Advanced Topics in Classification Multinomial logistic regression (++) July 14th, 2023

## Example: NFL Expected Points

What does football **play-by-play** data look like? Each row is a play with contextual information:

- Possession team: team with the ball, on offense (opposing team is on defense)
- Down: 4 downs to advance the ball 10 (or more) yards
  - New set of downs, else turnover to defense
- Yards to go: distance in yards to advance
- Yard line: distance in yards away from opponent's endzone (100 to 0) the field position
- Time remaining: seconds remaining in game, each game is 3600 seconds long
  - 4 quarters, halftime in between, followed by a potential overtime (900 seconds)

## Example: NFL Expected Points

Drive: a series of plays, changes with possession and the types of scoring events:

- No Score: 0 points turnover the ball or half/game ends
- Field Goal: 3 points kick through opponent's goal post
- Touchdown: 7 points enter opponent's end zone
- Safety: 2 points for opponent tackled in own endzone

Next Score: type of next score (current drive or future drives) with respect to possession team

- For: Touchdown (7), Field Goal (3), Safety (2)
- Against: -Touchdown (-7), -Field Goal (-3), -Safety (-2)
- No Score

Note: treating point-after-touchdown attempts (PATs) separately

## Example: NFL Expected Points

**Expected Points:** Measure the value of play in terms of  $\mathbb{E}[\text{points of next scoring play}]$ 

• i.e., historically, how many points have teams scored when in similar situations?

**Explanatory variables**:  $\mathbf{X} = \{\text{down, yards to go, yard line, ...}\}$ 

Want to estimate the probabilities of each scoring event to compute expected points:

- Outcome probabilities:  $P(Y=y|\mathbf{X})$
- + Expected Points  $= E(Y|\mathbf{X}) = \sum_{y \in Y} y \cdot P(Y=y|\mathbf{X})$

How do we model more than two categories???

### Review: logistic regression

Response variable Y has two possible values: 1 or 0, we estimate the probability

$$p(x) = P(Y = 1 | X = x)$$

Assuming that we are dealing with two classes, the possible observed values for Y are 0 and 1,

$$Y|x \sim \mathrm{Binomial}(n=1, p=\mathbb{E}[Y|x]) = \mathrm{Bernoulli}(p=\mathbb{E}[Y|x])$$

To limit the regression betweewn [0, 1]: use the **logit** function, aka the **log-odds ratio** 

$$ext{logit}(p(x)) = ext{log}igg[rac{p(x)}{1-p(x)}igg] = eta_0 + eta_1 x_1 + \dots + eta_p x_p$$

meaning

$$p(x)=rac{e^{eta_0+eta_1x_1+\cdots+eta_px_p}}{1+e^{eta_0+eta_1x_1+\cdots+eta_px_p}}$$

### Multinomial logistic regression

We can extend this to K classes (via the softmax function):

$$P(Y=k^* \mid X=x) = rac{e^{eta_{0k^*}+eta_{1k^*}x_1+\dots+eta_{pk^*}x_p}}{\sum_{k=1}^K e^{eta_{0k}+eta_{1k}x_1+\dots+eta_{pk}x_p}}$$

We only estimate coefficients for K - 1 classes **relative to reference class** For example, let K be the reference then we use K - 1 logit transformations

- Use  $oldsymbol{eta}$  for vector of coefficients and  ${f X}$  for matrix of predictors

$$egin{aligned} &\log\left(rac{P(Y=1|\mathbf{X})}{P(Y=K|\mathbf{X})}
ight) = oldsymbol{eta}_1\cdot\mathbf{X} \ &\log\left(rac{P(Y=2|\mathbf{X})}{P(Y=K|\mathbf{X})}
ight) = oldsymbol{eta}_2\cdot\mathbf{X} \ &\log\left(rac{P(Y=K-1|\mathbf{X})}{P(Y=K|\mathbf{X})}
ight) = oldsymbol{eta}_{K-1}\cdot\mathbf{X} \end{aligned}$$

### Multinomial logistic regression for next score

 $Y \in \{$ Touchdown (7), Field Goal (3), Safety (2), No Score (0), -Safety (-2), -Field Goal (-3), -Touchdown (-7) $\}$ 

 $\mathbf{X} = \{\text{down, yards to go, yard line, ...}\}$ 

Model is specified with **six logit transformations** relative to **No Score**:

$$egin{aligned} &\logigg(rac{P(Y= ext{Touchdown}\,|\mathbf{X})}{P(Y= ext{No}\, ext{Score}\,|\mathbf{X})}igg) = \mathbf{X}\cdotoldsymbol{eta}_{ ext{Touchdown}} \ &\logigg(rac{P(Y= ext{Field}\, ext{Goal}\,|\mathbf{X})}{P(Y= ext{No}\, ext{Score}\,|\mathbf{X})}igg) = \mathbf{X}\cdotoldsymbol{eta}_{ ext{Field}\, ext{Goal}}\,, \ &dots \ ˙$$

- Model is generating probabilities, agnostic of value associated with each next score type
- Fit multinomial logistic regression model in R with nnet package

### NFL play-by-play data (2010 to 2020)

Initialized NFL play-by-play dataset with next score in half for each play

• Followed steps in script by Ben Baldwin (which copies Prof. Yurko's steps here)

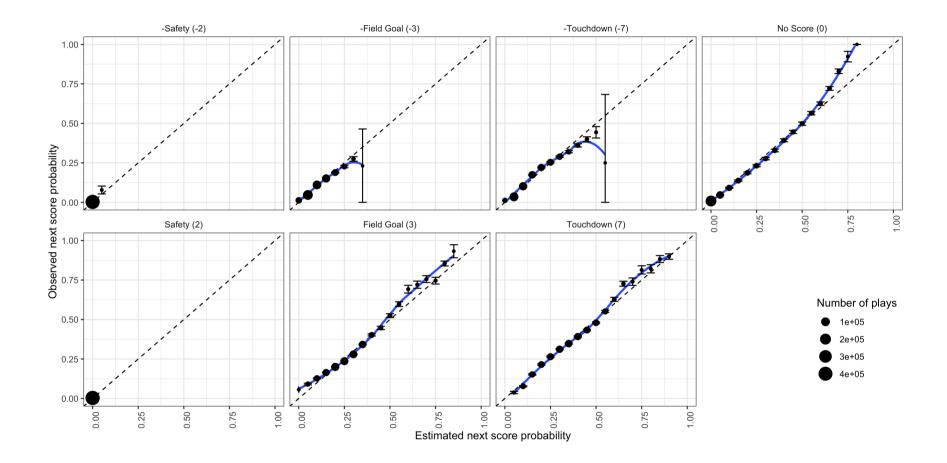
#### How to fit the model?

What does the summary() function return?

#### Leave-one-season-out cross-validation

```
library(nnet)
init_loso_cv_preds <-</pre>
 map_dfr(unique(nfl_ep_model_data$season),
          function(x) {
            # Separate test and training data:
            test data <- nfl ep model data %>% filter(season == x)
            train data <- nfl ep model data %>% filter(season != x)
            # Fit multinomial logistic regression model:
            ep model <-
              multinom(Next Score Half ~ half seconds remaining + yardline 100 + down +
                         log_ydstogo + log_ydstogo*down + yardline_100*down,
                       data = train data, maxit = 300)
            # Return dataset of class probabilities:
            predict(ep_model, newdata = test_data, type = "probs") %>%
              as tibble() %>%
              mutate(Next Score Half = test data$Next Score Half,
                     season = x)
              })
```

```
ep_cv_loso_calibration_results %>%
 mutate(next_score_type = fct_relevel(next_score_type, "Opp_Safety", "Opp_Field_Goal",
                                       "Opp_Touchdown", "No_Score", "Safety", "Field_Goal",
                                       "Touchdown"),
 next_score_type = fct_recode(next_score_type, "-Field Goal (-3)" = "Opp_Field_Goal",
                               "-Safety (-2)" = "Opp Safety", "-Touchdown (-7)" = "Opp Touchdown'
                               "Field Goal (3)" = "Field Goal", "No Score (0)" = "No Score",
                               "Touchdown (7)" = "Touchdown", "Safety (2)" = "Safety")) %>%
 ggplot(aes(x = bin_pred_prob, y = bin actual prob)) +
 geom abline(slope = 1, intercept = 0, color = "black", linetype = "dashed") +
 geom smooth(se = FALSE) +
 geom_point(aes(size = n_plays)) +
 geom errorbar(aes(ymin = bin lower, ymax = bin upper)) + #coord equal() +
 scale x continuous(limits = c(0,1)) +
 scale y continuous(limits = c(0,1)) +
 labs(size = "Number of plays", x = "Estimated next score probability",
       y = "Observed next score probability") +
 theme bw() +
 theme(strip.background = element blank(),
        axis.text.x = element text(angle = 90),
        legend.position = c(1, .05), legend.justification = c(1, 0)) +
 facet_wrap(~ next_score_type, ncol = 4)
```



## Multinomial classification with XGBoost

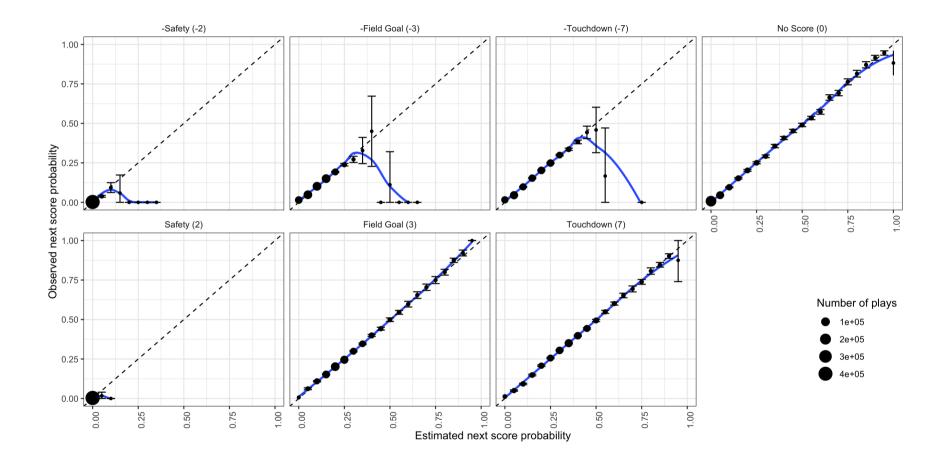
Use same NFL play-by-play dataset as before but get ready for XGBoost...

XGBoost requires the multinomial categories to be numeric starting at 0

#### Leave-one-season-out cross-validation

```
xgb_loso_cv_preds <-</pre>
 map_dfr(unique(nfl_ep_model_data$season), function(x) {
            # Separate test and training data - scale variables:
            test data <- nfl ep model data %>% filter(season == x)
            test data x <- as.matrix(dplyr::select(test data, model variables))</pre>
            train_data <- nfl_ep_model_data %>% filter(season != x)
            train data x <- as.matrix(dplyr::select(train data, model variables))</pre>
            train data y <- train data$next score label
            xgb model <- xgboost(data = train data x, label = train data y, nrounds = 100,
                                  max depth = 3, eta = 0.3, gamma = 0, colsample bytree = 1,
                                  min child weight = 1, subsample = 1, nthread = 1,
                                  objective = 'multi:softprob', num class = 7,
                                  eval metric = 'mlogloss', verbose = 0)
            xgb_preds <- matrix(predict(xgb_model, test_data_x), ncol = 7, byrow = TRUE) %>%
              as tibble()
            colnames(xgb_preds) <- c("No_Score", "Safety", "Field_Goal", "Touchdown",</pre>
                                      "Opp Safety", "Opp Field Goal", "Opp Touchdown")
            xgb_preds %>%
              mutate(Next Score Half = test data$Next Score Half, season = x)
            })
```

```
ep_cv_loso_calibration_results %>%
 mutate(next_score_type = fct_relevel(next_score_type, "Opp_Safety", "Opp_Field_Goal",
                                       "Opp_Touchdown", "No_Score", "Safety", "Field_Goal",
                                       "Touchdown"),
 next_score_type = fct_recode(next_score_type, "-Field Goal (-3)" = "Opp_Field_Goal",
                               "-Safety (-2)" = "Opp Safety", "-Touchdown (-7)" = "Opp Touchdown'
                               "Field Goal (3)" = "Field Goal", "No Score (0)" = "No Score",
                               "Touchdown (7)" = "Touchdown", "Safety (2)" = "Safety")) %>%
 ggplot(aes(x = bin_pred_prob, y = bin actual prob)) +
 geom abline(slope = 1, intercept = 0, color = "black", linetype = "dashed") +
 geom smooth(se = FALSE) +
 geom_point(aes(size = n_plays)) +
 geom errorbar(aes(ymin = bin lower, ymax = bin upper)) + #coord equal() +
 scale x continuous(limits = c(0,1)) +
 scale y continuous(limits = c(0,1)) +
 labs(size = "Number of plays", x = "Estimated next score probability",
       y = "Observed next score probability") +
 theme bw() +
 theme(strip.background = element blank(),
        axis.text.x = element text(angle = 90),
        legend.position = c(1, .05), legend.justification = c(1, 0)) +
 facet_wrap(~ next_score_type, ncol = 4)
```



# Model Evaluation for Classification

### Back to a binary example: NFL completion probability

```
Binary outcome model: Y \in \{ 	ext{Incomplete } (0), 	ext{Complete } (1) \}
```

```
library(tidyverse)
nfl_passing_plays <-
    read_csv("https://shorturl.at/ADMWZ") %>%
    # Only keep rows with passer and receiver information known:
    filter(!is.na(passer_player_id), !is.na(receiver_player_id),
        !is.na(epa), !is.na(air_yards), !is.na(pass_location)) %>%
    # Combine passer and receiver unique IDs:
    mutate(passer_name_id = paste0(passer_player_name, ":", passer_player_id),
        receiver_name_id = paste0(receiver_player_name, ":", receiver_player_id))
```

Create train and test folds based on games:

```
set.seed(1985)
game_fold_table <- tibble(game_id = unique(nfl_passing_plays$game_id)) %>%
    mutate(game_fold = sample(rep(1:5, length.out = n()), n()))
nfl_passing_plays <- nfl_passing_plays %>% dplyr::left_join(game_fold_table, by = "game_id")
```

## Logistic regression review

Generate data of test predictions with particular model:

```
logit_cv_preds <-</pre>
  map_dfr(unique(nfl_passing_plays$game_fold),
          function(test_fold) {
            # Separate test and training data:
            test data <- nfl passing plays %>%
              filter(game_fold == test_fold)
            train data <- nfl passing plays %>%
              filter(game fold != test fold)
            # Train model:
            logit_model <- glm(complete_pass ~ yardline_100 + shotgun + air_yards +</pre>
                                  pass location + qb hit,
                                data = train data, family = "binomial")
            # Return tibble of holdout results:
            tibble(test_pred_probs = predict(logit_model, newdata = test_data,
                                              type = "response"),
                   test_actual = test_data$complete_pass,
                   game fold = test fold)
          })
```

# Holdout performance by fold

```
logit_cv_preds %>%
  mutate(test_pred = ifelse(test_pred_probs < .5, 0, 1)) %>%
  group_by(game_fold) %>%
  summarize(mcr = mean(test_pred != test_actual))
```

Let's think more carefully about what's going on here...

### Evaluating the prediction threshold

We can really write our classification as a function of some cutoff *c*:

$$\hat{Y} = \hat{C}(x) = egin{cases} 1 & \hat{p}(x) > c \ 0 & \hat{p}(x) \leq c \end{cases}$$

#### Given the classifications, we can form a confusion matrix:





We want to **maximize** all of the following (positive means 1, negative means 0):

- Accuracy: How often is the classifier correct?  $\frac{TP+TN}{total}$
- **Precision**: How often is it right for predicted positives?  $\frac{TP}{TP+FP}$
- Sensitivity, aka true positive rate (TPR) or power: How often does it detect positives?  $\frac{TP}{TP+FN}$
- Specificity, aka true negative rate (TNR), or 1 false positive rate (FPR): How often does it detect negatives?  $\frac{TN}{TN+FP}$

#### So how do we handle this?

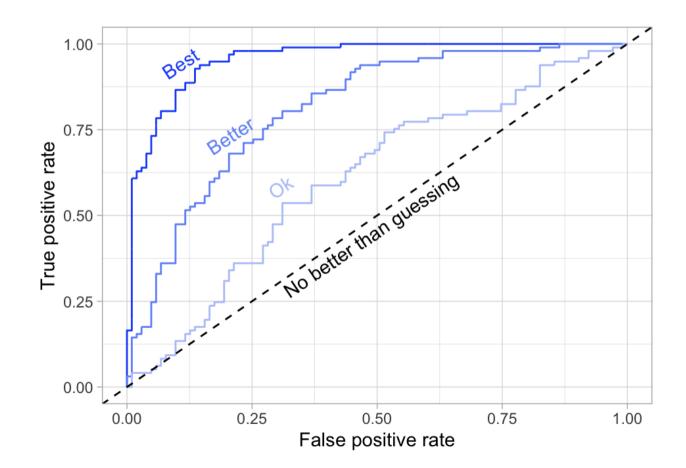
### We want to balance with high power and low false positive rate



### Receiver Operating Characteristic (ROC) curve

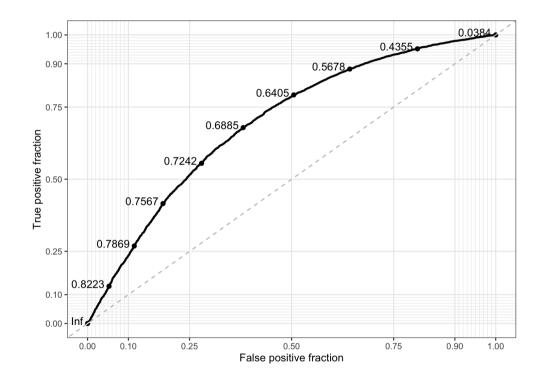
Check all possible values for the cutoff *c*, plot the power against false positive rate

Want to maximize the area under the curve (AUC)



### plotROC and holdout AUC

- d stands for disease status (the outcome)
- m stands for marker (the prediction)

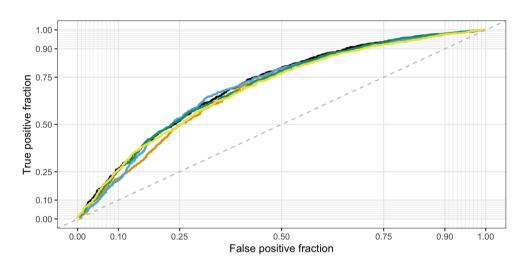


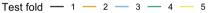
## [1] 0.6957778

### plotROC and holdout AUC by test fold

```
logit_cv_preds %>%
 ggplot() +
 geom_roc(aes(d = test_actual,
              m = test_pred_probs,
               color = as.factor(game_fold)),
           n.cuts = 0) +
 style_roc() +
 geom_abline(slope = 1, intercept = 0,
              linetype = "dashed",
              color = "gray") +
 ggthemes::scale_color_colorblind() +
 labs(color = "Test fold") +
 theme(legend.position = "bottom")
logit_cv_preds %>% group_by(game_fold) %>%
 summarize(auc = MLmetrics::AUC(test pred pr
                                 test actual)
```

*There is definitely room for improvement...* 





```
## # A tibble: 5 × 2
   game_fold
##
               auc
##
         <int> <dbl>
## 1
             1 0.707
## 2
             2 0.686
## 3
             3 0.699
## 4
             4 0.700
## 5
             5 0.690
```

# Tree-based approach?

We need to first convert categorical variables into dummy indicators:

```
model_data <- nfl_passing_plays %>%
mutate(play_id = 1:n(),
            complete_pass = as.factor(complete_pass)) %>%
dplyr::select(play_id, complete_pass, yardline_100, shotgun, air_yards, qb_hit,
            game_fold, pass_location) %>%
mutate(pass_location_val = 1) %>%
pivot_wider(id_cols = play_id:game_fold,
            names_from = pass_location, values_from = pass_location_val,
            values_fill = 0) %>%
dplyr::select(-play_id)
```

# Random forests using probability forest

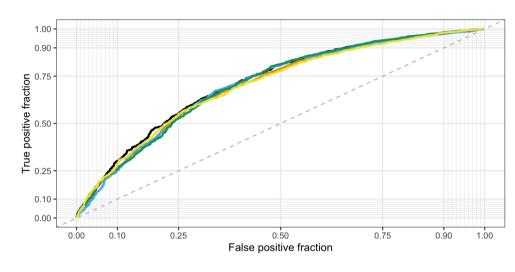
For each tree compute class proportion in terminal node, then take average across all trees

```
library(ranger)
rf prob cv preds <-
 map dfr(unique(model data$game fold),
          function(test fold) {
            # Separate test and training data - scale variables:
            test data <- model data %>% filter(game fold == test fold)
            train data <- model data %>% filter(game fold != test fold)
            rf prob model <-
              ranger(complete pass ~ ., data = dplyr::select(train data, -game fold),
                     probability = TRUE)
            # Return tibble of holdout results:
            tibble(test pred probs =
                     as.numeric(predict(rf_prob_model, data = test_data,
                                        type = "response")$predictions[,2]),
                   test_actual = as.numeric(test_data$complete_pass) - 1,
                   game fold = test fold)
          })
```

### Random forests using probability forest

```
rf_prob_cv_preds %>%
 ggplot() +
 geom_roc(aes(d = test_actual,
              m = test_pred_probs,
               color = as.factor(game_fold)),
          n.cuts = 0) +
 style_roc() +
 geom_abline(slope = 1, intercept = 0,
              linetype = "dashed",
              color = "gray") +
 ggthemes::scale_color_colorblind() +
 labs(color = "Test fold") +
 theme(legend.position = "bottom")
rf_prob_cv_preds %>% group_by(game_fold) %>%
 summarize(auc = MLmetrics::AUC(test_pred_pr
                                 test actual)
```

Looks like just a modest improvement



Test fold — 1 — 2 — 3 — 4 — 5

##	#	A tibble: 5 × 2
##		game_fold auc
##		<int> <dbl></dbl></int>
##	1	1 0.717
##	2	2 0.705
##	3	3 0.707
##	4	4 0.708
##	5	5 0.704

## XGBoost!

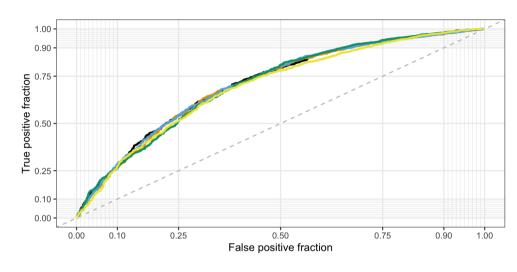
```
library(xgboost)
xgb_cv_preds <-</pre>
 map_dfr(unique(model_data$game_fold),
          function(test_fold) {
            # Separate test and training data - scale variables:
            test data <- model data %>% filter(game fold == test fold)
            test_data_x <- as.matrix(dplyr::select(test_data, -complete_pass, -game_fold))</pre>
            train_data <- model_data %>% filter(game_fold != test_fold)
            train_data_x <- as.matrix(dplyr::select(train_data, -complete_pass, -game_fold))</pre>
            train data y <- as.numeric(train data$complete pass) - 1</pre>
            xgb_model <- xgboost(data = train_data_x, label = train_data_y,</pre>
                                  nrounds = 100, max_depth = 3, eta = 0.3,
                                  gamma = 0, colsample by tree = 1, min child weight = 1,
                                  subsample = 1, nthread = 1,
                                  objective = 'binary:logistic', eval_metric = 'auc',
                                  verbose = 0)
            # Return tibble of holdout results:
            tibble(test pred probs =
                     as.numeric(predict(xgb_model, newdata = test_data_x, type = "response")),
                   test actual = as.numeric(test data$complete pass) - 1,
                   game fold = test fold)
```

```
1)
```

#### XGBoost

```
xgb_cv_preds %>%
 ggplot() +
 geom_roc(aes(d = test_actual,
              m = test_pred_probs,
               color = as.factor(game_fold)),
          n.cuts = 0) +
 style_roc() +
 geom_abline(slope = 1, intercept = 0,
              linetype = "dashed",
              color = "gray") +
 ggthemes::scale_color_colorblind() +
 labs(color = "Test fold") +
 theme(legend.position = "bottom")
xgb_cv_preds %>% group_by(game_fold) %>%
 summarize(auc = MLmetrics::AUC(test_pred_pr
                                 test_actual)
```

Should actually tune this more...

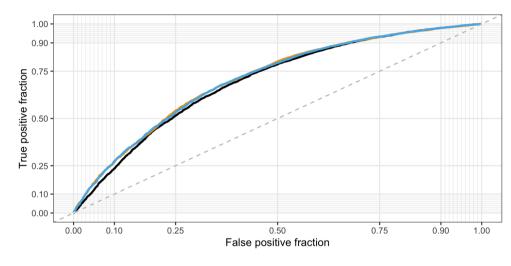


Test fold — 1 — 2 — 3 — 4 — 5

##	#	A tibble:	5 × 2
##		game_fold	auc
##		<int></int>	<dbl></dbl>
##	1	1	0.712
##	2	2	0.708
##	3	3	0.711
##	4	4	0.708
##	5	5	0.697

# All together now...

```
bind_rows(
 mutate(logit_cv_preds, type = "logit"),
 mutate(rf_prob_cv_preds, type = "RF"),
 mutate(xgb_cv_preds, type = "XGBoost")) %>%
 ggplot() +
 geom_roc(aes(d = test_actual,
              m = test_pred_probs,
               color = type),
           n.cuts = 0) +
 style_roc() +
 geom_abline(slope = 1, intercept = 0,
              linetype = "dashed",
              color = "gray") +
 ggthemes::scale_color_colorblind() +
 labs(color = "Model") +
 theme(legend.position = "bottom")
```





Pretty similar performance across all models...

### Explaining predictions with SHAP-values

SHAP-values are based on Shapley values (an idea from game theory) and are used to measure the contributions from each feature in the model to the prediction for an individual observation

Shapley value  $\phi_i^j$  for feature value j for observation i can be interpreted as:

- the value of feature j contributed  $\phi_i^j$  to the prediction of observation i compared to the average prediction for the dataset
- linear regression coefficients function in the same way

Can use them in multiple ways:

- View total importance:  $rac{1}{n}\sum |\phi_i^j|$
- View distribution of  $\phi_i^j$  for each feature
- Plot  $\phi_i^j$  against feature value for partial dependence

### SHAPforxgboost

#### Fit model on full data then extract SHAP-values with SHAPforxgboost

