_converged  
## <int> <dbl> <int>  
## 1 1 81.6 25  
## 2 2 -80.1 25

mumo$transforms$the\_multi$best\_model

##   
## Call:  
## flexmix::flexmix(formula = stats::formula(sprintf("%s ~ 1", var)), data = dat[idx, ], k = k)  
##   
## Cluster sizes:  
## 1 2   
## 218 142   
##   
## convergence after 43 iterations

flexmix::parameters(mumo$transforms$the\_multi$best\_model)

## Comp.1 Comp.2  
## coef.(Intercept) 0.2033608 0.6895610  
## sigma 0.0945754 0.1627811

flexmix::prior(mumo$transforms$the\_multi$best\_model)

## [1] 0.6004198 0.3995802

pcuts <- mumo$transforms$the\_multi$cut\_points  
mumo$transforms$the\_multi$transformed\_var

## [1] "the\_multi\_grp"

Lets create categorical variable for the\_multi and add it to the set:

toy\_data <- toy\_data %>% bind\_cols( mumo$data[,mumo$transforms$the\_multi$transformed\_var] )  
vars <- c(vars, mumo$transforms$the\_multi$transformed\_var )

# 2. Feature construction

Another task may be to see if standard transforms improve Normality of the features. The one-stop function in GameRank tries square root, cube root, log and z-score transformations. Those that increase the Shapiro-Wilk W-statistics are retrained and added to the dataset.

smp <- simple\_transforms( toy\_data, vars = vars )

## Adding simple transformed variables if they are better by Shapiro-Wilk statistic W (larger is better)   
## Evaluating the\_normal with W = 0.9955

## Warning in FUN(X[[i]], ...): NaNs produced  
  
## Warning in FUN(X[[i]], ...): NaNs produced

## Evaluating the\_squared with W = 0.9153   
## Evaluating the\_cubed with W = 0.8447

## Warning in FUN(X[[i]], ...): NaNs produced  
  
## Warning in FUN(X[[i]], ...): NaNs produced

## Evaluating the\_exped with W = 0.9854   
## Evaluating the\_multi with W = 0.9183

## Warning in FUN(X[[i]], ...): NaNs produced  
  
## Warning in FUN(X[[i]], ...): NaNs produced

## Evaluating the\_power with W = 0.2215

## Warning in FUN(X[[i]], ...): NaNs produced  
  
## Warning in FUN(X[[i]], ...): NaNs produced

## Evaluating rnd01 with W = 0.9968

## Warning in FUN(X[[i]], ...): NaNs produced  
  
## Warning in FUN(X[[i]], ...): NaNs produced

## Evaluating rnd02 with W = 0.9959

## Warning in FUN(X[[i]], ...): NaNs produced  
  
## Warning in FUN(X[[i]], ...): NaNs produced

## Evaluating rnd03 with W = 0.9959

## Warning in FUN(X[[i]], ...): NaNs produced  
  
## Warning in FUN(X[[i]], ...): NaNs produced

## Evaluating rnd04 with W = 0.9965

## Warning in FUN(X[[i]], ...): NaNs produced  
  
## Warning in FUN(X[[i]], ...): NaNs produced

## Evaluating rnd05 with W = 0.9974

## Warning in FUN(X[[i]], ...): NaNs produced  
  
## Warning in FUN(X[[i]], ...): NaNs produced

## Evaluating rnd06 with W = 0.9970

## Warning in FUN(X[[i]], ...): NaNs produced  
  
## Warning in FUN(X[[i]], ...): NaNs produced

## Evaluating rnd07 with W = 0.9934

## Warning in FUN(X[[i]], ...): NaNs produced  
  
## Warning in FUN(X[[i]], ...): NaNs produced

## Evaluating rnd08 with W = 0.9960

## Warning in FUN(X[[i]], ...): NaNs produced  
  
## Warning in FUN(X[[i]], ...): NaNs produced

## Evaluating rnd09 with W = 0.9937

## Warning in FUN(X[[i]], ...): NaNs produced  
  
## Warning in FUN(X[[i]], ...): NaNs produced

## Evaluating rnd10 with W = 0.9980

## Warning in FUN(X[[i]], ...): NaNs produced  
  
## Warning in FUN(X[[i]], ...): NaNs produced

## Evaluating rnd11 with W = 0.9919

## Warning in FUN(X[[i]], ...): NaNs produced  
  
## Warning in FUN(X[[i]], ...): NaNs produced

## Evaluating rnd12 with W = 0.9968

## Warning in FUN(X[[i]], ...): NaNs produced  
  
## Warning in FUN(X[[i]], ...): NaNs produced

## Evaluating rnd13 with W = 0.9985

## Warning in FUN(X[[i]], ...): NaNs produced  
  
## Warning in FUN(X[[i]], ...): NaNs produced

## Evaluating rnd14 with W = 0.9975

## Warning in FUN(X[[i]], ...): NaNs produced  
  
## Warning in FUN(X[[i]], ...): NaNs produced

## Evaluating rnd15 with W = 0.9971

## Warning in FUN(X[[i]], ...): NaNs produced  
  
## Warning in FUN(X[[i]], ...): NaNs produced

## Evaluating rnd16 with W = 0.9939

## Warning in FUN(X[[i]], ...): NaNs produced  
  
## Warning in FUN(X[[i]], ...): NaNs produced

## Evaluating rnd17 with W = 0.9919

## Warning in FUN(X[[i]], ...): NaNs produced  
  
## Warning in FUN(X[[i]], ...): NaNs produced

## Evaluating rnd18 with W = 0.9982

## Warning in FUN(X[[i]], ...): NaNs produced  
  
## Warning in FUN(X[[i]], ...): NaNs produced

## Evaluating rnd19 with W = 0.9935

## Warning in FUN(X[[i]], ...): NaNs produced  
  
## Warning in FUN(X[[i]], ...): NaNs produced

## Evaluating rnd20 with W = 0.9957

## Warning in FUN(X[[i]], ...): NaNs produced  
  
## Warning in FUN(X[[i]], ...): NaNs produced

tfs <- smp$transformations %>% Reduce( bind\_rows, ., NULL )  
tfs %>% group\_by( variable ) %>% filter( max(W)==W )

## # A tibble: 26 × 5  
## # Groups: variable [26]  
## variable transformed\_var term W transform  
## <chr> <chr> <chr> <dbl> <chr>   
## 1 the\_normal "" "( the\_normal )" 0.996 identity   
## 2 the\_squared "the\_squared\_sqrt" "sqrt( the\_squared )" 0.994 sqrt   
## 3 the\_cubed "the\_cubed\_cubert" "( the\_cubed )^(1/3)" 0.991 cube root  
## 4 the\_exped "the\_exped\_cubert" "( the\_exped )^(1/3)" 0.996 cube root  
## 5 the\_multi "the\_multi\_cubert" "( the\_multi )^(1/3)" 0.968 cube root  
## 6 the\_power "the\_power\_log" " log( the\_power ) " 0.849 log   
## 7 rnd01 "" "( rnd01 )" 0.997 identity   
## 8 rnd02 "" "( rnd02 )" 0.996 identity   
## 9 rnd03 "" "( rnd03 )" 0.996 identity   
## 10 rnd04 "" "( rnd04 )" 0.996 identity   
## # … with 16 more rows

tfs %>% pull( transform ) %>% table

## .  
## cube root identity log sqrt zscore   
## 5 26 4 5 3

Lets add some transformed variables.

svars <- tfs %>% group\_by( variable ) %>% filter( max(W)==W ) %>% filter( "identity"!=transform )  
svars

## # A tibble: 5 × 5  
## # Groups: variable [5]  
## variable transformed\_var term W transform  
## <chr> <chr> <chr> <dbl> <chr>   
## 1 the\_squared the\_squared\_sqrt "sqrt( the\_squared )" 0.994 sqrt   
## 2 the\_cubed the\_cubed\_cubert "( the\_cubed )^(1/3)" 0.991 cube root  
## 3 the\_exped the\_exped\_cubert "( the\_exped )^(1/3)" 0.996 cube root  
## 4 the\_multi the\_multi\_cubert "( the\_multi )^(1/3)" 0.968 cube root  
## 5 the\_power the\_power\_log " log( the\_power ) " 0.849 log

toy\_data <- toy\_data %>% bind\_cols( smp$data[,svars$transformed\_var] )  
vars <- c(vars, svars$transformed\_var )

Another feature construction approach that can be tried in a second round is searching for Power-Transformations via the Box-Cox transformation. However we will skip this here. Please take a look at the example code for box\_cox\_normal and box\_cox\_binomial.

# 3. Feature selection

Now, let’s run two feature selection algorithms, the bidirectional search that applies forward and backward selection and the GameRank algorithm. First, we’ll split the dataset into thirds: one for training the model, one for validating it and one final hold-out dataset.

rr <- rep\_len( c(1L,2L,3L), length.out = nrow(toy\_data) )   
rr <- rr[ order( runif( length(rr) ) )]  
df\_test <- toy\_data[which(3==rr),]  
df\_sel <- toy\_data[which(rr %in% c(1L,2L)),]  
ds <- prepare\_splits( ds = 3L, dat = df\_sel, resp = resp, vars = vars, fn\_train = fn\_train\_binomial, fn\_eval = fn\_eval\_binomial\_auroc )

## Generating 3 splits

## Warning: glm.fit: algorithm did not converge

## Warning: glm.fit: fitted probabilities numerically 0 or 1 occurred

## Warning: glm.fit: algorithm did not converge

## Warning: glm.fit: fitted probabilities numerically 0 or 1 occurred

## Warning: glm.fit: algorithm did not converge

## Warning: glm.fit: fitted probabilities numerically 0 or 1 occurred

Wrapper selection algorithms are slow combinatorial searches that are not guaranteed to find more than a local optimum. Their performance also depends - in some cases - on the ordering of input variables. Therefore it is a good idea to rerun each algorithm with varying ordering of features to obtain a varying selections that can be used to choose from.

Here we’ll sort variables by their the mutual information with regards to the response:

vck <- check\_variables( df\_sel, resp, vars )

## Evaluating variable resp   
## Evaluating variable the\_normal   
## Evaluating variable the\_squared   
## Evaluating variable the\_cubed   
## Evaluating variable the\_exped   
## Evaluating variable the\_multi   
## Evaluating variable the\_power

## Warning in KL.plugin(freqs2d, freqs.null, unit = unit): Vanishing value(s) in argument freqs2!

## Evaluating variable rnd01   
## Evaluating variable rnd02   
## Evaluating variable rnd03   
## Evaluating variable rnd04   
## Evaluating variable rnd05   
## Evaluating variable rnd06   
## Evaluating variable rnd07   
## Evaluating variable rnd08   
## Evaluating variable rnd09   
## Evaluating variable rnd10   
## Evaluating variable rnd11   
## Evaluating variable rnd12   
## Evaluating variable rnd13   
## Evaluating variable rnd14   
## Evaluating variable rnd15   
## Evaluating variable rnd16   
## Evaluating variable rnd17   
## Evaluating variable rnd18   
## Evaluating variable rnd19   
## Evaluating variable rnd20   
## Evaluating variable the\_multi\_grp   
## Evaluating variable the\_squared\_sqrt   
## Evaluating variable the\_cubed\_cubert   
## Evaluating variable the\_exped\_cubert

## Warning in KL.plugin(freqs2d, freqs.null, unit = unit): Vanishing value(s) in argument freqs2!

## Evaluating variable the\_multi\_cubert   
## Evaluating variable the\_power\_log

## Warning in KL.plugin(freqs2d, freqs.null, unit = unit): Vanishing value(s) in argument freqs2!

vars <- vck %>% filter( !is\_response) %>% arrange( desc(mutual\_information) ) %>% pull( variable )

Let’s run the first wrapper: bidirectional search, an algorithm that performs a forward and backward selection step per iteration and ensures that it converges to the same partition by constraining the search variables for the forward and backward steps.

bds <- bidirectional( dat = df\_sel, resp = resp, vars = vars, fn\_train = fn\_train\_binomial, fn\_eval = fn\_eval\_binomial\_auroc, m = 6L, ds = ds, maximize = TRUE )

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## Warning in max(.data$mean\_validation, na.rm = TRUE): no non-missing arguments to max; returning -Inf

bds$variable\_selections

## [[1]]  
## [1] "1" "rnd03" "rnd20" "the\_cubed\_cubert" "the\_exped\_cubert" "the\_multi\_grp" "the\_normal" "the\_squared"   
##   
## [[2]]  
## [1] "1" "rnd03" "rnd20" "the\_cubed\_cubert" "the\_exped\_cubert" "the\_multi" "the\_normal" "the\_squared"

bds$agg\_results %>% arrange( desc(mean\_validation) )

## # A tibble: 399 × 10  
## ch\_selection added selection m mean\_train mean\_validation mean\_bias opt k removed  
## <chr> <chr> <list> <int> <dbl> <dbl> <dbl> <lgl> <dbl> <chr>   
## 1 1,rnd03,rnd20,the\_cubed\_cubert,the\_exped\_cubert,the\_multi\_grp,the\_normal,the\_squared the\_mul… <chr [8]> 8 NaN 0.960 NaN TRUE 7 <NA>   
## 2 1,rnd03,rnd20,the\_cubed\_cubert,the\_exped\_cubert,the\_multi,the\_normal,the\_squared the\_mul… <chr [8]> 8 NaN 0.960 NaN TRUE 7 <NA>   
## 3 1,rnd03,rnd20,the\_cubed\_cubert,the\_exped\_cubert,the\_normal,the\_squared rnd03 <chr [7]> 7 NaN 0.958 NaN TRUE 6 <NA>   
## 4 1,rnd20,the\_cubed\_cubert,the\_exped\_cubert,the\_multi,the\_normal,the\_squared the\_mul… <chr [7]> 7 NaN 0.958 NaN TRUE 6 <NA>   
## 5 1,rnd03,rnd08,rnd20,the\_cubed\_cubert,the\_exped\_cubert,the\_normal,the\_squared rnd08 <chr [8]> 8 NaN 0.958 NaN FALSE 7 <NA>   
## 6 1,rnd03,rnd14,rnd20,the\_cubed\_cubert,the\_exped\_cubert,the\_normal,the\_squared rnd14 <chr [8]> 8 NaN 0.958 NaN FALSE 7 <NA>   
## 7 1,rnd03,rnd18,rnd20,the\_cubed\_cubert,the\_exped\_cubert,the\_normal,the\_squared rnd18 <chr [8]> 8 NaN 0.958 NaN FALSE 7 <NA>   
## 8 1,rnd08,rnd20,the\_cubed\_cubert,the\_exped\_cubert,the\_normal,the\_squared rnd08 <chr [7]> 7 NaN 0.957 NaN FALSE 6 <NA>   
## 9 1,rnd03,rnd15,rnd20,the\_cubed\_cubert,the\_exped\_cubert,the\_normal,the\_squared rnd15 <chr [8]> 8 NaN 0.957 NaN FALSE 7 <NA>   
## 10 1,rnd03,rnd19,rnd20,the\_cubed\_cubert,the\_exped\_cubert,the\_normal,the\_squared rnd19 <chr [8]> 8 NaN 0.957 NaN FALSE 7 <NA>   
## # … with 389 more rows

bds$agg\_results %>% arrange( desc(mean\_validation) ) %>% filter( opt )

## # A tibble: 10 × 10  
## ch\_selection added selection m mean\_train mean\_validation mean\_bias opt k removed  
## <chr> <chr> <list> <int> <dbl> <dbl> <dbl> <lgl> <dbl> <chr>   
## 1 1,rnd03,rnd20,the\_cubed\_cubert,the\_exped\_cubert,the\_multi\_grp,the\_normal,the\_squared the\_mul… <chr [8]> 8 NaN 0.960 NaN TRUE 7 <NA>   
## 2 1,rnd03,rnd20,the\_cubed\_cubert,the\_exped\_cubert,the\_multi,the\_normal,the\_squared the\_mul… <chr [8]> 8 NaN 0.960 NaN TRUE 7 <NA>   
## 3 1,rnd03,rnd20,the\_cubed\_cubert,the\_exped\_cubert,the\_normal,the\_squared rnd03 <chr [7]> 7 NaN 0.958 NaN TRUE 6 <NA>   
## 4 1,rnd20,the\_cubed\_cubert,the\_exped\_cubert,the\_multi,the\_normal,the\_squared the\_mul… <chr [7]> 7 NaN 0.958 NaN TRUE 6 <NA>   
## 5 1,rnd20,the\_cubed\_cubert,the\_exped\_cubert,the\_normal,the\_squared rnd20 <chr [6]> 6 NaN 0.953 NaN TRUE 5 <NA>   
## 6 1,the\_cubed\_cubert,the\_exped\_cubert,the\_normal,the\_squared the\_exp… <chr [5]> 5 NaN 0.949 NaN TRUE 4 <NA>   
## 7 1,the\_cubed\_cubert,the\_exped,the\_normal,the\_squared the\_exp… <chr [5]> 5 NaN 0.949 NaN TRUE 4 <NA>   
## 8 1,the\_cubed\_cubert,the\_normal,the\_squared the\_cub… <chr [4]> 4 NaN 0.934 NaN TRUE 3 <NA>   
## 9 1,the\_normal,the\_squared the\_squ… <chr [3]> 3 0.878 0.922 0.0447 TRUE 2 <NA>   
## 10 1,the\_normal the\_nor… <chr [2]> 2 0.877 0.902 0.0299 TRUE 1 <NA>

Now let’s run GameRank. Since GameRank doesn’t use a validation set, the dsi parameter receives an index vector of 1s and 2s that is then repeated to the length of the dataset and thereby defines the relative proportions of training to validation split per round. In small sample feature selection scenarios it contains just 2s such that all data are put into the validation split where the fn\_eval function performs a bootstrap or cross-validation (see small sample example code for details).

gmr <- game\_rank( dat = df\_sel, resp = resp, vars = vars, fn\_train = fn\_train\_binomial, fn\_eval = fn\_eval\_binomial\_auroc, m = 6L, dsi = c(1L,2L), maximize = TRUE,   
 team\_size = 4L, rounds = 10L, min\_matches\_per\_var = 7L )

## Comparing variable selections (# matches 45)---   
## Iteration 1 of 45 -- (+) : (-) scored 0 : 10   
## Iteration 2 of 45 -- (+) : (-) scored 2 : 8   
## Iteration 3 of 45 -- (+) : (-) scored 1 : 0

## Warning: glm.fit: fitted probabilities numerically 0 or 1 occurred

## Iteration 4 of 45 -- (+) : (-) scored 10 : 0   
## Iteration 5 of 45 -- (+) : (-) scored 2 : 8   
## Iteration 6 of 45 -- (+) : (-) scored 2 : 0   
## Iteration 7 of 45 -- (+) : (-) scored 10 : 0   
## Iteration 8 of 45 -- (+) : (-) scored 2 : 8   
## Iteration 9 of 45 -- (+) : (-) scored 0 : 10   
## Iteration 10 of 45 -- (+) : (-) scored 0 : 10   
## Iteration 11 of 45 -- (+) : (-) scored 10 : 0

## Warning: glm.fit: fitted probabilities numerically 0 or 1 occurred

## Iteration 12 of 45 -- (+) : (-) scored 10 : 0   
## Iteration 13 of 45 -- (+) : (-) scored 0 : 10   
## Iteration 14 of 45 -- (+) : (-) scored 4 : 0   
## Iteration 15 of 45 -- (+) : (-) scored 3 : 7   
## Iteration 16 of 45 -- (+) : (-) scored 10 : 0   
## Iteration 17 of 45 -- (+) : (-) scored 3 : 7   
## Iteration 18 of 45 -- (+) : (-) scored 10 : 0   
## Iteration 19 of 45 -- (+) : (-) scored 10 : 0   
## Iteration 20 of 45 -- (+) : (-) scored 0 : 10   
## Iteration 21 of 45 -- (+) : (-) scored 10 : 0   
## Iteration 22 of 45 -- (+) : (-) scored 10 : 0   
## Iteration 23 of 45 -- (+) : (-) scored 10 : 0   
## Iteration 24 of 45 -- (+) : (-) scored 1 : 9   
## Iteration 25 of 45 -- (+) : (-) scored 0 : 10   
## Iteration 26 of 45 -- (+) : (-) scored 0 : 10   
## Iteration 27 of 45 -- (+) : (-) scored 4 : 0   
## Iteration 28 of 45 -- (+) : (-) scored 10 : 0   
## Iteration 29 of 45 -- (+) : (-) scored 0 : 10   
## Iteration 30 of 45 -- (+) : (-) scored 7 : 3   
## Iteration 31 of 45 -- (+) : (-) scored 8 : 2   
## Iteration 32 of 45 -- (+) : (-) scored 0 : 10   
## Iteration 33 of 45 -- (+) : (-) scored 10 : 0   
## Iteration 34 of 45 -- (+) : (-) scored 9 : 1

## Warning: glm.fit: fitted probabilities numerically 0 or 1 occurred

## Iteration 35 of 45 -- (+) : (-) scored 10 : 0   
## Iteration 36 of 45 -- (+) : (-) scored 0 : 10   
## Iteration 37 of 45 -- (+) : (-) scored 10 : 0

## Warning: glm.fit: fitted probabilities numerically 0 or 1 occurred

## Iteration 38 of 45 -- (+) : (-) scored 7 : 3   
## Iteration 39 of 45 -- (+) : (-) scored 10 : 0

## Warning: glm.fit: fitted probabilities numerically 0 or 1 occurred

## Iteration 40 of 45 -- (+) : (-) scored 4 : 6   
## Iteration 41 of 45 -- (+) : (-) scored 1 : 9   
## Iteration 42 of 45 -- (+) : (-) scored 4 : 5   
## Iteration 43 of 45 -- (+) : (-) scored 0 : 10   
## Iteration 44 of 45 -- (+) : (-) scored 10 : 0   
## Iteration 45 of 45 -- (+) : (-) scored 8 : 2   
## Optimizing maximum likelihood   
## Calculating score vector   
## Calculating Hessian matrix   
## Compiling results

gmr$variable\_ranking %>% as.data.frame

## variable vs vs.var selected  
## 1 the\_power\_log 6.867916e-16 252.488648 TRUE  
## 2 the\_multi\_cubert 6.803158e-16 2.802317 TRUE  
## 3 rnd15 5.560074e-16 245.071142 TRUE  
## 4 rnd02 4.337223e-16 952.071304 TRUE  
## 5 rnd01 4.141868e-16 360.234923 TRUE  
## 6 rnd16 3.802199e-16 23.488695 TRUE  
## 7 rnd08 3.610430e-16 81.163179 TRUE  
## 8 the\_squared\_sqrt 3.542573e-16 440.710263 TRUE  
## 9 the\_exped\_cubert 2.489840e-16 1441.862336 TRUE  
## 10 rnd03 2.452569e-16 199.587314 TRUE  
## 11 rnd13 2.094530e-16 13.428061 TRUE  
## 12 rnd11 2.068503e-16 7.947741 TRUE  
## 13 rnd12 2.061149e-16 259.567178 TRUE  
## 14 rnd17 1.699038e-16 956.335867 TRUE  
## 15 rnd19 1.324089e-16 25.163597 TRUE  
## 16 rnd05 1.293503e-16 13.952415 TRUE  
## 17 the\_multi 8.086849e-17 12333.102850 TRUE  
## 18 rnd10 5.839794e-17 98.452916 TRUE  
## 19 rnd20 3.417190e-18 7217.535738 TRUE  
## 20 rnd09 -2.602748e-18 7721.102787 FALSE  
## 21 the\_cubed -1.874344e-17 1065.912404 FALSE  
## 22 the\_squared -4.169608e-17 54.495151 FALSE  
## 23 the\_normal -4.812324e-17 253.482945 FALSE  
## 24 the\_power -6.343128e-17 474.751180 FALSE  
## 25 rnd14 -1.252464e-16 18.882880 FALSE  
## 26 rnd04 -1.703110e-16 1608.533173 FALSE  
## 27 rnd06 -1.850482e-16 1836.586078 FALSE  
## 28 the\_exped -2.541408e-16 13028.280449 FALSE  
## 29 the\_cubed\_cubert -2.545481e-16 1185.216294 FALSE  
## 30 rnd07 -3.319994e-16 97.245474 FALSE  
## 31 the\_multi\_grp -3.325039e-16 202.207919 FALSE  
## 32 rnd18 -4.185292e-16 12417.604048 FALSE

gmr$game\_rank\_selection

## [1] "the\_power\_log" "the\_multi\_cubert" "rnd15" "rnd02" "rnd01" "rnd16"

# 4. Model evaluation

Having obtained a potential variable selection, the model needs to assessed for calibration, that is whether it’s predictions correlate with the observed outcome. This may be easy for regression problems, for probability predictions or survival predictions it involves estimating the observed distribution.

bds\_fsel <- bds %>% purrr::pluck( "variable\_selections" ) %>% purrr::pluck( 1L)  
mod\_bds <- fn\_train\_binomial( dat = df\_sel, resp = resp, selection = bds\_fsel )  
mod\_bds

##   
## Call: stats::glm(formula = fo, family = stats::binomial, data = dat)  
##   
## Coefficients:  
## (Intercept) rnd03 rnd20 the\_cubed\_cubert the\_exped\_cubert the\_multi\_grpgroup[2] the\_normal   
## 1.3628 -0.4893 -2.2657 1.8288 -8.2253 1.6528 2.6690   
## the\_squared   
## -2.5303   
##   
## Degrees of Freedom: 236 Total (i.e. Null); 229 Residual  
## (3 observations deleted due to missingness)  
## Null Deviance: 201.9   
## Residual Deviance: 105.5 AIC: 121.5

gplot\_predictions\_binomial( dat = df\_sel, resp = resp, selection = bds\_fsel, mod = mod\_bds )

## `geom\_smooth()` using formula 'y ~ x'

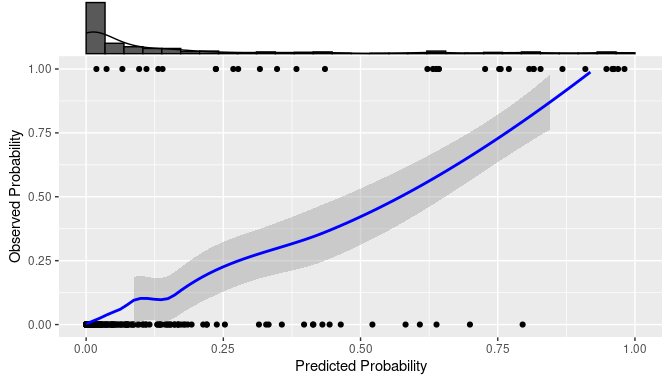
## Warning: Removed 3 rows containing non-finite values (stat\_smooth).

## `geom\_smooth()` using formula 'y ~ x'

## Warning: Removed 3 rows containing non-finite values (stat\_smooth).

## Warning: Removed 3 rows containing missing values (geom\_point).

## Warning: Removed 5 rows containing missing values (geom\_smooth).



gmr\_fsel <- gmr %>% purrr::pluck( "game\_rank\_selection" )   
mod\_gmr <- fn\_train\_binomial( dat = df\_sel, resp = resp, selection = gmr\_fsel )  
mod\_gmr

##   
## Call: stats::glm(formula = fo, family = stats::binomial, data = dat)  
##   
## Coefficients:  
## (Intercept) the\_power\_log the\_multi\_cubert rnd15 rnd02 rnd01 rnd16   
## -4.48511 0.03896 3.87955 -0.02675 0.19350 0.24416 -0.09275   
##   
## Degrees of Freedom: 177 Total (i.e. Null); 171 Residual  
## (62 observations deleted due to missingness)  
## Null Deviance: 129.2   
## Residual Deviance: 121.1 AIC: 135.1

gplot\_predictions\_binomial( dat = df\_sel, resp = resp, selection = bds\_fsel, mod = mod\_gmr )

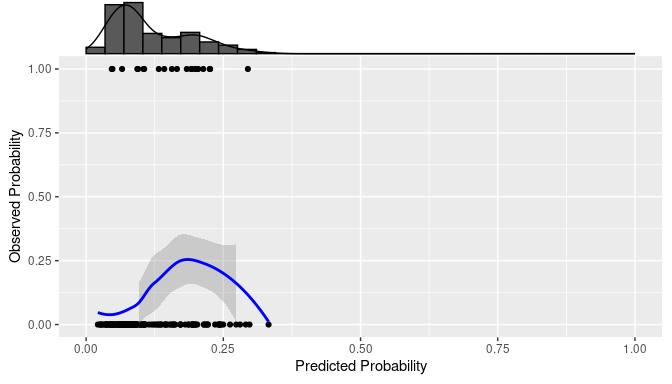
## `geom\_smooth()` using formula 'y ~ x'

## Warning: Removed 62 rows containing non-finite values (stat\_smooth).

## `geom\_smooth()` using formula 'y ~ x'

## Warning: Removed 62 rows containing non-finite values (stat\_smooth).

## Warning: Removed 62 rows containing missing values (geom\_point).



To finally understand the model, it is a good idea to also identify influential observations that impact the model fit. With influential\_observations we can generate a list of observations that, if they are removed, reduce or increase a model parameter by more than Q1 - 1.5 x IQR and Q3 + 1.5 x IQR of the distribution of difference to the reference model.

ifo <- influential\_observations( df\_sel, resp, gmr\_fsel, fn\_train\_binomial, fn\_eval\_binomial\_auroc, fn\_infl\_coefficients, fn\_predict\_glm )

## Warning: The `x` argument of `as\_tibble.matrix()` must have unique column names if `.name\_repair` is omitted as of tibble 2.0.0.  
## Using compatibility `.name\_repair`.  
## This warning is displayed once every 8 hours.  
## Call `lifecycle::last\_lifecycle\_warnings()` to see where this warning was generated.

ifo

## # A tibble: 241 × 14  
## row is\_influential is\_influential\_co ei deval yi dffit `(Intercept)\_df… the\_power\_log\_d… the\_multi\_cuber… rnd15\_dfbeta rnd02\_dfbeta rnd01\_dfbeta  
## <int> <lgl> <chr> <lgl> <dbl> <dbl> <dbl> <dbl> <dbl> <dbl> <dbl> <dbl> <dbl>  
## 1 NA NA <NA> NA NA NA NA -4.49 0.0390 3.88 -0.0267 0.194 0.244   
## 2 1 FALSE "" NA NA 0.0724 -0.00209 -0.0288 -0.000272 0.0279 0.000220 0.0201 0.00470  
## 3 2 TRUE "dffit (Intercept)\_dfb… NA NA 0.159 0.0248 0.0749 0.00746 0.0645 -0.111 -0.00612 0.00302  
## 4 3 FALSE "" NA NA NaN NaN 0 0 0 0 0 0   
## 5 4 FALSE "" NA NA 0.0430 -0.000981 -0.0325 -0.0000147 0.0391 -0.00460 0.0000558 -0.00994  
## 6 5 FALSE "" NA NA 0.104 -0.00293 -0.0408 -0.000909 0.0346 -0.0299 -0.00451 -0.0179   
## 7 6 TRUE "rnd16\_dfbeta" NA NA 0.0958 -0.00396 -0.0269 0.000138 0.0292 0.00377 0.0281 0.00186  
## 8 7 FALSE "" NA NA 0.0461 -0.000732 -0.0154 0.000782 0.0266 -0.00490 -0.00516 -0.00148  
## 9 8 TRUE "dffit (Intercept)\_dfb… NA NA 0.209 -0.0139 0.0509 0.00109 -0.0661 -0.0385 0.0639 -0.0137   
## 10 9 FALSE "" NA NA 0.166 -0.00327 0.00201 -0.000479 -0.0211 -0.0179 0.0237 0.0127   
## # … with 231 more rows, and 1 more variable: rnd16\_dfbeta <dbl>

ifo %>% filter( is\_influential )

## # A tibble: 87 × 14  
## row is\_influential is\_influential\_co ei deval yi dffit `(Intercept)\_dfb… the\_power\_log\_d… the\_multi\_cuber… rnd15\_dfbeta rnd02\_dfbeta rnd01\_dfbeta  
## <int> <lgl> <chr> <lgl> <dbl> <dbl> <dbl> <dbl> <dbl> <dbl> <dbl> <dbl> <dbl>  
## 1 2 TRUE dffit (Intercept)\_dfbeta … NA NA 0.159 0.0248 0.0749 0.00746 0.0645 -0.111 -0.00612 0.00302   
## 2 6 TRUE rnd16\_dfbeta NA NA 0.0958 -0.00396 -0.0269 0.000138 0.0292 0.00377 0.0281 0.00186   
## 3 8 TRUE dffit (Intercept)\_dfbeta … NA NA 0.209 -0.0139 0.0509 0.00109 -0.0661 -0.0385 0.0639 -0.0137   
## 4 10 TRUE (Intercept)\_dfbeta the\_po… NA NA 0.183 -0.0102 0.0951 0.00398 -0.0851 -0.0238 -0.0274 0.0188   
## 5 14 TRUE dffit (Intercept)\_dfbeta … NA NA 0.276 -0.0262 0.0848 -0.00164 -0.151 -0.0485 -0.0736 0.0758   
## 6 22 TRUE dffit the\_power\_log\_dfbet… NA NA 0.319 -0.0212 0.0352 -0.00462 -0.127 0.0841 0.0163 -0.0194   
## 7 28 TRUE rnd15\_dfbeta rnd02\_dfbeta NA NA 0.205 -0.00986 0.00727 -0.00150 -0.0418 -0.0676 -0.0456 0.00332   
## 8 30 TRUE the\_multi\_cubert\_dfbeta NA NA 0.223 -0.00612 0.00437 -0.00224 -0.0501 -0.0168 0.0222 -0.0000773  
## 9 35 TRUE dffit the\_multi\_cubert\_df… NA NA 0.168 0.0584 -0.0597 0.000627 0.143 -0.0613 -0.178 0.289   
## 10 36 TRUE rnd15\_dfbeta NA NA 0.0954 -0.00365 -0.0132 0.000614 0.0174 0.0445 -0.00717 -0.00267   
## # … with 77 more rows, and 1 more variable: rnd16\_dfbeta <dbl>