03_MachineLearning

May 12, 2022

1 Install libraries (if needed)

[1]:
```
#install.packages( "tictoc" )
library( tictoc )
```

[2]:
```
# This took ~ 7 minutes for me to complete in Google Colab
# tic()
# install.packages( c(
#     "tidymodels",
#     "GGally",
#     "ggfortify",
#     "ROCit",
#     "ranger",
#     "xgboost"
# ))
# toc()
```

2 Import Libraries

[3]:
```
library( tidyverse )
library( tidymodels )
library( GGally )
library( ggfortify )
library( ROCit )
```

```
Attaching packages
```

```
                      tidyverse 1.3.1
```

```
ggplot2 3.3.5      purrr   0.3.4
tibble  3.1.6      dplyr   1.0.8
tidyr   1.2.0      stringr 1.4.0
readr   2.1.2      forcats 0.5.1
```

```
Conflicts
```

```
                    tidyverse_conflicts()
```

```
  dplyr::filter() masks stats::filter()
  dplyr::lag()    masks stats::lag()
```

```
  Attaching packages
```

```
                        tidymodels 0.2.0
```

```
  broom        0.8.0       rsample
0.1.1
  dials        0.1.1       tune
0.2.0
  infer        1.0.0       workflows
0.2.6
  modeldata    0.1.1       workflowsets
0.2.1
  parsnip      0.2.1       yardstick
0.0.9
  recipes      0.2.0
```

```
  Conflicts
```

```
                     tidymodels_conflicts()
  scales::discard() masks
purrr::discard()
  dplyr::filter()   masks
stats::filter()
  recipes::fixed()  masks
stringr::fixed()
  dplyr::lag()      masks stats::lag()
  yardstick::spec() masks readr::spec()
  recipes::step()   masks stats::step()
• Use suppressPackageStartupMessages() to eliminate package startup
messages
```

```
Registered S3 method overwritten by 'GGally':
  method from
  +.gg   ggplot2
```

```
Registered S3 method overwritten by 'ggfortify':
  method          from
  autoplot.glmnet parsnip
```

3 Non-linearly separable data

[4]:
```
funkydata <- read_csv( 'https://raw.githubusercontent.com/colettace/
↪Revue_of_Models_for_StatInf_ML/master/day04_materials/funkydata.csv' )
```

```
Rows: 200 Columns: 7
  Column specification
```

```
Delimiter: ","
dbl (7): Gaussian1, Gaussian2, Moon1, Moon2, Circle1, Circle2, Y

 Use `spec()` to retrieve the full column specification for this
data.
 Specify the column types or set `show_col_types = FALSE` to quiet
this message.
```

[5]:
```
dim( funkydata )
```

1. 200 2. 7

[6]:
```
head( funkydata )
```

A tibble: 6 × 7

Gaussian1 <dbl>	Gaussian2 <dbl>	Moon1 <dbl>	Moon2 <dbl>	Circle1 <dbl>	Circle2 <dbl>	Y <dbl>
-0.7994022	0.1545466	0.3378872	0.7223668	-0.5261698	0.9038196	0
-0.3301211	2.3876841	0.2182633	1.0285021	-0.7966583	0.5804428	0
1.6558677	0.6681260	-0.7572982	0.6764793	0.1200559	-1.0731062	0
1.4185881	-0.8775885	1.8573782	0.2101548	0.3124032	-0.1364299	1
-0.1880097	2.6413564	-0.3005245	0.7175567	-0.6291578	-0.9690414	0
-1.1174380	1.8842391	-0.5581630	0.9105472	-0.6317169	-0.7896364	0

[7]:
```
funkydata$Y <- factor( funkydata$Y  )
```

[8]:
```
options(repr.plot.width=10, repr.plot.height=10)
funkydata %>% ggpairs( aes( color=Y ) )
```

```
`stat_bin()` using `bins = 30`. Pick better value with `binwidth`.

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```
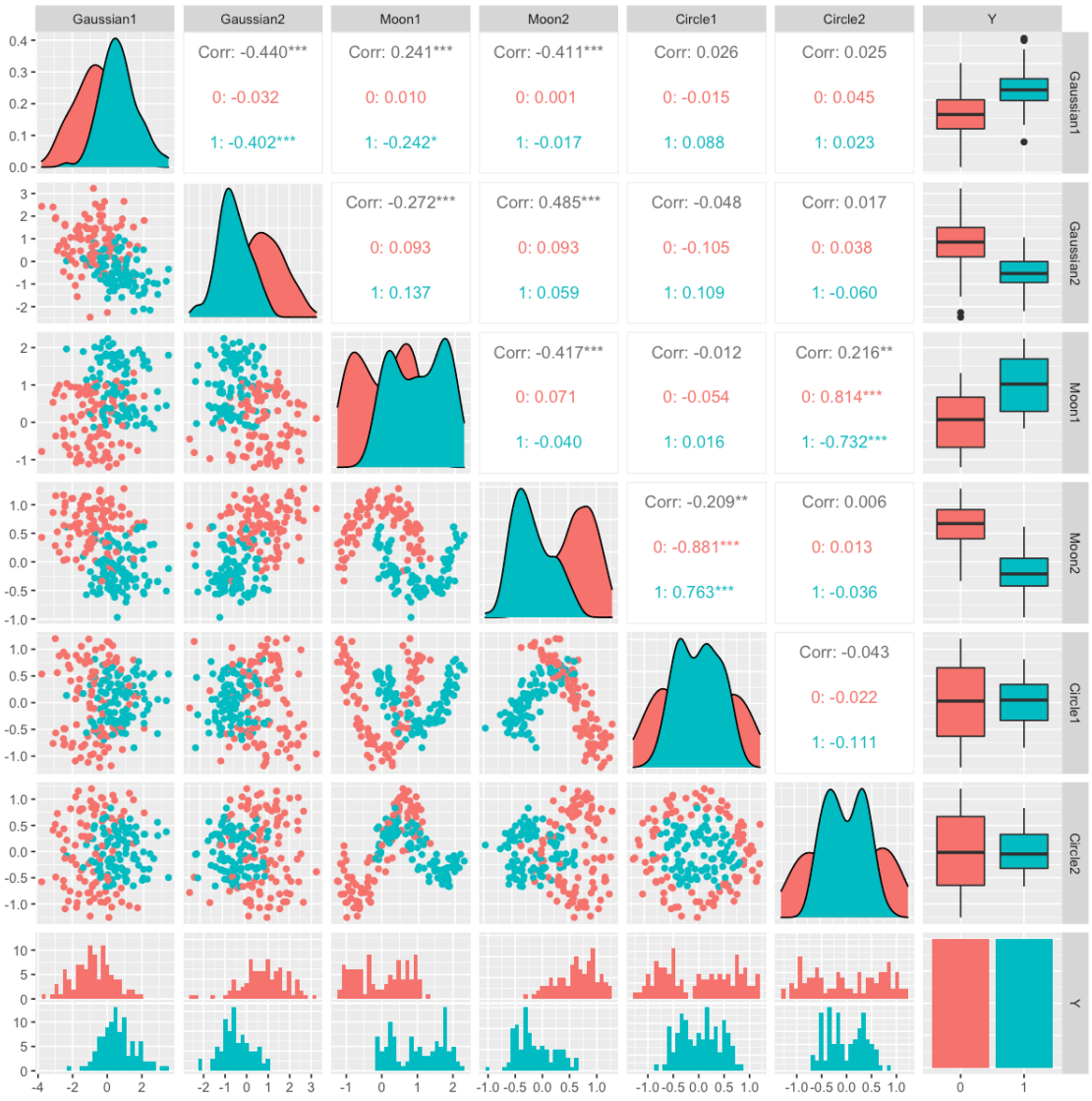

```
`stat_bin()` using `bins = 30`. Pick better value with `binwidth`.
```



[9]:
```
read_csv( 'https://raw.githubusercontent.com/colettace/
↪Revue_of_Models_for_StatInf_ML/master/day04_materials/unequal_variance_data.
↪csv' ) %>%
   mutate( Y=factor(Y) ) %>%
   ggpairs( aes( color=Y, alpha=0.1 ) )
```

```
Rows: 200 Columns: 11
```

```
  Column specification

Delimiter: ","
dbl (11): 0, 1, 2, 3, 4, 5, 6, 7, 8, 9, Y

 Use `spec()` to retrieve the full column specification for this
data.
 Specify the column types or set `show_col_types = FALSE` to quiet
this message.
`stat_bin()` using `bins = 30`. Pick better value with `binwidth`.

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`stat_bin()` using `bins = 30`. Pick better value with `binwidth`.

`stat_bin()` using `bins = 30`. Pick better value with `binwidth`.
```

4 Funkydata: Hold some test data in reserve to assess model fit

[10]:
```
set.seed( 42 )
data_splitter <- initial_split( funkydata, prop=0.8 )
train_data <- training( data_splitter )
test_data <- testing( data_splitter )
```

[11]:
```
dim( train_data )
```

1. 160 2. 7

[12]:
```
dim( test_data )
```

1. 40 2. 7

5 Train a Logistic Regression model

- Plain vanilla logistic regression

[13]:
```
model0 <- glm( Y ~ 1, train_data, family='binomial' )
```

[14]:
```
summary( model0 )
```

```
Call:
glm(formula = Y ~ 1, family = "binomial", data = train_data)

Deviance Residuals:
   Min      1Q  Median      3Q     Max
-1.209  -1.209   1.146   1.146   1.146

Coefficients:
            Estimate Std. Error z value Pr(>|z|)
(Intercept)  0.07504    0.15823   0.474    0.635

(Dispersion parameter for binomial family taken to be 1)

    Null deviance: 221.58  on 159  degrees of freedom
Residual deviance: 221.58  on 159  degrees of freedom
AIC: 223.58

Number of Fisher Scoring iterations: 3
```

[15]:
```
model1 <- glm( Y ~ Gaussian1 + Gaussian2, train_data, family='binomial' )
```

[16]:
```
summary( model1 )
```

```
Call:
glm(formula = Y ~ Gaussian1 + Gaussian2, family = "binomial",
    data = train_data)

Deviance Residuals:
     Min        1Q    Median        3Q       Max
-2.07395  -0.41709   0.07468   0.46161   2.02121

Coefficients:
            Estimate Std. Error z value Pr(>|z|)
(Intercept)   0.6363     0.2550   2.496   0.0126 *
Gaussian1     1.0805     0.2541   4.252 2.12e-05 ***
```

```
Gaussian2    -1.8837     0.3471  -5.427 5.73e-08 ***
---
Signif. codes:  0 ‘***’ 0.001 ‘**’ 0.01 ‘*’ 0.05 ‘.’ 0.1 ‘ ’ 1

(Dispersion parameter for binomial family taken to be 1)

    Null deviance: 221.58  on 159  degrees of freedom
Residual deviance: 110.72  on 157  degrees of freedom
AIC: 116.72

Number of Fisher Scoring iterations: 6
```

[17]:
```
anova( model0, model1 )
```

A anova: 2 × 4

	Resid. Df <dbl>	Resid. Dev <dbl>	Df <dbl>	Deviance <dbl>
1	159	221.5820	NA	NA
2	157	110.7177	2	110.8643

5.1 Use augment() function to attached fitted values to original data frame

[18]:
```
augmented_funky1 <- augment( model1 )
```

[19]:
```
augmented_funky1 %>% head
```

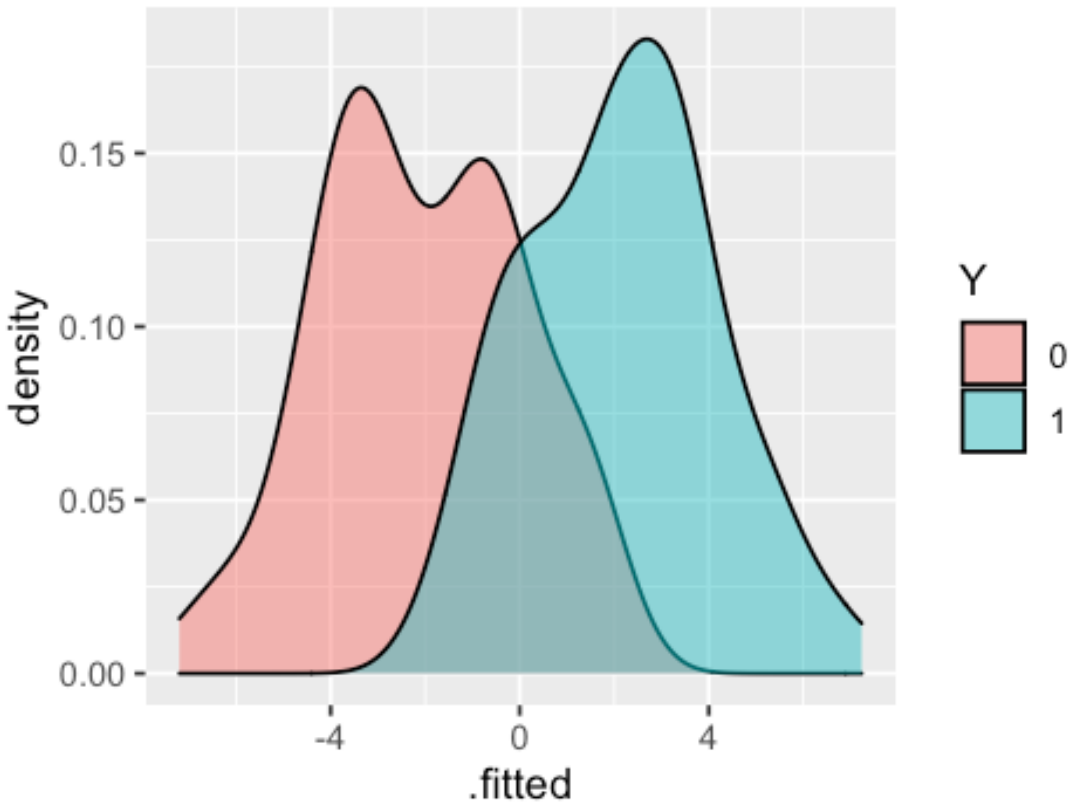
A tibble: 6 × 9

Y <fct>	Gaussian1 <dbl>	Gaussian2 <dbl>	.fitted <dbl>	.resid <dbl>	.std.resid <dbl>	.hat <dbl>	.sigma <dbl>
0	-2.47702641	0.92347223	-3.779734	-0.21247157	-0.21366669	0.01115548	0.8422
0	-1.96080333	0.44304474	-2.316974	-0.43361422	-0.43867256	0.02292908	0.8417
1	0.05830344	-0.90737792	2.408470	0.41505273	0.41847694	0.01629817	0.8417
1	1.61237531	0.07494858	2.237273	0.45039344	0.45589873	0.02400557	0.8416
0	-1.75746682	1.05942979	-3.258341	-0.27470445	-0.27642794	0.01243084	0.8421
1	2.78549049	-1.45826253	6.392927	0.05782651	0.05788017	0.00185325	0.8424

5.2 Plot distribution of TRAINING set fitted values colored by class

[20]:
```
options(repr.plot.width=4, repr.plot.height=3)
```

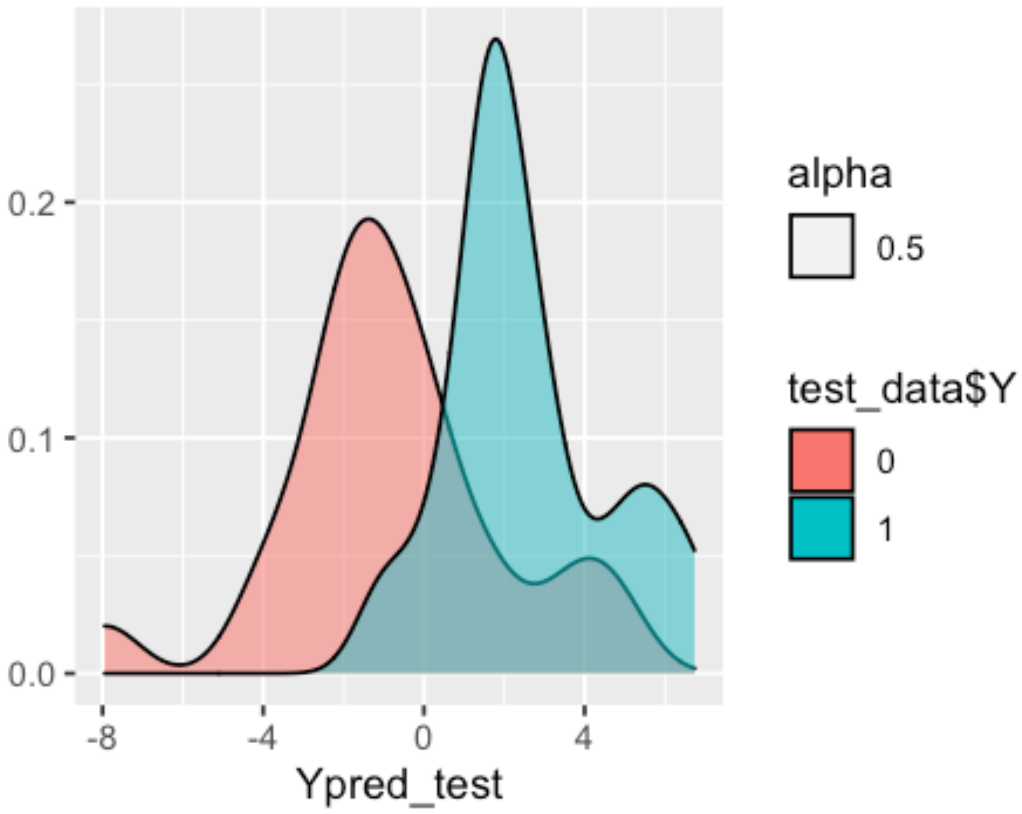
[21]:
```
augmented_funky1 %>% ggplot( aes( x=.fitted, fill=Y) ) + geom_density( alpha=0.
↪5 )
```



5.3 Plot distribution of TEST set fitted values colored by class

[22]:
```
Ypred_test <- predict( model1, test_data )
```

[23]:
```
qplot( Ypred_test, geom='density', fill=test_data$Y, alpha=0.5 )
```



6 Logit link function

- The target variable Y is binary (0/1, loss/win)
- The output is not a 0/1 directly, but the probability of a win
- Linear regression involves solving simultaneous linear equations => linear combinations
- Predicted values of a linear regression MUST also be linear. Consider:
  - $\hat{y}_i = \hat{\beta}_0 + \hat{\beta}_1 x_1 + \hat{\beta}_2 x_2 + ... + \hat{\beta}_n x_n + \epsilon$
  - Use logit link function
  - $logit = log(Odds) = log(\frac{p}{1-p}) = \hat{\beta}_0 + \hat{\beta}_1 x_1 + ... + \hat{\beta}_n x_n + \epsilon$
  - logit function is a "sigmoid" function
- Exponentiate the coefficient to get the odds ratio - if bigger than 1, a 1 unit change in x is an increase
  - Odds ratio estimates = "times more likely" - probability of a win over probability of a loss

[24]:
```
summary( model1 )
```

```
Call:
glm(formula = Y ~ Gaussian1 + Gaussian2, family = "binomial",
    data = train_data)
```

```
Deviance Residuals:
     Min        1Q    Median        3Q       Max
-2.07395  -0.41709   0.07468   0.46161   2.02121

Coefficients:
            Estimate Std. Error z value Pr(>|z|)
(Intercept)   0.6363     0.2550   2.496   0.0126 *
Gaussian1     1.0805     0.2541   4.252 2.12e-05 ***
Gaussian2    -1.8837     0.3471  -5.427 5.73e-08 ***
---
Signif. codes:  0 ‘***’ 0.001 ‘**’ 0.01 ‘*’ 0.05 ‘.’ 0.1 ‘ ’ 1

(Dispersion parameter for binomial family taken to be 1)

    Null deviance: 221.58  on 159  degrees of freedom
Residual deviance: 110.72  on 157  degrees of freedom
AIC: 116.72

Number of Fisher Scoring iterations: 6
```

[25]:
```
coef( model1 )
```

(Intercept) 0.63625825846748 **Gaussian1** 1.08051384014923 **Gaussian2** -1.88368522422804

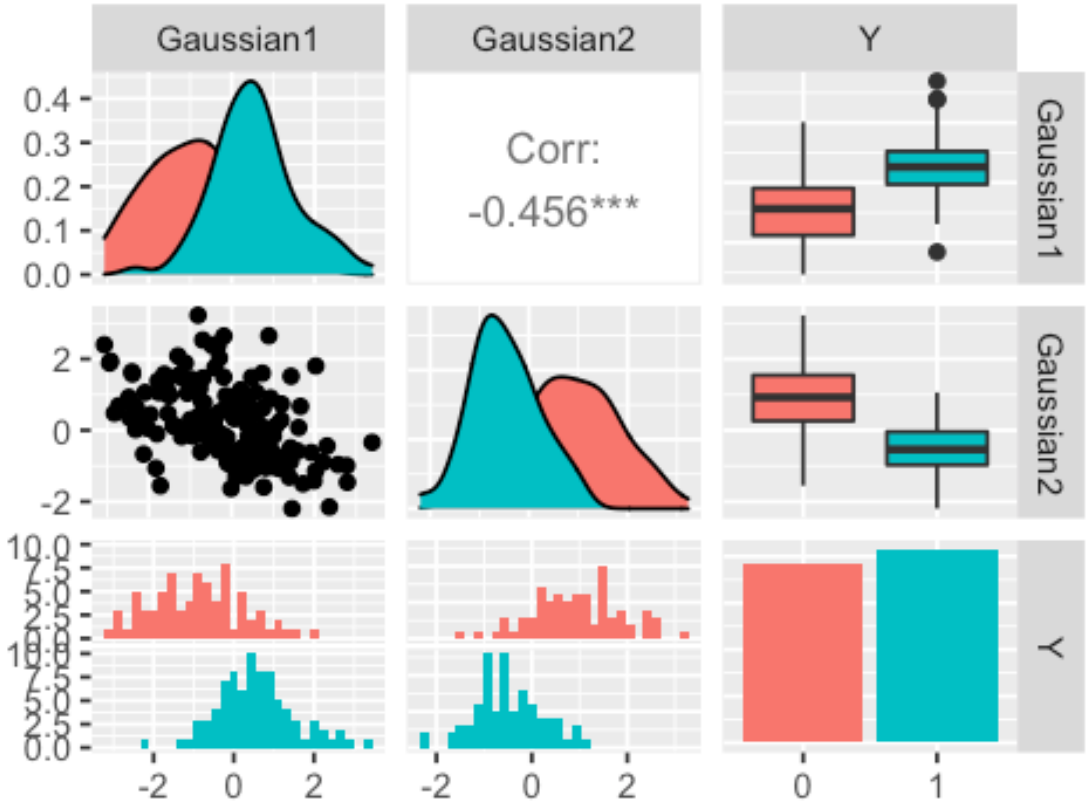
[26]:
```
exp( coef( model1 ) )
```

(Intercept) 1.88939799745355 **Gaussian1** 2.94619303445645 **Gaussian2** 0.152028811884316

[27]:
```
train_data %>%
    select( Gaussian1, Gaussian2, Y ) %>%
    ggpairs( aes( fill=Y ) )
```

```
`stat_bin()` using `bins = 30`. Pick better value with `binwidth`.

`stat_bin()` using `bins = 30`. Pick better value with `binwidth`.
```



[28]:
```
Ypred_test <- predict( model1, test_data )
```

[29]:
```
head( Ypred_test )
```

1 -0.776657624025814 **2** 4.19971262911796 **3** -1.50326617304229 **4** -4.02780804178211 **5** -1.95492268296168 **6** 0.346337686461873

6.1 Use type="response" argument to predict() to get probabilities

[30]:
```
Ypred_test <- predict( model1, test_data, type='response' )
```

[31]:
```
head(Ypred_test)
```

1 0.315040691278714 **2** 0.985221784821913 **3** 0.18193889087942 **4** 0.0175015719397043 **5** 0.124017581035379 **6** 0.585729196604246

6.2 Classification metrics

- Goodness of fit is not adjusted R-squared, but rather accuracy, F1, ROC curve AUC, others...

[32]:
```
length( Ypred_test )
```

40

[33]:
```
head( Ypred_test )
```

1 0.315040691278714 **2** 0.985221784821913 **3** 0.18193889087942 **4** 0.0175015719397043 **5** 0.124017581035379 **6** 0.585729196604246

[34]:
```
mean( as.numeric( Ypred_test > 0.5 ) == test_data$Y )
```

0.8

[35]:
```
# In class activity 1: How to get test prediction accuracy?
```

[36]:
```
# Homework: How to get four-square confusion matrix of TP/FP/FN/TN?
```

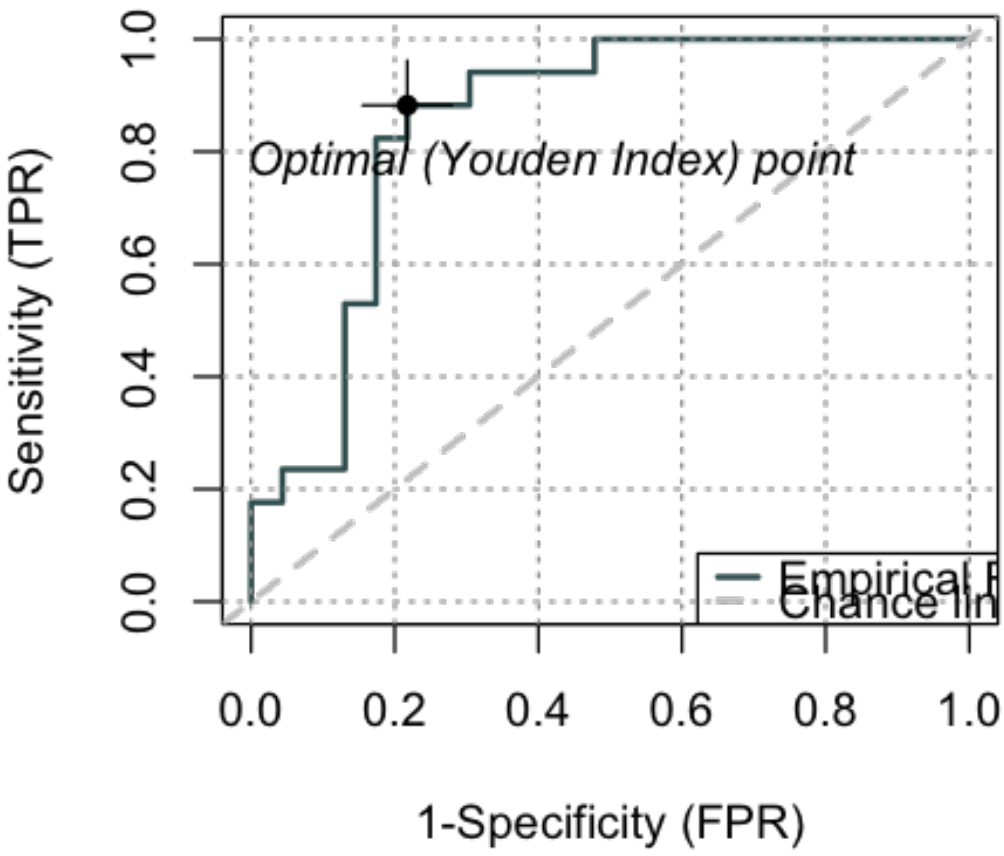
6.3 ROC Curve

- Receiver operator characteristic
- REquires probabilities to work
- How to create a ROC curve

[37]:
```
ROCit_obj <- rocit( score = Ypred_test, class = test_data$Y )
```

[38]:
```
options(repr.plot.width=4, repr.plot.height=4)
```

[39]:
```
plot(ROCit_obj)
```



6.4 Other Logistic regression considerations

6.4.1 Categorical/nominal predictor variables

- One hot encoding: the creation of a dummy variable for each level, e.g.,
  - If you have a nominal variable with 12 cases, you just picked up 11 variables. Each one is going to have it's own coefficient.
- Options: change variable type to interval like an ordinal, or bin into "other" category

7 Retrain GLM model with Parsnip interface (Tidyverse for modelling!)

- Parsnip is a unified modelling interface, allowing you to swap in and out classification algorithms easily

[40]:
```
glm_fit <- logistic_reg() %>%
    set_engine( "glm" ) %>%
    fit( Y ~ Gaussian1 + Gaussian2, train_data )
```

[41]:
```
glm_fit
```

```
parsnip model object


Call:  stats::glm(formula = Y ~ Gaussian1 + Gaussian2, family = stats::binomial,
    data = data)

Coefficients:
(Intercept)    Gaussian1    Gaussian2
     0.6363       1.0805      -1.8837

Degrees of Freedom: 159 Total (i.e. Null);  157 Residual
Null Deviance:            221.6
Residual Deviance: 110.7        AIC: 116.7
```

[42]:
```
glm_test_predictions <- glm_fit %>%
    predict( test_data ) %>%
    bind_cols( test_data )
```

[43]:
```
sample_n( glm_test_predictions, 7 )
```

A tibble: 7 × 8

.pred_class <fct>	Gaussian1 <dbl>	Gaussian2 <dbl>	Moon1 <dbl>	Moon2 <dbl>	Circle1 <dbl>	Circle2 <dbl>
1	1.5704620	0.5242194	-0.08266246	-0.29561727	0.17115858	0.47415826
1	1.5457122	-1.1098034	0.28370608	-0.43815627	-0.04300102	0.27852605
1	-0.1300116	0.1871431	-0.07821408	0.27825127	0.57927695	0.09949454
1	2.0589611	-1.2810525	0.11145428	-0.23824116	0.06435647	0.33150403
1	-0.5710477	-0.4590166	1.73303412	-0.02129662	0.08584222	-0.36298196
1	1.0441428	-0.7342579	1.62134124	-0.29756429	-0.11499781	-0.53755393
1	1.2134165	-0.6016433	0.37254033	-0.24177992	-0.24111067	0.46080170

[44]:
```
glm_test_predictions %>%
    yardstick::metrics( Y, .pred_class )
```

A tibble: 2 × 3

.metric <chr>	.estimator <chr>	.estimate <dbl>
accuracy	binary	0.800000
kap	binary	0.608802

8 Random Forest classifier

- RF YouTube explainer

[45]:
```
rf_fit <- rand_forest() %>%
    set_engine( "ranger" ) %>%
    set_mode( "classification" ) %>%
    fit( Y ~ Gaussian1 + Gaussian2, train_data )
```

[46]:
```
rf_fit
```

```
parsnip model object

Ranger result

Call:
 ranger::ranger(x = maybe_data_frame(x), y = y, num.threads = 1,      verbose =␣
 ↪FALSE, seed = sample.int(10^5, 1), probability = TRUE)

Type:                             Probability estimation
Number of trees:                  500
Sample size:                      160
Number of independent variables:  2
Mtry:                             1
Target node size:                 10
Variable importance mode:         none
Splitrule:                        gini
OOB prediction error (Brier s.):  0.1286279
```

[47]:
```
rf_test_predictions <- rf_fit %>%
    predict( test_data ) %>%
    bind_cols( test_data )
```

[48]:
```
sample_n( rf_test_predictions, 7 )
```

A tibble: 7 × 8

.pred_class <fct>	Gaussian1 <dbl>	Gaussian2 <dbl>	Moon1 <dbl>	Moon2 <dbl>	Circle1 <dbl>	Circle2 <dbl>
1	3.26366961	-0.8788645	0.44887539	-0.5111791	0.037088069	0.3786367
0	0.81184413	1.8763646	-0.08713043	0.9500149	-0.877042683	-0.3308256
0	-0.90289741	0.6402446	0.81652354	0.5629166	0.214471135	0.8439254
0	0.05448866	1.0087876	-0.95066569	0.6080864	0.006890235	-1.2584722
0	-0.69256180	1.3947951	0.80678982	0.6053824	0.572456174	0.8752464
0	-0.97017491	0.9474368	-0.39114679	0.8247762	-0.983245353	-0.2062242
0	-1.11067539	0.9533176	0.28494349	1.1407795	-1.117022375	0.2236662

[49]:
```
rf_test_predictions %>%
    yardstick::metrics( Y, .pred_class )
```

A tibble: 2 × 3

.metric	.estimator	.estimate
<chr>	<chr>	<dbl>
accuracy	binary	0.8250000
kap	binary	0.6551724

9 XGBoost classifier

- Gradient-boosted classification trees YouTube explainer

[50]:
```
xgb_fit <- boost_tree() %>%
    set_engine( "xgboost" ) %>%
    set_mode( "classification" ) %>%
    fit( Y ~ Gaussian1 + Gaussian2, train_data )
```

```
[12:19:34] WARNING: ../../amalgamation/../src/learner.cc:1115: Starting in
XGBoost 1.3.0, the default evaluation metric used with the objective
'binary:logistic' was changed from 'error' to 'logloss'. Explicitly set
eval_metric if you'd like to restore the old behavior.
```

[51]:
```
xgb_fit
```

```
parsnip model object

##### xgb.Booster
raw: 28.2 Kb
call:
  xgboost::xgb.train(params = list(eta = 0.3, max_depth = 6, gamma = 0,
    colsample_bytree = 1, colsample_bynode = 1, min_child_weight = 1,
    subsample = 1, objective = "binary:logistic"), data = x$data,
    nrounds = 15, watchlist = x$watchlist, verbose = 0, nthread = 1)
params (as set within xgb.train):
  eta = "0.3", max_depth = "6", gamma = "0", colsample_bytree = "1",␣
 ↪colsample_bynode = "1", min_child_weight = "1", subsample = "1", objective =␣
 ↪"binary:logistic", nthread = "1", validate_parameters = "TRUE"
xgb.attributes:
  niter
callbacks:
  cb.evaluation.log()
# of features: 2
niter: 15
nfeatures : 2
evaluation_log:
    iter training_logloss
       1         0.525383
       2         0.425617
---
      14         0.144400
      15         0.139690
```

[52]:
```
xgb_test_predictions <- xgb_fit %>%
    predict( test_data ) %>%
    bind_cols( test_data )
```

[53]:
```
sample_n( xgb_test_predictions, 7 )
```

A tibble: 7 × 8

.pred_class <fct>	Gaussian1 <dbl>	Gaussian2 <dbl>	Moon1 <dbl>	Moon2 <dbl>	Circle1 <dbl>	Circle2 <dbl>	Y <fct>
1	1.2134165	-0.60164334	0.37254033	-0.24177992	-0.2411107	0.4608017	1
1	0.3938438	-0.08247521	1.04137506	0.58091150	0.7810910	0.4032936	0
1	1.4293675	-0.64325092	0.66148906	0.59075731	0.1314410	0.9877415	0
0	0.0715979	1.17688822	-0.96693899	0.06382244	0.8893231	-0.1691161	0
0	-0.8358316	0.40048561	1.20377759	-0.52041253	-0.3737893	0.2450463	1
1	1.0451760	0.02597667	-0.06489091	0.24542509	0.2278580	0.1448821	1
0	-0.9947197	0.17949256	-0.66451551	0.89679138	-0.2940818	-1.2318677	0

[54]:
```
xgb_test_predictions %>%
    yardstick::metrics( Y, .pred_class )
```

A tibble: 2 × 3

.metric <chr>	.estimator <chr>	.estimate <dbl>
accuracy	binary	0.7500000
kap	binary	0.5037221

[55]:
```
mean( as.character(xgb_test_predictions$.pred_class) ==
 as.character(xgb_test_predictions$Y) )
```

0.75