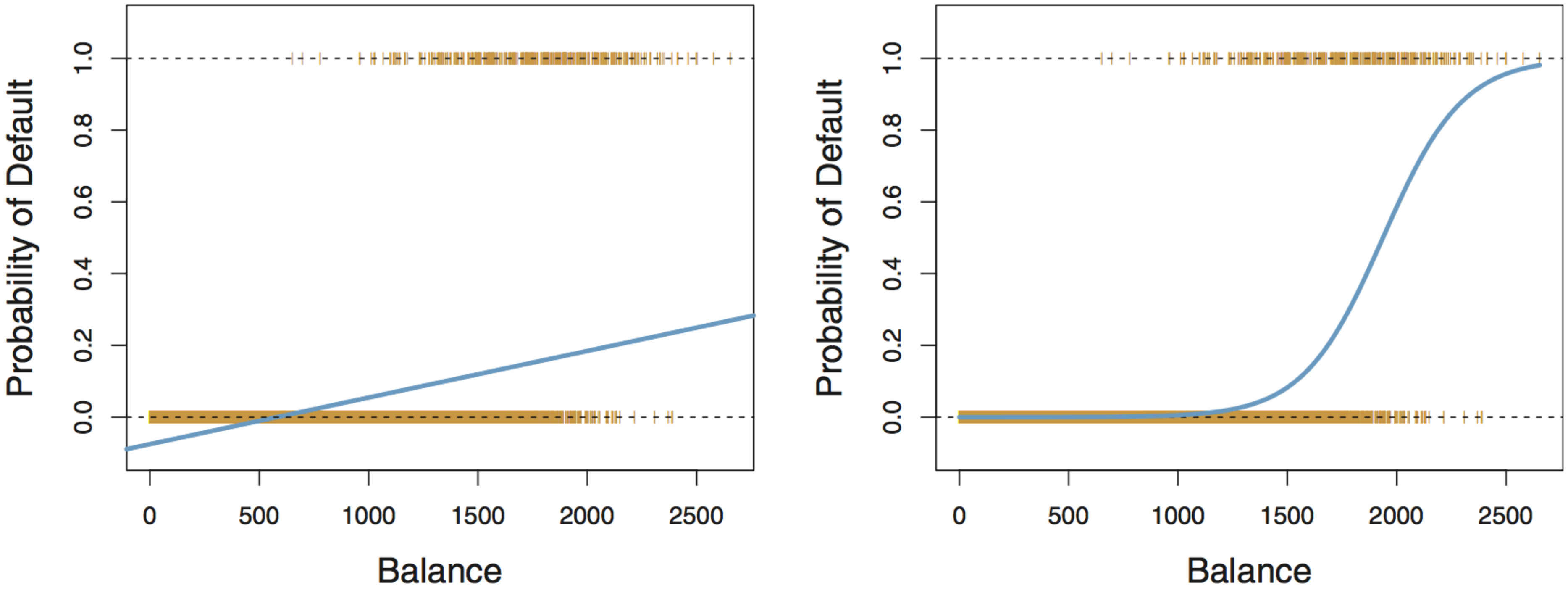
# Supervised Learning

## Logistic regression

June 29th, 2023

# The setting: Figure 4.2 (ISLR)




Left: Linear regression

- **not limited to be within [0, 1]!**

Right: **Logistic regression**

- **respects the observed range of outcomes!**

# Generalized linear models (GLMs) review

Linear regression: estimate **mean value** of response variable $Y$, given predictor variables $x_1, \ldots, x_p$:

$$\mathbb{E}[Y|x] = \beta_0 + \beta_1 x_1 + \cdots + \beta_p x_p$$

In a **GLM**, we include a **link function** $g$ that transforms the linear model:

$$g(\mathbb{E}[Y|x]) = \beta_0 + \beta_1 x_1 + \cdots + \beta_p x_p$$

- Use $g$ to reduce the range of possible values for $\mathbb{E}[Y|x]$ from $(-\infty, \infty)$ to, e.g., $[0, 1]$ or $[0, \infty)$, etc.

In a GLM you specify a **probability distribution family** that governs the observed response values

- e.g. if $Y$ are zero and the positive integers, the family could be Poisson
- e.g. if $Y$ are just 0 and 1, the family is Bernoulli and extends to Binomial for $n$ independent trials

# Logistic regression

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

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

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

$$\text{logit}(p(x)) = \log\left[\frac{p(x)}{1 - p(x)}\right] = \log\left[\frac{\mathbb{E}[Y|x]}{1 - \mathbb{E}[Y|x]}\right] = \beta_0 + \beta_1 x_1 + \cdots + \beta_p x_p$$

meaning

$$p(x) = \mathbb{E}[Y|x] = \frac{e^{\beta_0 + \beta_1 x_1 + \cdots + \beta_p x_p}}{1 + e^{\beta_0 + \beta_1 x_1 + \cdots + \beta_p x_p}}$$

# Major difference between linear and logistic regression

Logistic regression **involves numerical optimization**

- $y_i$ is observed response for $n$ observations - either 0 or 1
- we need to use an iterative algorithm to find $\beta$'s that maximize the **likelihood**

$$\prod_{i=1}^{n} p(x_i)^{y_i} (1 - p(x_i))^{1-y_i}$$

- **Newton's method**: start with initial guess, calculate gradient of log-likelihood, add amount proportional to the gradient to parameters, moving up log-likelihood surface
- means logistic regression runs more slowly than linear regression
- if you're interested: you use iteratively re-weighted least squares, Section 12.3.1

# Inference with logistic regression

**Major motivation** for logistic regression (and all GLMs) is **inference**

- how does the response change when we change a predictor by one unit?

For linear regression, the answer is straightforward

$$\mathbb{E}[Y|x] = \beta_0 + \beta_1 x_1$$

For logistic regression… it is a little *less* straightforward,

$$E[Y|x] = \frac{e^{\beta_0 + \beta_1 x_1 + \cdots + \beta_p x_p}}{1 + e^{\beta_0 + \beta_1 x_1 + \cdots + \beta_p x_p}}$$

- the predicted response varies **non-linearly** with the predictor variable values
- one convention is to fall back upon the concept of **odds**

# The odds interpretation

Pretend the predicted probability is 0.8 given a particular predictor variable value

- just pretend we only have one predictor variable

This means that if we were to repeatedly sample response values given that predictor variable value: **we expect class 1 to appear 4 times as often as class 0**

$$Odds = \frac{\mathbb{E}[Y|x]}{1-\mathbb{E}[Y|x]} = \frac{0.8}{1-0.8} = 4 = e^{\beta_0+\beta_1 x}$$

Thus we say that for the given predictor variable value, the $Odds$ are 4 (or 4-1) in favor of class 1

How does the odds change if I change the value of a predictor variable by one unit?

$$Odds_{\text{new}} = e^{\beta_0+\beta_1(x+1)} = e^{\beta_0+\beta_1 x}e^{\beta_1} = e^{\beta_1}Odds_{\text{old}}$$

For every unit change in $x$, the odds change by a **factor** $e^{\beta_1}$

# Example data: NFL field goal attempts

Created dataset using `nflscrapR-data` of all NFL field goal attempts from 2009 to 2019

```
nfl_fg_attempts <- read_csv("https://shorturl.at/mCGN2")
nfl_fg_attempts
```

```
## # A tibble: 10,811 × 11
##    kicker_player_id kicker_player_name   qtr score_differential home_team
##    <chr>            <chr>              <dbl>              <dbl> <chr>
##  1 00-0020962       R.Bironas              1                  0 PIT
##  2 00-0020962       R.Bironas              2                  0 PIT
##  3 00-0020962       R.Bironas              4                  0 PIT
##  4 00-0020737       J.Reed                 4                 -3 PIT
##  5 00-0020737       J.Reed                 5                  0 PIT
##  6 00-0004091       P.Dawson               1                  0 CLE
##  7 00-0010072       R.Longwell             1                 -3 CLE
##  8 00-0004091       P.Dawson               2                 -7 CLE
##  9 00-0010072       R.Longwell             4                 12 CLE
## 10 00-0006800       J.Hanson               1                -14 NO
## # ℹ 10,801 more rows
## # ℹ 6 more variables: posteam <chr>, posteam_type <chr>, kick_distance <dbl>,
## #   pbp_season <dbl>, abs_score_diff <dbl>, is_fg_made <dbl>
```

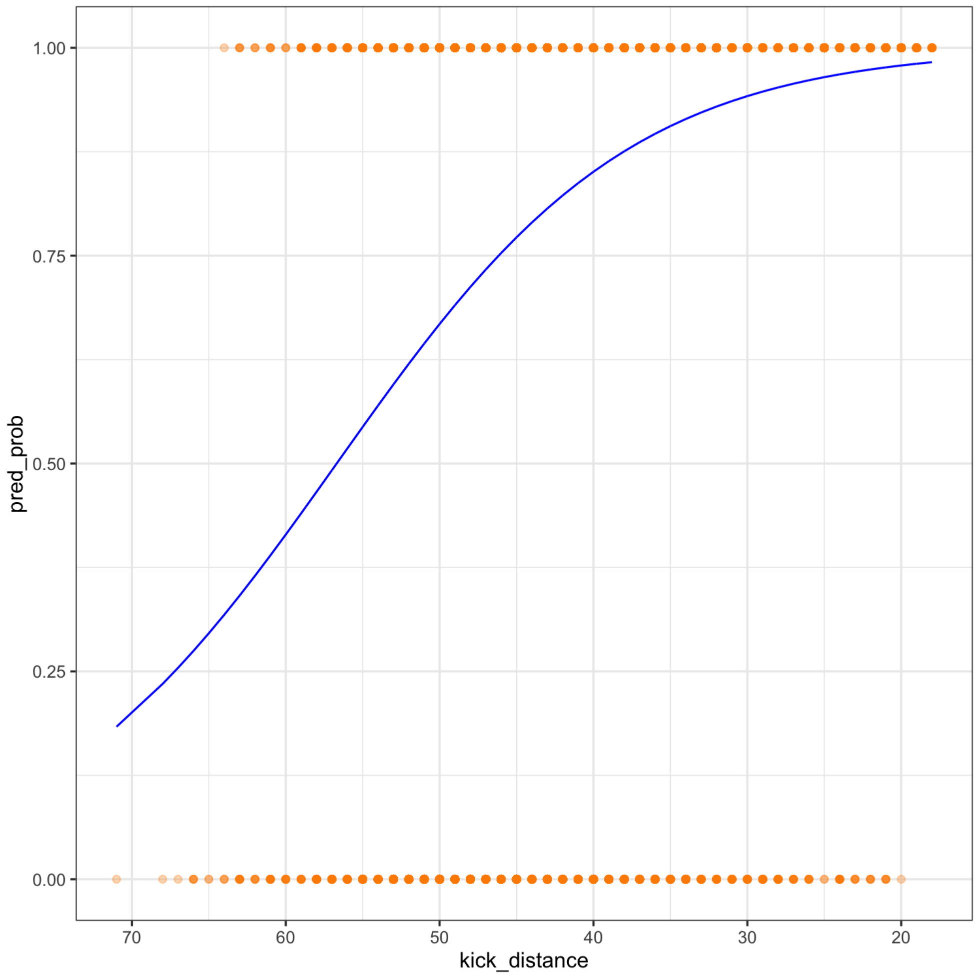
# Fitting a logistic regression model

- We use the `glm` function (similar to `lm`)
- **Specify the family is `binomial`**

```
init_logit <- glm(is_fg_made ~ kick_distance,
                  data = nfl_fg_attempts,
                  family = "binomial")
```

- View predicted probability relationship

```
nfl_fg_attempts %>%
  mutate(pred_prob = init_logit$fitted.values
  ggplot(aes(x = kick_distance)) +
  geom_line(aes(y = pred_prob),
            color = "blue") +
  geom_point(aes(y = is_fg_made),
             alpha = 0.3,
             color = "darkorange") +
  scale_x_reverse() +
  theme_bw()
```



```r
summary(init_logit)
```

```
##
## Call:
## glm(formula = is_fg_made ~ kick_distance, family = "binomial",
##     data = nfl_fg_attempts)
##
## Coefficients:
##                Estimate Std. Error z value Pr(>|z|)
## (Intercept)    5.916656   0.145371   40.70   <2e-16 ***
## kick_distance -0.104365   0.003255  -32.06   <2e-16 ***
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## (Dispersion parameter for binomial family taken to be 1)
##
##     Null deviance: 9593.1  on 10810  degrees of freedom
## Residual deviance: 8277.5  on 10809  degrees of freedom
## AIC: 8281.5
##
## Number of Fisher Scoring iterations: 5
```

# What is Deviance?

For model of interest $\mathcal{M}$ the total deviance is:

$$D_{\mathcal{M}} = -2\log\frac{\mathcal{L}_{\mathcal{M}}}{\mathcal{L}_{\mathcal{S}}} = 2\left(\log\mathcal{L}_{\mathcal{S}} - \log\mathcal{L}_{\mathcal{M}}\right)$$

- $\mathcal{L}_{\mathcal{M}}$ is the likelihood for model $\mathcal{M}$
- $\mathcal{L}_{\mathcal{S}}$ is the likelihood for the **saturated** model, with $n$ parameters! (i.e., a perfect fit)
- Can think of $\mathcal{L}_{\mathcal{S}}$ as some constant that does not change

**Deviance is a measure of goodness of fit**: the smaller the deviance, the better the fit

- Generalization of RSS in linear regression to any distribution family

# Logistic regression output

```
Deviance Residuals:
    Min       1Q   Median       3Q      Max
-2.7752   0.2420   0.4025   0.6252   1.5136
```

The **deviance residuals** are contributions to total deviance (signed square roots of unit deviances)

$$d_i = \text{sign}(y_i - \hat{p}_i)\sqrt{-2[y_i \log \hat{p}_i + (1 - y_i)\log(1 - \hat{p}_i)]}$$

where $y_i$ is the $i^{\text{th}}$ observed response and $\hat{p}_i$ is the estimated probability of success

```
Coefficients:
              Estimate Std. Error z value Pr(>|z|)
(Intercept)    5.916656   0.145371   40.70   <2e-16 ***
kick_distance -0.104365   0.003255  -32.06   <2e-16 ***
```

The intercept of the prediction curve is $e^{5.916656}$.

# Logistic regression output

```
    Null deviance: 9593.1  on 10810  degrees of freedom
Residual deviance: 8277.5  on 10809  degrees of freedom
AIC: 8281.5
```

```
logLik(init_logit)   # the maximum log-likelihood value
```

```
## 'log Lik.' -4138.732 (df=2)
```

- **Residual deviance** is -2 times -4138.732, or 8277.5 (*What about the saturated model?*)
    - Null deviance corresponds to intercept-only model
- AIC is $2k - 2\log\mathcal{L}$ = $2 \cdot k - 2 \cdot (-4138.732)$ = 8281.5
    - where $k$ is the number of degrees of freedom (here, `df` = 2)
- These are all metrics of quality of fit of the model
- **We will consider these to be less important than test-set performances**

# Logistic regression predictions

To generate logistic regression predictions there are few things to keep in mind...

- the `fitted.values` **are on the probability scale**: all are between 0 and 1
- but the **default** for `predict(init_logit)` is **the log-odds scale!**
- we change this with the `type` argument: `predict(init_logit, type = "response")`

How do we predict the class? e.g make or miss field goal?

```
pred_fg_outcome <- ifelse(init_logit$fitted.values > 0.5,
                          "make", "miss")
```

- typically if predicted probability is > 0.5 then we predict success, else failure

# Model assessment

Most straight-forward way is the **confusion matrix** (rows are predictions, and columns are observed):

```
table("Predictions" = pred_fg_outcome, "Observed" = nfl_fg_attempts$is_fg_made)
```

```
##              Observed
## Predictions     0    1
##         make 1662 8994
##         miss   94   61
```

**In-sample misclassification rate**:

```
mean(ifelse(fitted(init_logit) < 0.5, 0, 1) != nfl_fg_attempts$is_fg_made)
```

```
## [1] 0.1593747
```

**Brier score**:

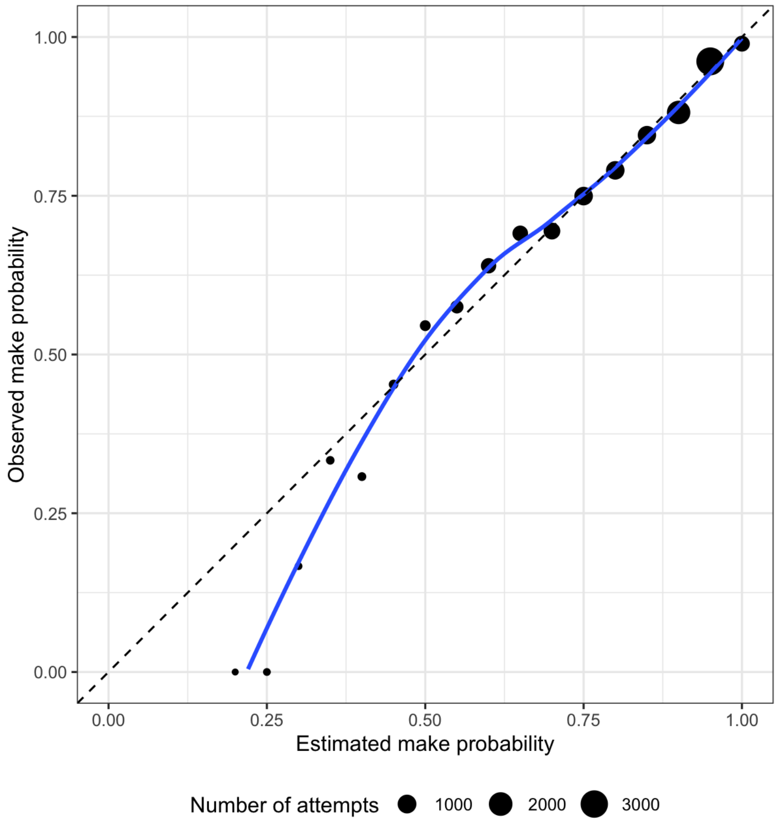
```
mean((nfl_fg_attempts$is_fg_made - fitted(init_logit))^2)
```

```
## [1] 0.1197629
```

# **Well-calibrated** if actual probabilities match predicted probabilities

```
nfl_fg_attempts %>%
  mutate(pred_prob = init_logit$fitted.values
         bin_pred_prob = round(pred_prob / 0.
  # Group by bin_pred_prob:
  group_by(bin_pred_prob) %>%
  # Calculate the calibration results:
  summarize(n_attempts = n(),
            bin_actual_prob = mean(is_fg_made
  ggplot(aes(x = bin_pred_prob, y = bin_actua
  geom_point(aes(size = n_attempts)) +
  geom_smooth(method = "loess", se = FALSE) +
  geom_abline(slope = 1, intercept = 0,
              color = "black", linetype = "da
  coord_equal() +
  scale_x_continuous(limits = c(0,1)) +
  scale_y_continuous(limits = c(0,1)) +
  labs(size = "Number of attempts",
       x = "Estimated make probability",
       y = "Observed make probability") +
  theme_bw() +
  theme(legend.position = "bottom")
```

If model says the probability of rain for a group of days is 50%, it better rain on half those days... **or something is incorrect about the probability!**



## BONUS: Leave-one-season-out cross validation (with `purrr`)

In many datasets rather than random holdout folds, you might have particular holdouts of interest (e.g. seasons, games, etc.)

```
nfl_fg_loso_cv_preds <- # generate holdout predictions for every row based season
  map_dfr(unique(nfl_fg_attempts$pbp_season),
          function(season) {
            # Separate test and training data:
            test_data <- nfl_fg_attempts %>%
              filter(pbp_season == season)
            train_data <- nfl_fg_attempts %>%
              filter(pbp_season != season)

            # Train model:
            fg_model <- glm(is_fg_made ~ kick_distance, data = train_data,
                            family = "binomial")

            # Return tibble of holdout results:
            tibble(test_pred_probs = predict(fg_model, newdata = test_data,
                                             type = "response"),
                   test_actual = test_data$is_fg_made,
                   test_season = season)
          })
```

# Overall holdout performance

**Misclassification rate**:

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

```
## # A tibble: 1 × 1
##     mcr
##   <dbl>
## 1 0.160
```

**Brier score**:

```
nfl_fg_loso_cv_preds %>%
  summarize(brier_score = mean((test_actual - test_pred_probs)^2))
```

```
## # A tibble: 1 × 1
##   brier_score
##         <dbl>
## 1       0.120
```

# Holdout performance by season

```
nfl_fg_loso_cv_preds %>%
  mutate(test_pred = ifelse(test_pred_probs < .5, 0, 1)) %>%
  group_by(test_season) %>%
  summarize(mcr = mean(test_pred != test_actual)) %>%
  ggplot(aes(x = test_season, y = mcr)) +
  geom_bar(stat = "identity", width = .1) + geom_point(size = 5) +
  theme_bw() +
  scale_x_continuous(breaks = unique(nfl_fg_loso_cv_preds$test_season))
```