Regression and Classification

Stat 220

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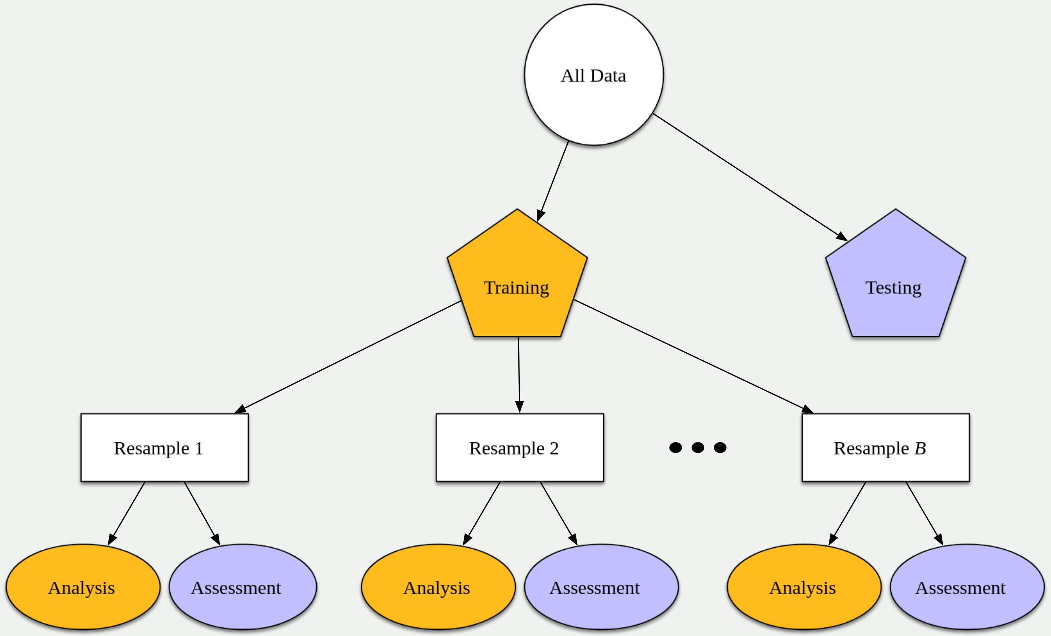
March 02 2022

Resampling methods

Create a series of data sets similar to the training/testing split, always used with the training set



Kuhn and Johnson (2019)

First, simple linear regression (SLR)

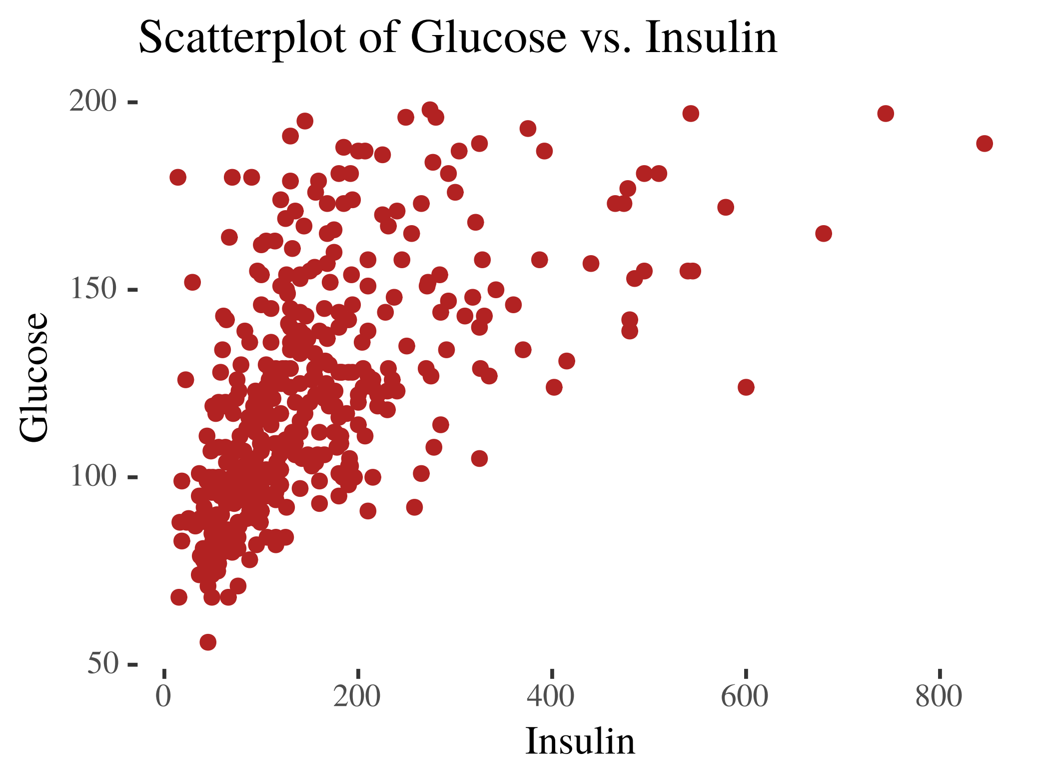
Predicting a numeric outcome when there is just one predictor

$$Y = \beta_0 + \beta_1 X$$

- β values are the coefficients and X is the only model predictor or feature.

Bivariate data from `PimaIndiansDiabetes2`

	glucose	insulin
4	89	94
5	137	168
7	78	88
9	197	543
14	189	846
15	166	175
17	118	230
19	103	83
20	115	96
21	126	235
25	143	146
26	125	115
28	97	140
29	145	110
32	158	245



Specification for a linear regression model

```
lm_spec <- linear_reg() %>%
  set_mode("regression") %>%
  set_engine("lm")
```

```
lm_spec
Linear Regression Model Specification (regression)

Computational engine: lm
```

Fitting the model

```
lm_fit <- lm_spec %>%
  fit(glucose ~ insulin, data = db_slr)

lm_fit
parsnip model object

Fit time:  6ms

Call:
stats::lm(formula = glucose ~ insulin, data = data)

Coefficients:
(Intercept)      insulin
    99.0737       0.1509
```

Getting the fit

```
lm_fit %>%
  pluck("fit")

Call:
stats::lm(formula = glucose ~ insulin, data = data)

Coefficients:
(Intercept)      insulin
    99.0737       0.1509
```

```r
lm_fit %>%
  pluck("fit") %>%
  summary()
```

```

Call:
stats::lm(formula = glucose ~ insulin, data = data)

Residuals:
    Min      1Q  Median      3Q     Max 
-65.633 -17.361  -5.807  12.626  78.813 

Coefficients:
            Estimate Std. Error t value Pr(>|t|)    
(Intercept)  99.0737     2.0979   47.23   <2e-16 ***
insulin       0.1509     0.0107   14.11   <2e-16 ***
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

Residual standard error: 25.14 on 390 degrees of freedom
Multiple R-squared:  0.3378,	Adjusted R-squared:  0.3361 
F-statistic:   199 on 1 and 390 DF,  p-value: < 2.2e-16
```

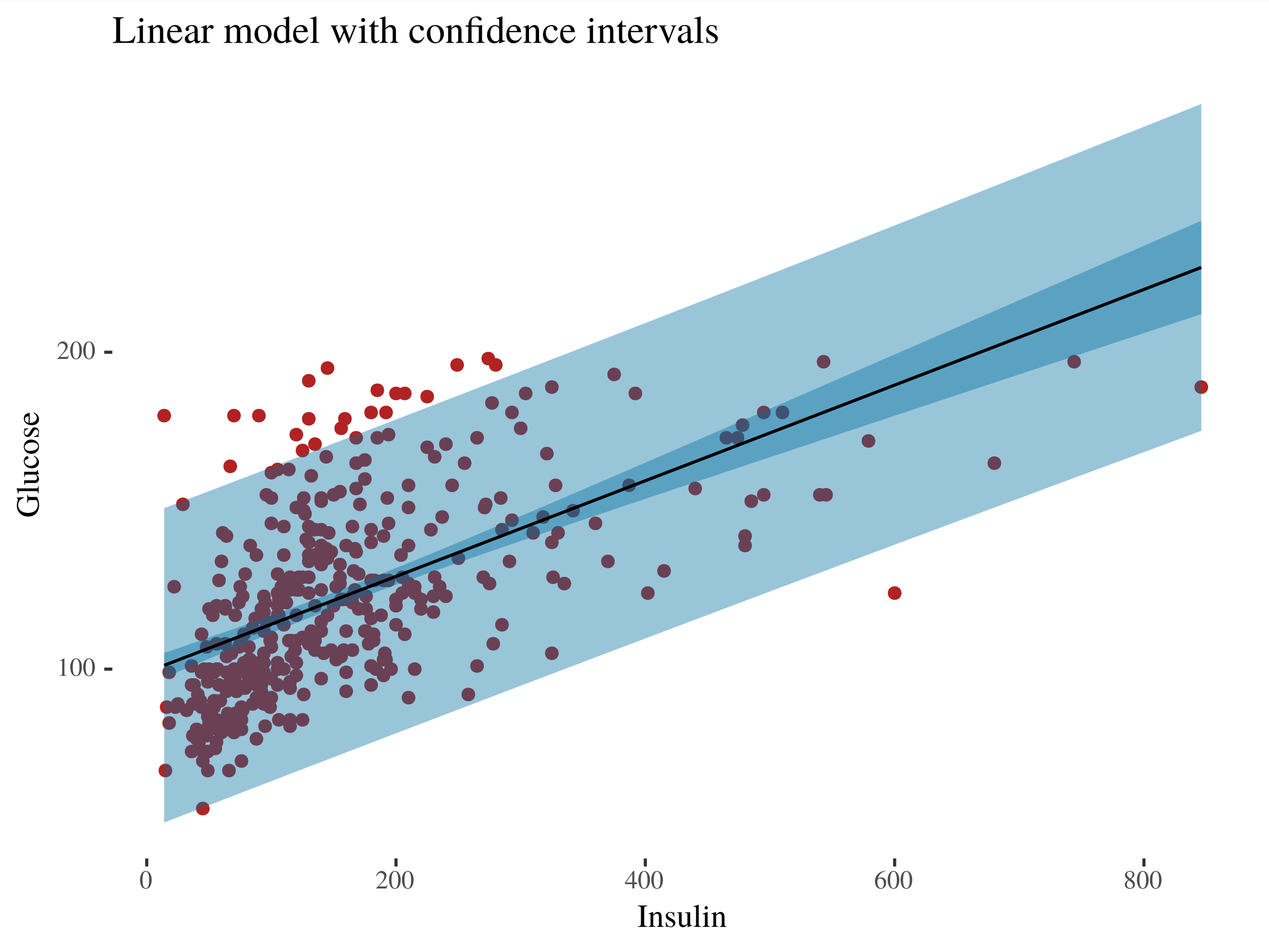
```
predict(lm_fit, new_data = db_slr)
# A tibble: 392 × 1
   .pred
   <dbl>
 1  113.
 2  124.
 3  112.
 4  181.
 5  227.
 6  125.
 7  134.
 8  112.
 9  114.
10  135.
# … with 382 more rows
```

Confidence and Prediction intervals

```
predict(lm_fit, new_data = db_slr,
          type = "conf_int")
# A tibble: 392 × 2
   .pred_lower .pred_upper
         <dbl>       <dbl>
 1        110.        116.
 2        122.        127.
 3        109.        115.
 4        173.        190.
 5        212.        241.
 6        123.        128.
 7        131.        137.
 8        109.        115.
 9        111.        116.
10        132.        138.
# … with 382 more rows
```

```
predict(lm_fit, new_data = db_slr,
          type = "pred_int")
# A tibble: 392 × 2
   .pred_lower .pred_upper
         <dbl>       <dbl>
 1        63.7        163.
 2        74.9        174.
 3        62.8        162.
 4       131.         231.
 5       175.         278.
 6        76.0        175.
 7        84.3        183.
 8        62.1        161.
 9        64.0        163.
10        85.0        184.
# … with 382 more rows
```

Confidence and Prediction intervals



Multiple linear regression (MLR)

Predicting a continuous response with a set of p predictors. predioc

$$Y = \beta_0 + \beta_1 X_1 + \beta_2 X_2 + \cdots + \beta_k X_k$$

- β_i's are the coefficients of the model and X_i's are the predictors.

Fitting a MLR

```
db_mlr <- db %>% select(-diabetes)

lm_fit2 <- lm_spec %>%
  fit(glucose ~ ., data = db_mlr)
```

Extract parameter estimates

```
tidy(lm_fit2)
# A tibble: 8 × 5
  term        estimate std.error statistic  p.value
  <chr>          <dbl>     <dbl>     <dbl>    <dbl>
1 (Intercept)  60.0       8.44       7.11  5.65e-12
2 pregnant      0.0738    0.523      0.141 8.88e- 1
3 pressure      0.213     0.108      1.98  4.82e- 2
4 triceps       0.0743    0.158      0.471 6.38e- 1
5 insulin       0.133     0.0108    12.3   1.62e-29
6 mass          0.130     0.244      0.535 5.93e- 1
7 pedigree      4.18      3.62       1.15  2.50e- 1
8 age           0.577     0.172      3.36  8.57e- 4
```

Predict new values

```
predict(lm_fit2, new_data = db_mlr)
# A tibble: 392 × 1
   .pred
   <dbl>
 1  105.
 2  128.
 3  105.
 4  186.
 5  227.
 6  136.
 7  138.
 8  106.
 9  115.
10  137.
# … with 382 more rows
```

Actual and predicted values

```
bind_cols(
  predict(lm_fit, new_data = db_mlr), db_mlr) %>% select(glucose, .pred)
# A tibble: 392 × 2
   glucose .pred
     <dbl> <dbl>
 1      89  113.
 2     137  124.
 3      78  112.
 4     197  181.
 5     189  227.
 6     166  125.
 7     118  134.
 8     103  112.
 9     115  114.
10     126  135.
# … with 382 more rows
```

Data Splitting

```
set.seed(1234)

db_split <- initial_split(db_mlr,
                          prop = 0.80,
                          strata = age,
                          breaks = 5)

db_train <- training(db_split)
db_test <- testing(db_split)
```

Recipe

```r
db_recipe <- recipe(glucose ~ ., data = db_train) %>%
  step_scale(all_predictors()) %>%
  step_center(all_predictors()) %>% prep()
```

```
db_recipe
Recipe

Inputs:

      role #variables
   outcome          1
 predictor          7

Training data contained 311 data points and no missing data.

Operations:

Scaling for pregnant, pressure, triceps, insulin, mass, ped... [trained]
Centering for pregnant, pressure, triceps, insulin, mass, ped... [trained]
```

Model Building

```
lm_spec <- # your model specification
  linear_reg() %>%  # model type
  set_engine(engine = "lm") %>%  # model engine
  set_mode("regression") # model mode
```

```
# Show your model specification
lm_spec
Linear Regression Model Specification (regression)

Computational engine: lm
```

Create workflow

```
lm_wflow <-
 workflow() %>%
 add_model(lm_spec) %>%
 add_recipe(db_recipe)
```

Create Validation Set

```
set.seed(1234)

cv_folds <- vfold_cv(db_train,
           v = 5,
           strata = age,
           breaks = 5)
```

```
cv_folds
#  5-fold cross-validation using stratification
# A tibble: 5 × 2
  splits            id
  <list>            <chr>
1 <split [247/64]> Fold1
2 <split [247/64]> Fold2
3 <split [249/62]> Fold3
4 <split [250/61]> Fold4
5 <split [251/60]> Fold5
```

Common metrics for regression

Root mean square error (RMSE)

- the standard deviation of the residuals (prediction errors)
- smaller is better

Coefficient of determination, R^2

- proportion of the variation in the outcome that is predictable from the predictors
- larger is better

Fit the model

```r
get_model <- function(x) {   # Function to extract fit
  extract_fit_parsnip(x) %>% tidy()
}
```

```r
lm_wflow_eval <- lm_wflow %>%
  fit_resamples(
    resamples = cv_folds,
    metrics = metric_set(rmse, rsq),
    control = control_resamples(
      save_pred = TRUE,
      extract = get_model)
    )
lm_wflow_eval%>%collect_metrics()
# A tibble: 2 × 6
  .metric .estimator   mean     n std_err .config
  <chr>   <chr>       <dbl> <int>   <dbl> <chr>
1 rmse    standard   24.8       5  0.870  Preprocessor1_Model1
2 rsq     standard    0.417     5  0.0442 Preprocessor1_Model1
```

Last fit and evaluation

```
last_fit_lm <- last_fit(lm_wflow, split = db_split)
```

```
last_fit_lm %>%
  collect_metrics()
# A tibble: 2 × 4
  .metric .estimator .estimate .config
  <chr>   <chr>          <dbl> <chr>
1 rmse    standard      24.4   Preprocessor1_Model1
2 rsq     standard       0.312 Preprocessor1_Model1
```

Extract the estimates

```
lm_wflow_eval$.extracts[[1]][[1]]
[[1]]
# A tibble: 8 × 5
  term        estimate std.error statistic   p.value
  <chr>          <dbl>     <dbl>     <dbl>     <dbl>
1 (Intercept)  124.         1.56    79.5   6.74e-174
2 pregnant      -1.19       2.17    -0.547 5.85e-  1
3 pressure       4.08       1.73     2.36  1.91e-  2
4 triceps        0.392      2.13     0.184 8.54e-  1
5 insulin       15.8        1.68     9.42  4.13e- 18
6 mass           0.923      2.18     0.424 6.72e-  1
7 pedigree       0.323      1.61     0.201 8.41e-  1
8 age            5.85       2.25     2.60  9.92e-  3
```

Logistic Regression

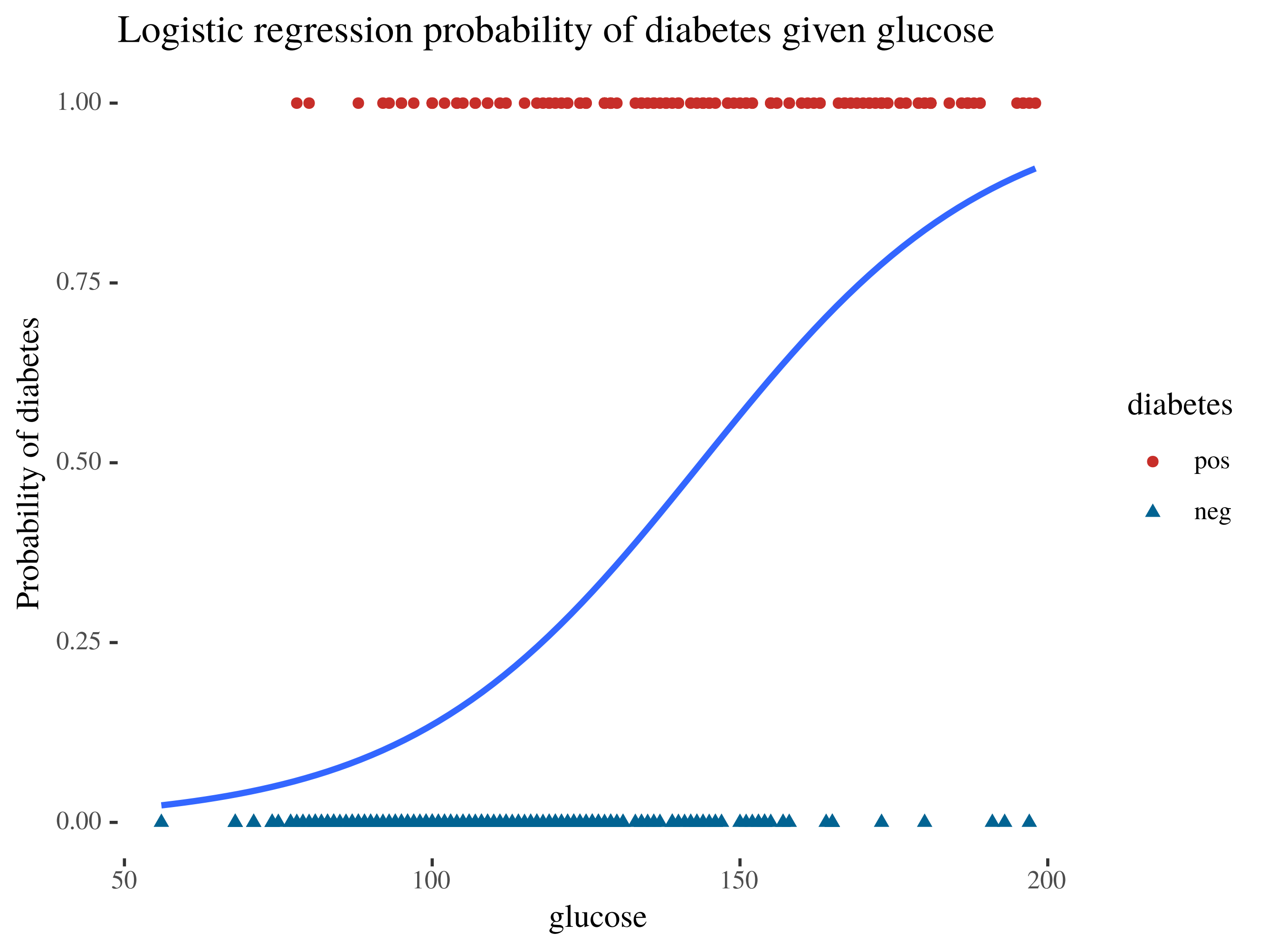
Binary response, Y, with a set of p explanatory (predictor, features) variables, $X_1, \ldots . X_p$. We model the probability that Y belongs to a particular category.

$$P(Y = 1) = \frac{e^{\beta_0 + \beta_1 + \cdots + \beta_p X_p}}{1 + e^{\beta_0 + \beta_1 + \cdots + \beta_p X_p}}$$

$$\text{Odds} = \frac{P(Y = 1)}{1 - P(Y = 1)} = e^{\beta_0 + \beta_1 + \cdots + \beta_p X_p}$$

$$\text{Log Odds} = \beta_0 + \beta_1 + \cdots + \beta_p X_p$$

Logistic regression with just one predictor



Train and Test Split

```
# Create data split for train and test
set.seed(1234)
db_single <- db %>% select(diabetes, glucose)
db_split <- initial_split(db_single, prop = 0.80, strata = diabetes)
```

```
# Create training data
db_train <- db_split %>%
                    training()

# Create testing data
db_test <- db_split %>%
                    testing()
```

Steps

1. Call the model function

2. Supply the family of the model

3. Supply the type of model you want to fit

4. Fit the model

```r
fitted_logistic_model <- logistic_reg() %>% # Call the model function
        # Set the engine/family of the model
        set_engine("glm") %>%
        # Set the mode
        set_mode("classification") %>%
        # Fit the model
        fit(diabetes~., data = db_train)
```

Tidy the Summary

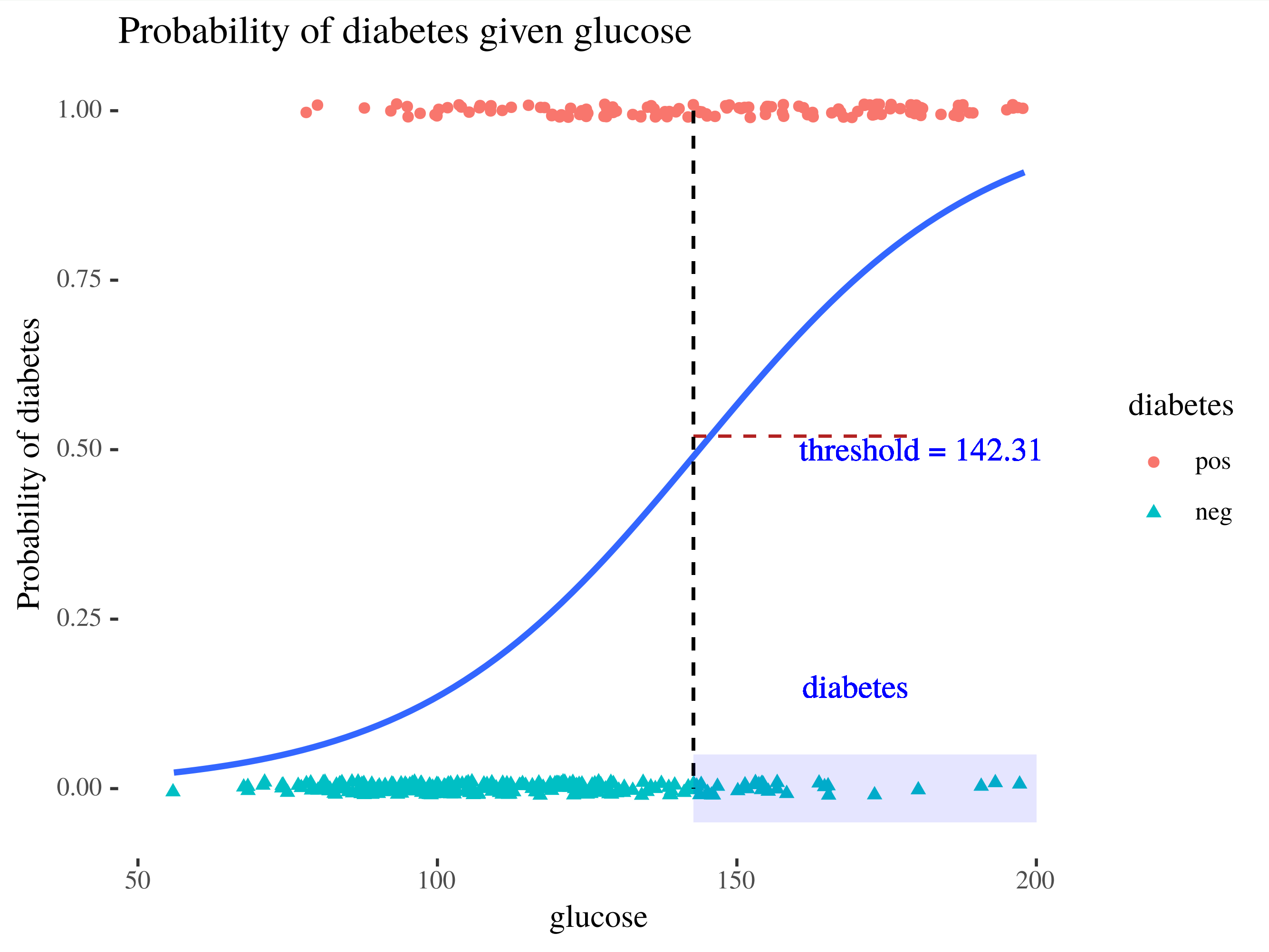
```
tidy(fitted_logistic_model)
# A tibble: 2 × 5
  term        estimate std.error statistic  p.value
  <chr>          <dbl>     <dbl>     <dbl>    <dbl>
1 (Intercept)   6.26     0.718        8.72 2.90e-18
2 glucose      -0.0439   0.00545     -8.04 8.81e-16
```

Odds Ratio

$$ODDS = \frac{probability}{1 - probability}$$

```
tidy(fitted_logistic_model, exponentiate = TRUE)
# A tibble: 2 × 5
  term        estimate std.error statistic  p.value
  <chr>          <dbl>     <dbl>     <dbl>    <dbl>
1 (Intercept)  523.      0.718        8.72 2.90e-18
2 glucose        0.957   0.00545     -8.04 8.81e-16
```

Threshold for classification



Your Turn 1

05:00

Please clone the repository on logistic regression to your local folder.

$$P(Y = 1) = \frac{e^{\beta_0 + \beta_1 X}}{1 + e^{\beta_0 + \beta_1 X}}$$

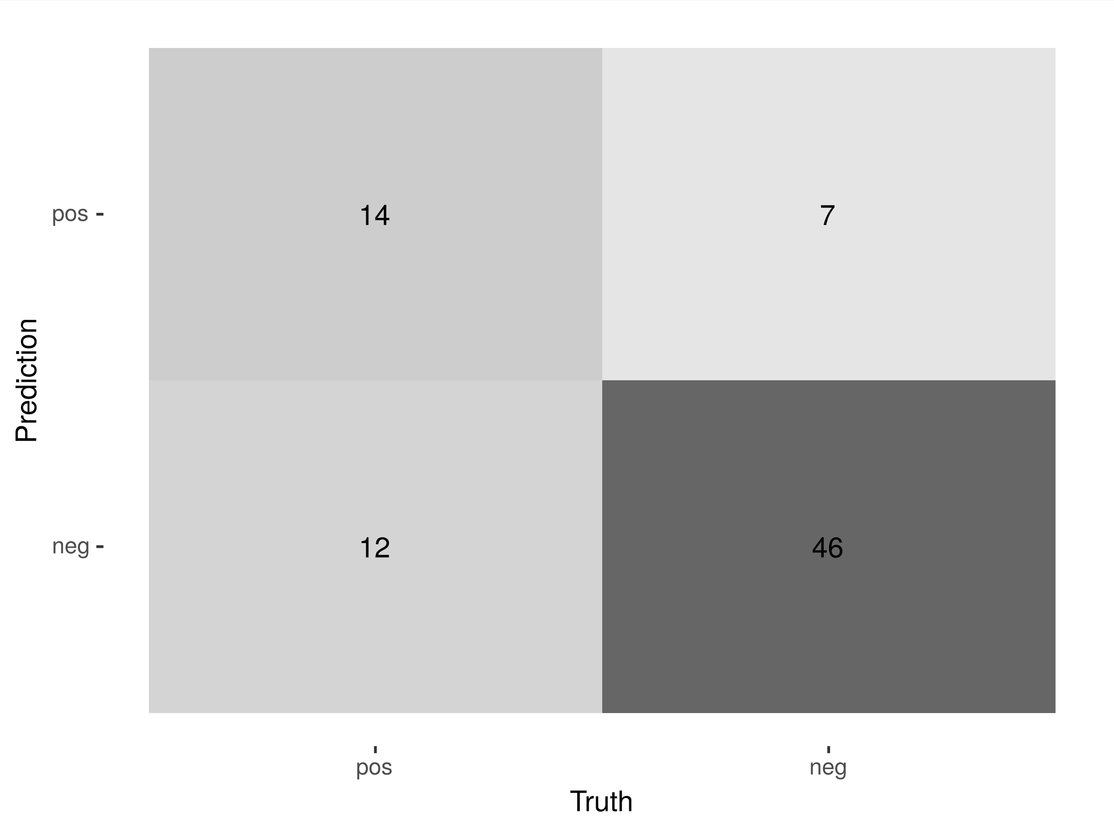
- Verify that the glucose value of 142.31 gives the probability of having diabetes as 1/2.
- What value of glucose gives us have a probability threshold (of having diabetes) of 0.75?

Class Prediction

Use the predict function and supply the trained model object, test dataset and the type of variable to predict

```
# Class prediction
pred_class <- predict(fitted_logistic_model, new_data = db_test,
                      type = "class")  # default 0.5 probability threshold
```

```r
bind_cols(db_test %>% select(diabetes), pred_class) %>%
  conf_mat(diabetes, .pred_class) %>%
  autoplot(type = "heatmap")
```



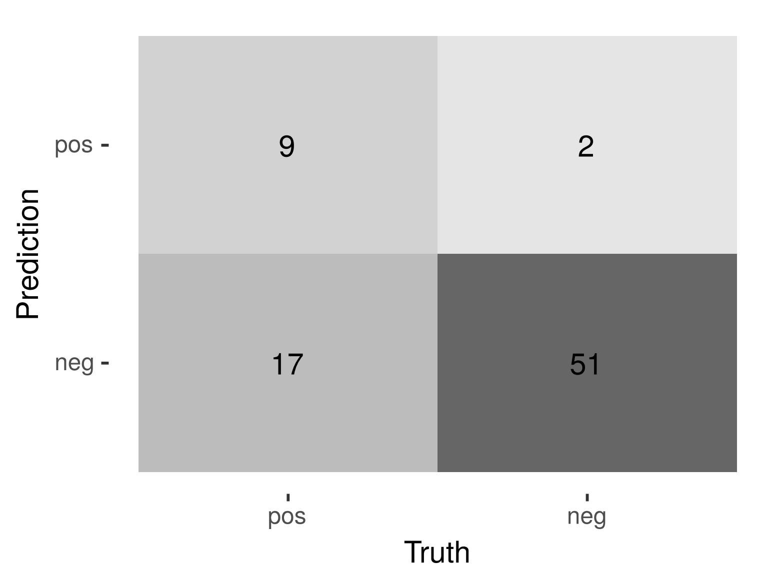
Class Probabilities

```r
# Prediction Probabilities
pred_prob <- predict(fitted_logistic_model,
                      new_data = db_test,
                      type = "prob")
```

```r
db_results <- db_test %>%
  bind_cols(pred_prob) %>%
  mutate(.pred_class = make_two_class_pred(.pred_pos, levels(diabetes),
                                           threshold = .75)) %>%
  select(diabetes, glucose, contains(".pred"))
```

Results

```
head(db_results,12)
   diabetes glucose  .pred_pos  .pred_neg .pred_class
4       neg      89 0.08650244 0.91349756         neg
5       pos     137 0.43727088 0.56272912         neg
9       pos     197 0.91519888 0.08480112         pos
20      pos     115 0.22846937 0.77153063         neg
25      pos     143 0.50271555 0.49728445         neg
26      pos     125 0.31465164 0.68534836         neg
29      neg     145 0.52462130 0.47537870         neg
40      pos     111 0.19902817 0.80097183         neg
44      pos     171 0.77533744 0.22466256         pos
58      neg     100 0.13299378 0.86700622         neg
69      neg      95 0.10968133 0.89031867         neg
89      pos     136 0.42651192 0.57348808         neg
```



Custom Metrics

```
custom_metrics <- metric_set(accuracy, sens, spec, ppv)

custom_metrics(db_results,
               truth = diabetes,
               estimate = .pred_class)
# A tibble: 4 × 3
  .metric  .estimator .estimate
  <chr>    <chr>          <dbl>
1 accuracy binary         0.759
2 sens     binary         0.346
3 spec     binary         0.962
4 ppv      binary         0.818
```

ROC-AUC (Receiver Operator Characteristic- Area Under Curve)

Uses the class probability estimates to give us a sense of performance across the entire set of potential probability cutoffs

```
db_results %>% roc_auc(truth = diabetes, .pred_pos)
# A tibble: 1 × 3
  .metric .estimator .estimate
  <chr>   <chr>          <dbl>
1 roc_auc binary         0.802
```

- ROC_AUC tells how much the model is capable of distinguishing between classes.

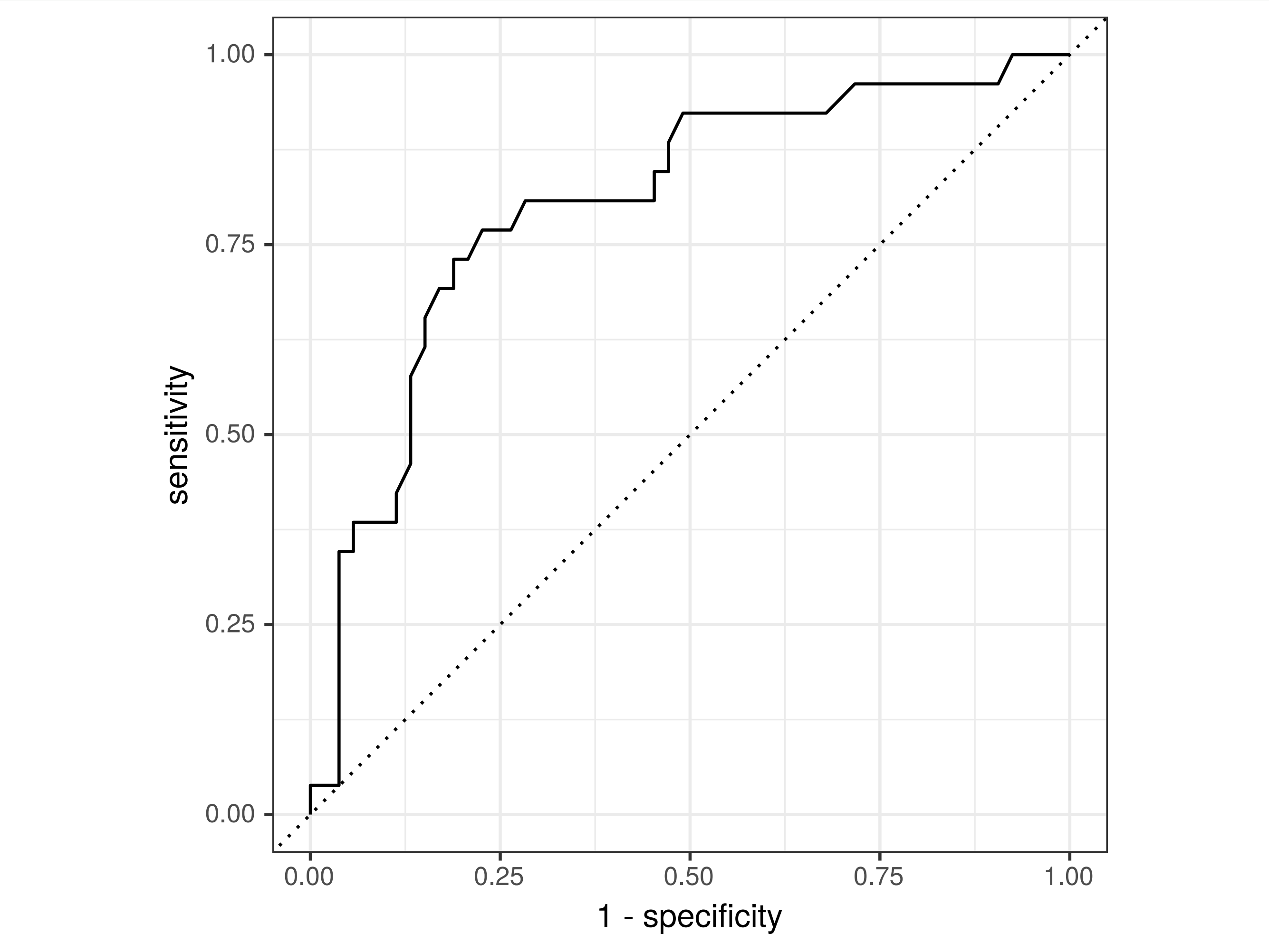
ROC-AUC

plotted with TPR/Recall/Sensitivity against the FPR/ (1- Specificity), where TPR is on the y-axis and FPR is on the x-axis

- ROC curves with area = 1 under the curve (AUC) are perfect classifiers
- ROC curves with area = 0.5 AUC are just as good as random guesses

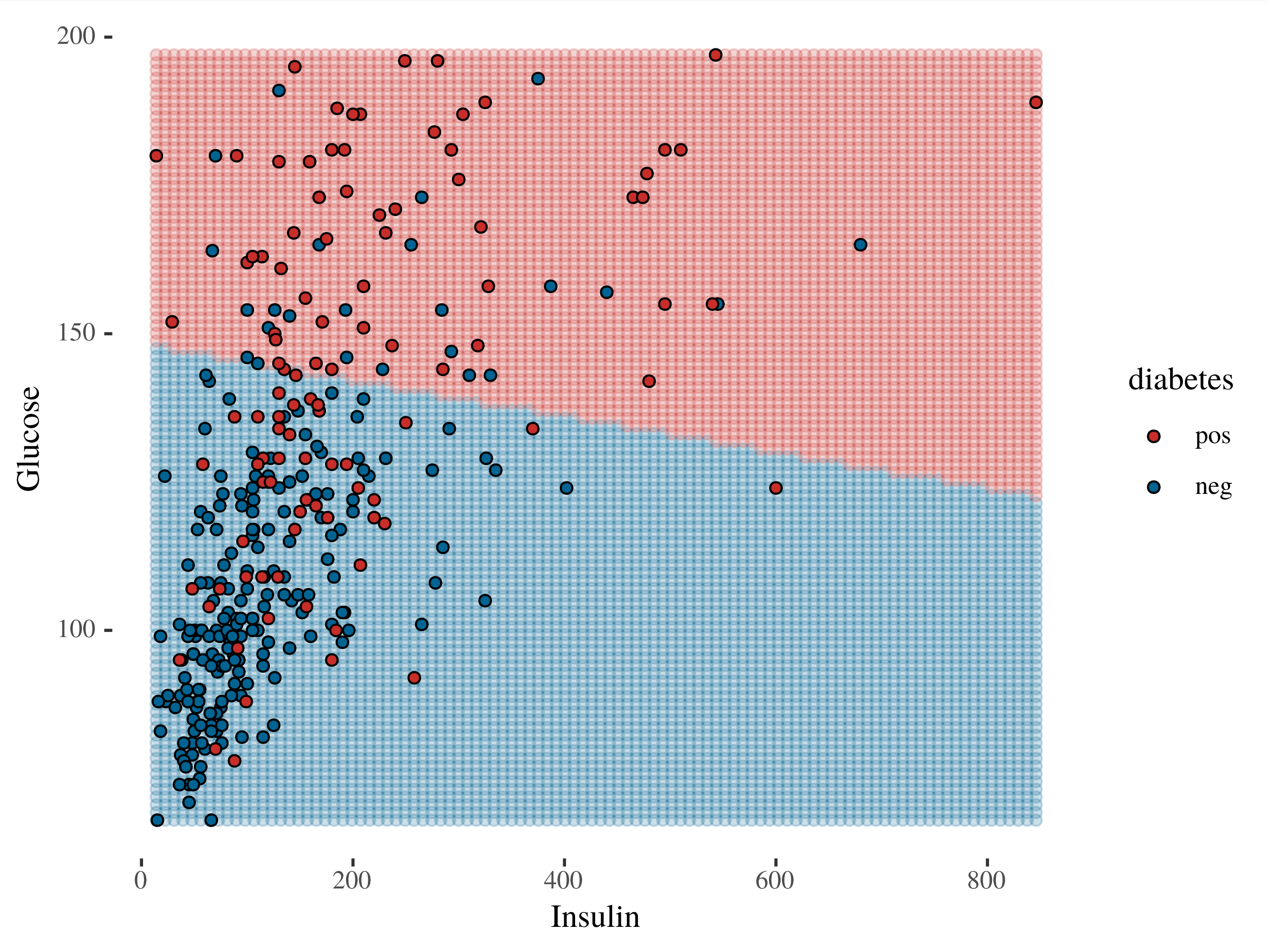
```
db_results %>%
  roc_curve(truth = diabetes, .pred_pos) %>%
  autoplot()
```

ROC Curve



1.00
0.75
0.50
0.25
0.00
sensitivity
0.00
0.25
0.50
0.75
1.00
1 - specificity

Decision boundary



Let's look at the full model

```r
# Create data split for train and test
set.seed(1234)
db_split <- initial_split(db, prop = 0.80, strata = diabetes)
```

```r
# Create training data
db_train <- db_split %>%
                    training()

# Create testing data
db_test <- db_split %>%
                    testing()
```

Model Tuning with a Cross Validation

```
set.seed(100)

cv_folds <-
 vfold_cv(db_train,
          v = 5,
          strata = diabetes)
```

Recipe

```
db_recipe <- recipe(diabetes ~ ., data = db_train) %>%
  step_scale(all_predictors()) %>%
  step_center(all_predictors()) %>% prep()
```

Specify the model

```
log_spec <- # your model specification
  logistic_reg() %>%  # model type
  set_engine(engine = "glm") %>%  # model engine
  set_mode("classification") # model mode
```

Workflow

```
log_wflow <- # new workflow object
 workflow() %>% # use workflow function
 add_recipe(db_recipe) %>%   # use the new recipe
 add_model(log_spec)   # add your model spec
```

Fit, tune, and evaluate

```
log_res_2 <-
  log_wflow %>%
  fit_resamples(
    resamples = cv_folds,
    metrics = metric_set(
      recall, precision,
      accuracy, kap,
      roc_auc, sens, spec),
    control = control_resamples(
      save_pred = TRUE,
      extract = get_model) # use extract function as before
    )
```

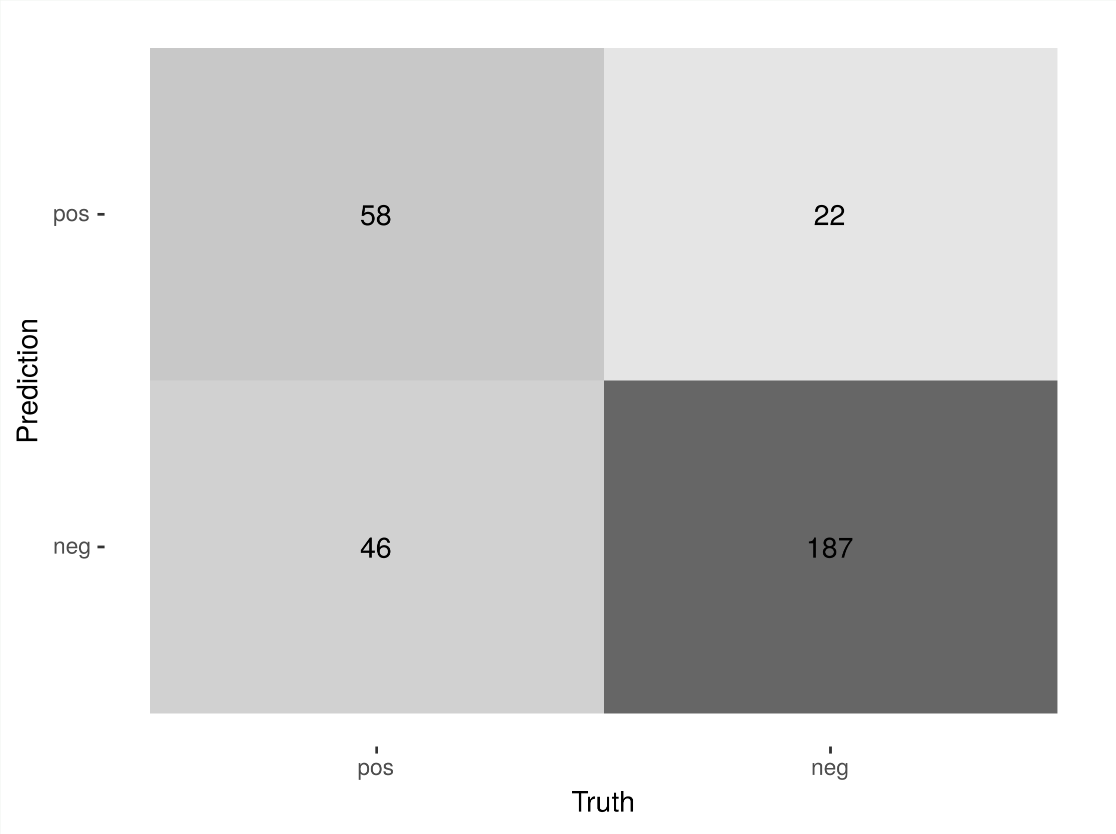
Extract the model

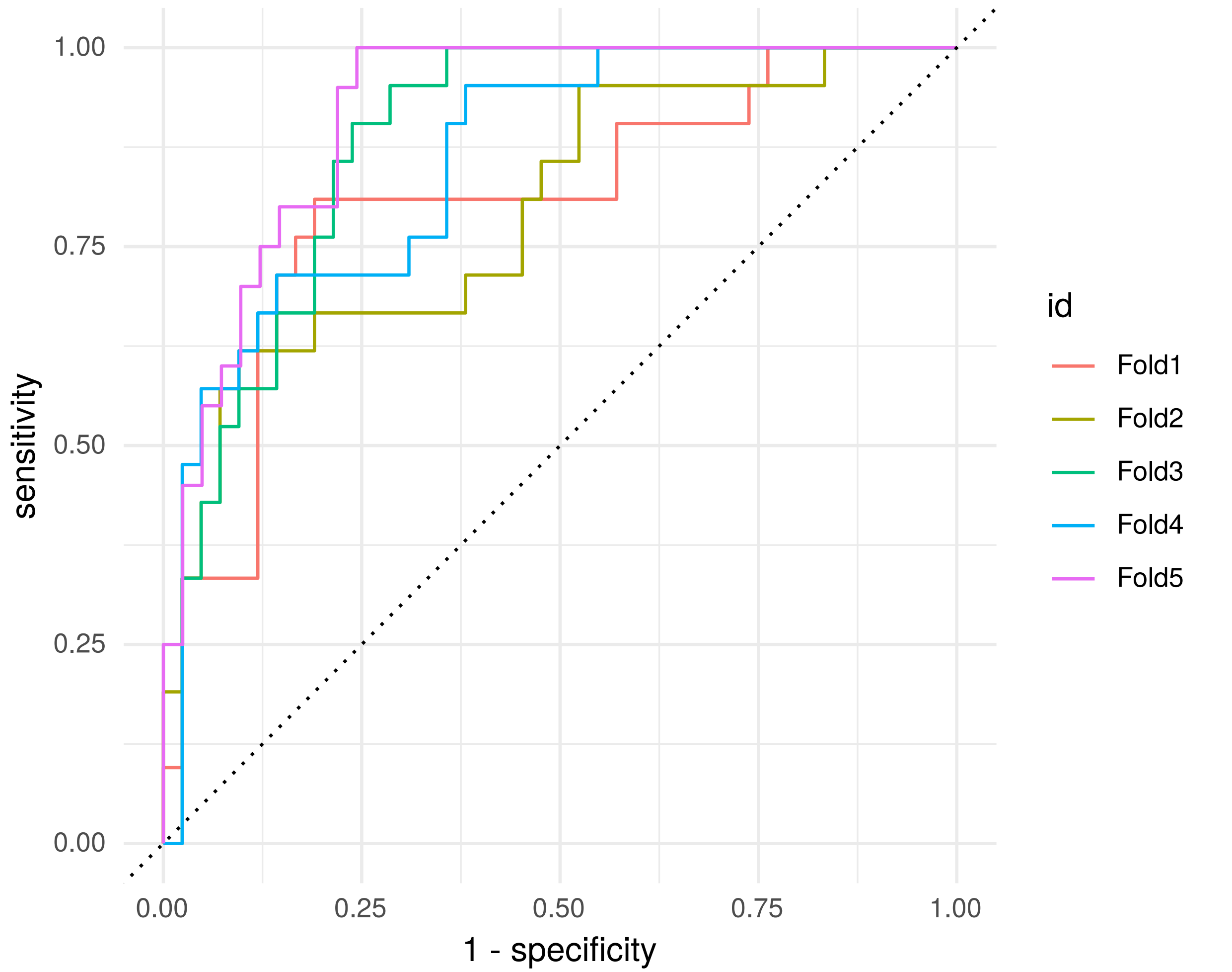
```
log_res_2$.extracts[[1]][[1]]
[[1]]
# A tibble: 9 × 5
  term        estimate std.error statistic      p.value
  <chr>          <dbl>     <dbl>     <dbl>        <dbl>
1 (Intercept)   1.05       0.188     5.58  0.0000000242
2 pregnant     -0.379      0.237    -1.60  0.110
3 glucose      -1.30       0.239    -5.42  0.0000000580
4 pressure      0.102      0.182     0.560 0.576
5 triceps      -0.326      0.225    -1.45  0.147
6 insulin       0.225      0.198     1.14  0.255
7 mass         -0.461      0.238    -1.94  0.0530
8 pedigree     -0.422      0.184    -2.29  0.0219
9 age          -0.367      0.241    -1.52  0.128
```

Collect eh metrics

```
log_res_2 %>%  collect_metrics(summarize = TRUE)
# A tibble: 7 × 6
  .metric   .estimator  mean     n std_err .config
  <chr>     <chr>      <dbl> <int>   <dbl> <chr>
1 accuracy  binary     0.783     5  0.0159 Preprocessor1_Model1
2 kap       binary     0.480     5  0.0405 Preprocessor1_Model1
3 precision binary     0.726     5  0.0313 Preprocessor1_Model1
4 recall    binary     0.558     5  0.0381 Preprocessor1_Model1
5 roc_auc   binary     0.851     5  0.0234 Preprocessor1_Model1
6 sens      binary     0.558     5  0.0381 Preprocessor1_Model1
7 spec      binary     0.895     5  0.0141 Preprocessor1_Model1
```

```r
log_pred <- log_res_2 %>%
  collect_predictions()
```





1.00
0.75
0.50
0.25
0.00
sensitivity
0.00
0.25
0.50
0.75
1.00
1 - specificity
id
Fold1
Fold2
Fold3
Fold4
Fold5

Optimal cut-off