432 Class 03

Thomas E. Love, Ph.D.

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Today's Agenda

- A First Example: Space Shuttle O-Rings
- Predicting a Binary outcome using a single predictor
  - using a linear probability model
  - using logistic regression and `glm`

See Chapters 19-20 in our Course Notes for more on logistic regression and related models.

Today's R Setup

```
knitr::opts_chunk$set(comment = NA)

library(janitor)
library(naniar)

library(broom)
library(caret)   # for confusion matrix
library(faraway) # data source
library(gt)
library(patchwork)

library(easystats)
library(tidyverse)

theme_set(theme_bw())
```


Challenger Space Shuttle Data

The US space shuttle Challenger exploded on 1986-01-28. An investigation ensued into the reliability of the shuttle's propulsion system. The explosion was eventually traced to the failure of one of the three field joints on one of the two solid booster rockets. Each of these six field joints includes two O-rings which can fail.

- The discussion among engineers and managers raised concern that the probability of failure of the O-rings depended on the temperature at launch, which was forecast to be 31 degrees F.
- There are strong engineering reasons based on the composition of O-rings to support the judgment that failure probability may rise monotonically as temperature drops.

We have data on 23 space shuttle flights that preceded *Challenger* on primary O-ring erosion and/or blowby and on the temperature in degrees Fahrenheit. No previous liftoff temperature was under 53 degrees F.

The "O-rings" data

- `damage` = number of damage incidents out of 6 possible
- we set `burst` = 1 if `damage` > 0

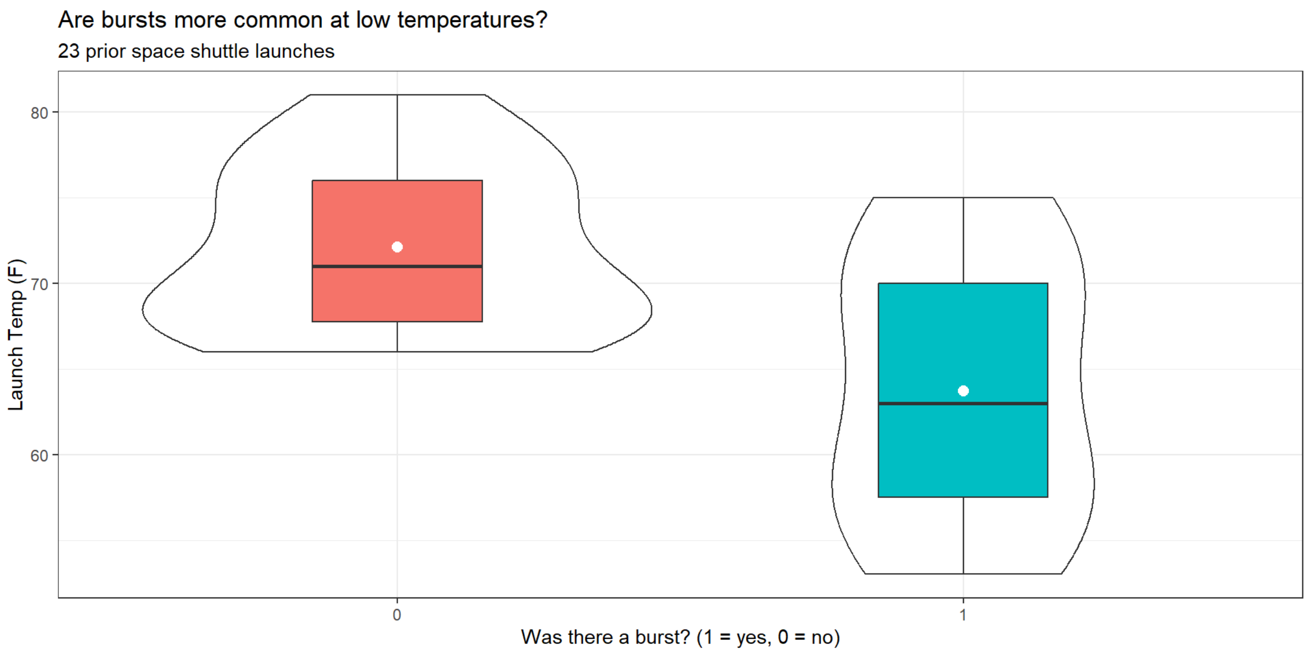
```r
orings1 <- faraway::orings |> tibble() |>
    mutate(burst = case_when( damage > 0 ~ 1, TRUE ~ 0))

orings1 |> summary()
```

```
      temp           damage           burst
 Min.   :53.00   Min.   :0.0000   Min.   :0.0000
 1st Qu.:67.00   1st Qu.:0.0000   1st Qu.:0.0000
 Median :70.00   Median :0.0000   Median :0.0000
 Mean   :69.57   Mean   :0.4783   Mean   :0.3043
 3rd Qu.:75.00   3rd Qu.:1.0000   3rd Qu.:1.0000
 Max.   :81.00   Max.   :5.0000   Max.   :1.0000
```


Association of `burst` and `temp`

```r
ggplot(orings1, aes(x = factor(burst), y = temp)) +
    geom_violin() +
    geom_boxplot(aes(fill = factor(burst)), width = 0.3) +
    stat_summary(geom = "point", fun = mean, col = "white", size = 2.5) +
    guides(fill = "none") +
    labs(title = "Are bursts more common at low temperatures?",
         subtitle = "23 prior space shuttle launches",
         x = "Was there a burst? (1 = yes, 0 = no)",
         y = "Launch Temp (F)")
```

Association of `burst` and `temp`



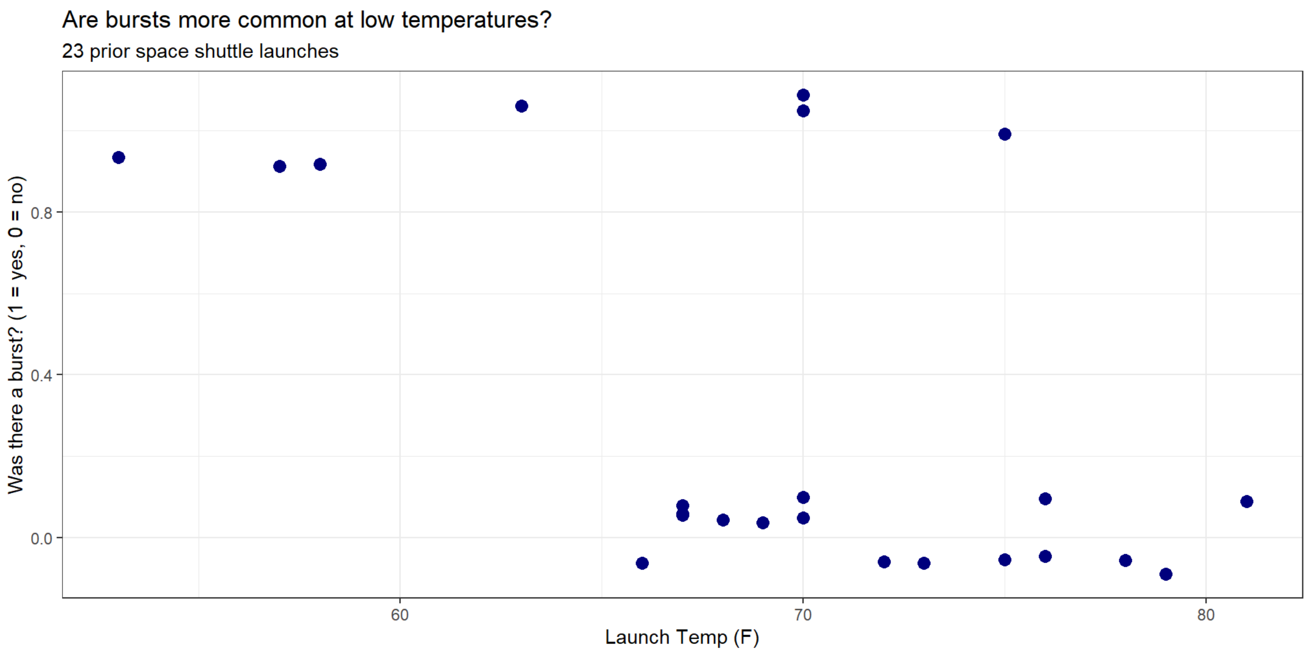
Predict Prob(burst) using temperature?

We want to treat the binary variable `burst` as the outcome, and `temp` as the predictor.

- We'll jitter the points vertically so that they don't overlap completely if we have two launches with the same temperature.

```
ggplot(orings1, aes(x = temp, y = burst)) +
    geom_jitter(col = "navy", size = 3, width = 0, height = 0.1) +
    labs(title = "Are bursts more common at low temperatures?",
         subtitle = "23 prior space shuttle launches",
         y = "Was there a burst? (1 = yes, 0 = no)",
         x = "Launch Temp (F)")
```

Predict Prob(burst) using temperature?



A Linear Probability Model, fit with `lm()`

Linear model to predict Prob(burst)?

```
fit1 <- lm(burst ~ temp, data = orings1)

tidy(fit1, conf.int = T) |> gt() |>
  fmt_number(decimals = 3) |> tab_options(table.font.size = 20)
```

term	estimate	std.error	statistic	p.value	conf.low	conf.high
(Intercept)	2.905	0.842	3.450	0.002	1.154	4.656
temp	−0.037	0.012	−3.103	0.005	−0.062	−0.012

- This is a **linear probability model.**

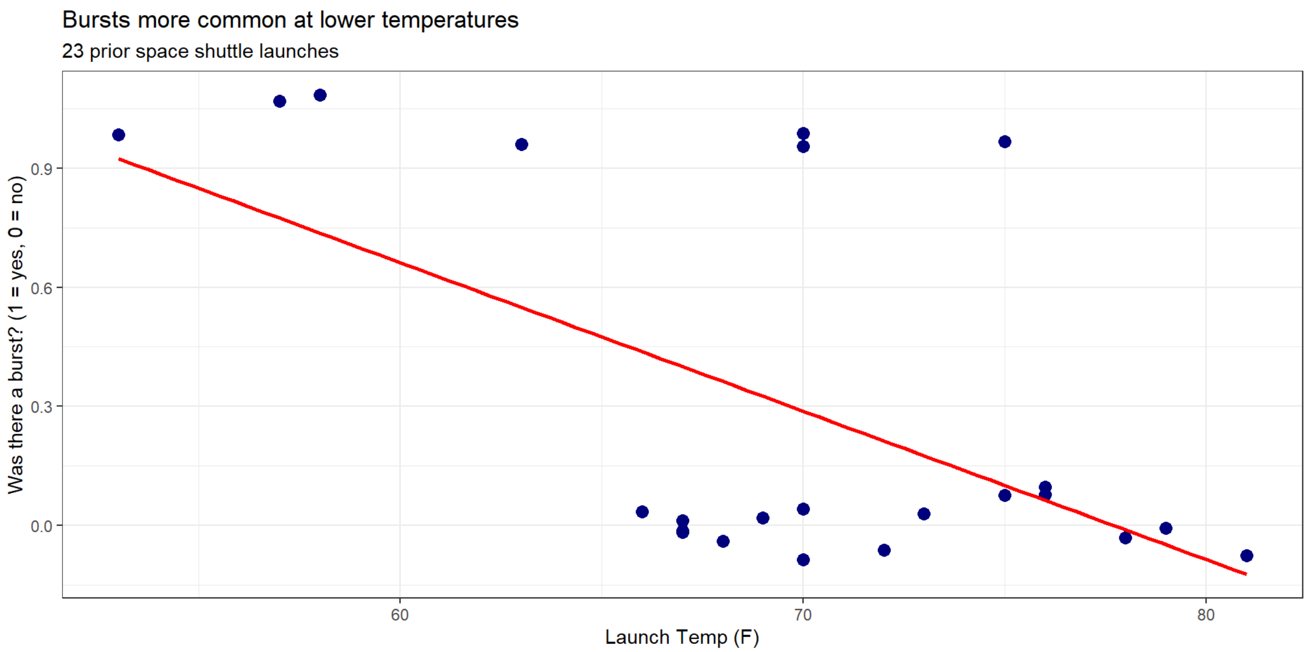
$$\widehat{\text{burst}} = 2.905 - 0.037(\text{temp})$$

Plot linear probability model?

```
ggplot(orings1, aes(x = temp, y = burst)) +
    geom_jitter(col = "navy", size = 3, width = 0, height = 0.1) +
    geom_smooth(method = "lm", se = F, col = "red",
                formula = y ~ x) +
    labs(title = "Bursts more common at lower temperatures",
         subtitle = "23 prior space shuttle launches",
         y = "Was there a burst? (1 = yes, 0 = no)",
         x = "Launch Temp (F)")
```

- It would help if we could see the individual launches…

Plot linear probability model?



Making Predictions with `fit1`

```
fit1$coefficients
```

```
(Intercept)        temp 
 2.90476190 -0.03738095 
```

- What does `fit1` predict for the probability of a burst if the temperature at launch is 70 degrees F?

```
predict(fit1, newdata = tibble(temp = 70))
```

```
        1 
0.2880952 
```

- What if the temperature was actually 60 degrees F?

Making Predictions with `fit1`

Let's use our linear probability model `fit1` to predict the probability of a burst at some other temperatures…

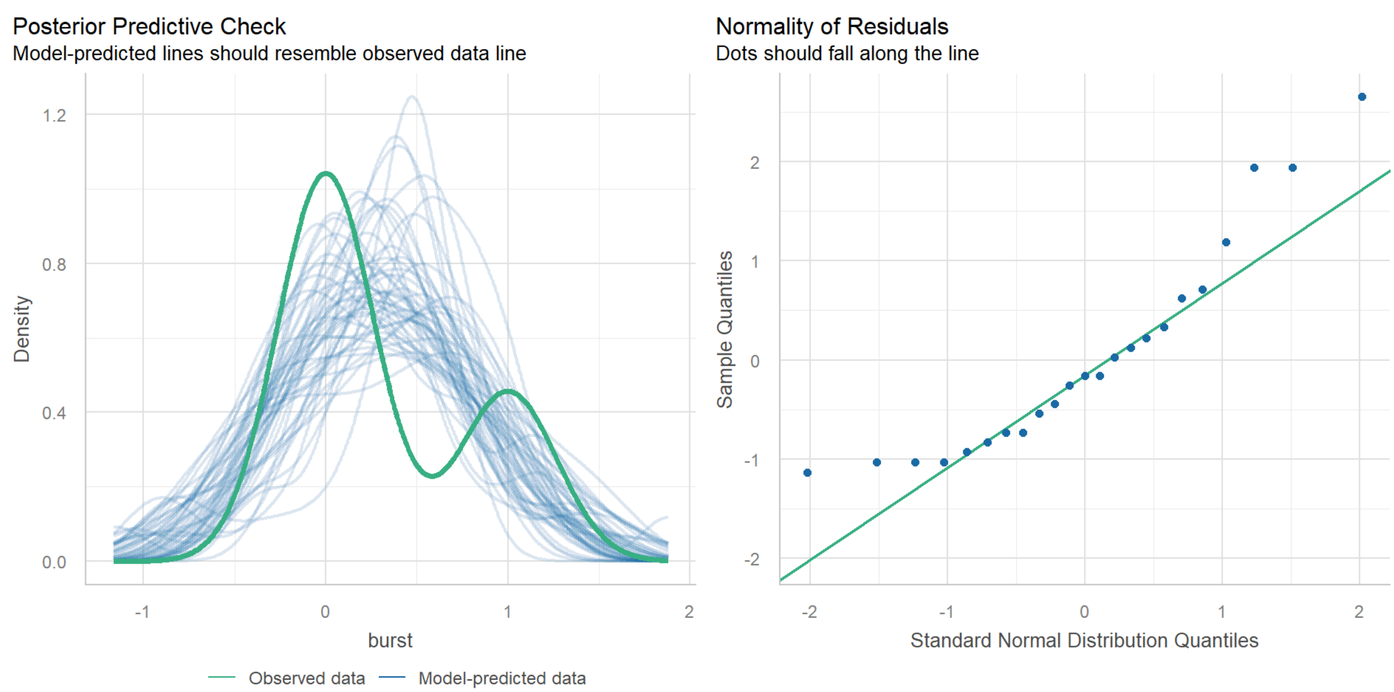
```
newtemps <- tibble(temp = c(80, 70, 60, 50, 31))

augment(fit1, newdata = newtemps)
```

```
# A tibble: 5 × 2
   temp .fitted
  <dbl>   <dbl>
1    80 -0.0857
2    70  0.288
3    60  0.662
4    50  1.04
5    31  1.75
```

- Uh, oh.

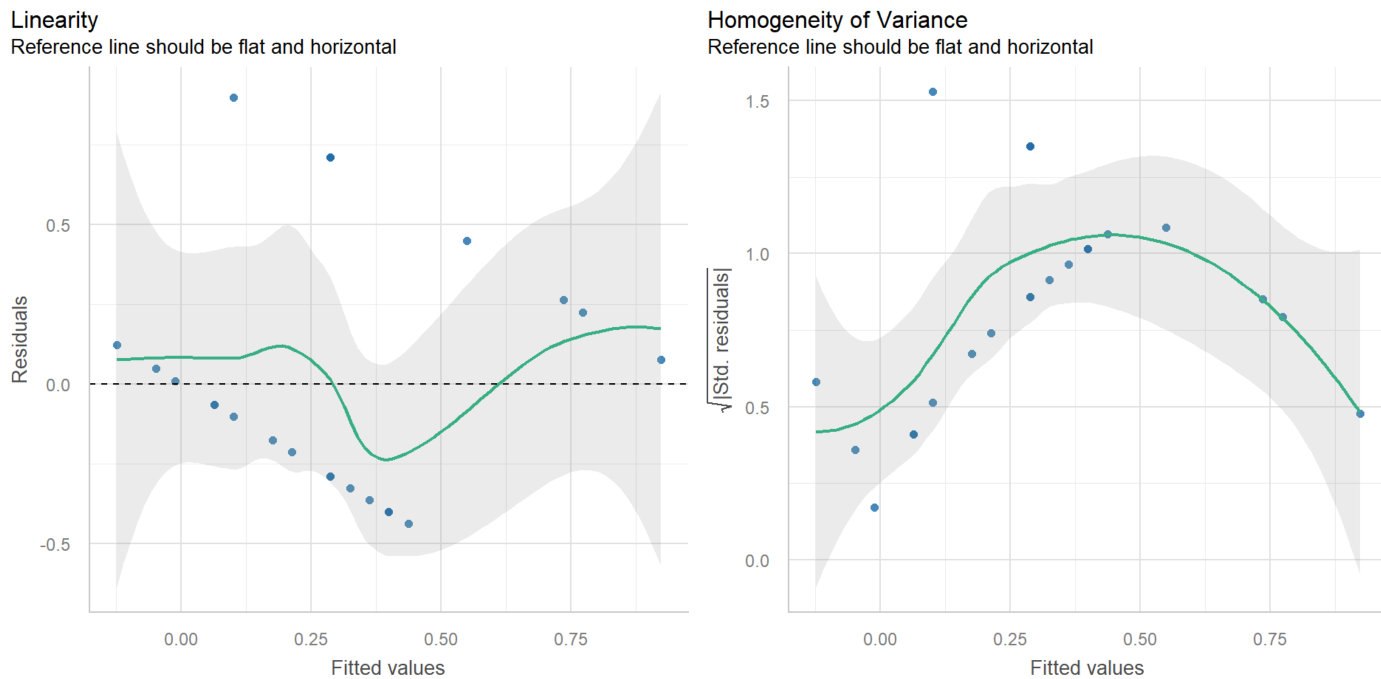
Checking model `fit1` (1/2)

```
check_model(fit1, detrend = FALSE, check = c("pp_check", "qq"))
```



Checking model `fit1` (2/2)

```r
check_model(fit1, detrend = FALSE, check = c("linearity", "homogeneity"))
```



Models to predict a Binary Outcome

Our outcome takes on two values (zero or one) and we then model the probability of a "one" response given a linear function of predictors.

Idea 1: Use a *linear probability model*

- Main problem: predicted probabilities that are less than 0 and/or greater than 1
- Also, how can we assume Normally distributed residuals when outcomes are 1 or 0?

Models to predict a Binary Outcome

Idea 2: Build a *non-linear* regression approach

- Most common approach: logistic regression, part of the class of *generalized* linear models

A Logistic Regression Model, fit with `glm()`

The Logit Link and Logistic Function

The function we use in logistic regression is called the **logit link.**

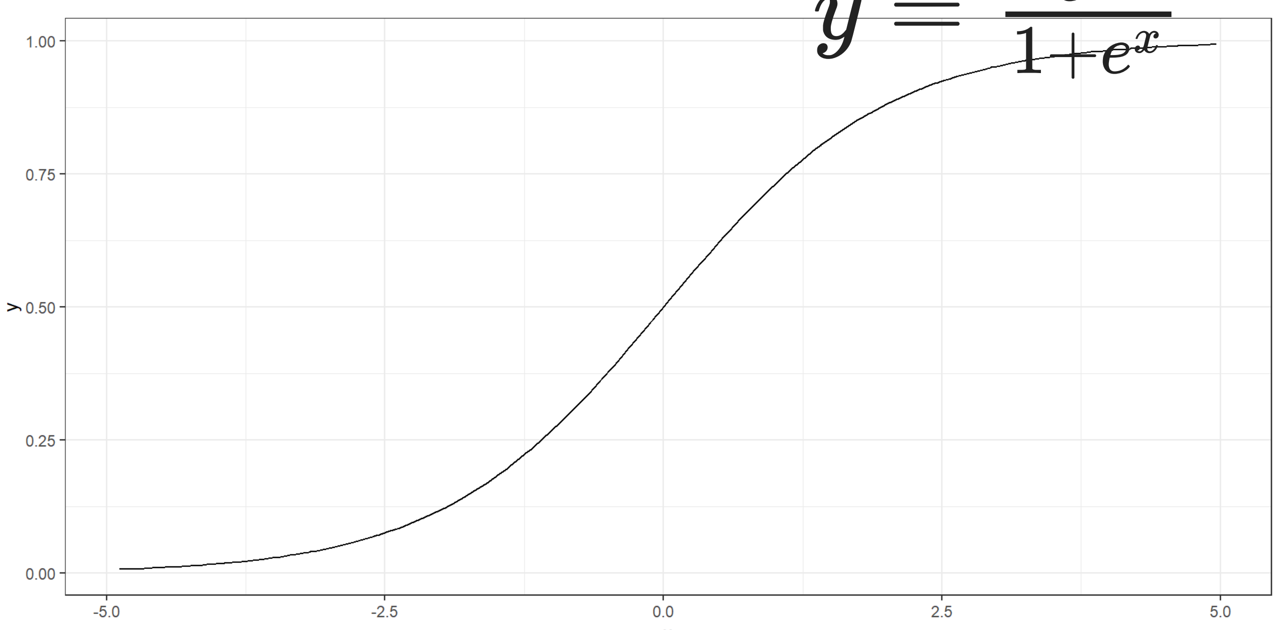
$$logit(\pi) = log\left(\frac{\pi}{1-\pi}\right) = \beta_0$$

The inverse of the logit function is called the **logistic function**. If logit(π) = η, then $\pi = \frac{exp(\eta)}{1+exp(\eta)}$.

- The logistic function $\frac{e^x}{1+e^x}$ takes any value x in the real numbers and returns a value between 0 and 1.

The Logistic Function

$$y = \frac{e^x}{1+e^x}$$



The logit or log odds

We usually focus on the **logit** in statistical work, which is the inverse of the logistic function.

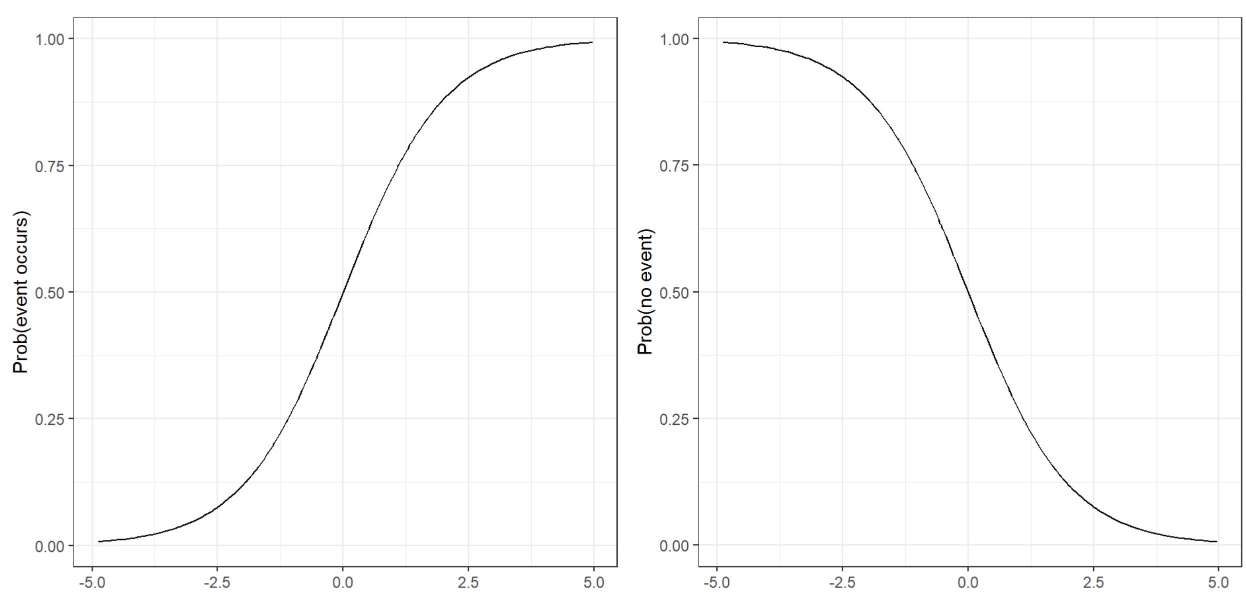
- If we have a probability $\pi < 0.5$, then $logit(\pi) < 0$.
- If our probability $\pi > 0.5$, then $logit(\pi) > 0$.
- Finally, if $\pi = 0.5$, then $logit(\pi) = 0$.

Why is this helpful?

- log(odds(Y = 1)) or logit(Y = 1) covers all real numbers.
- Prob(Y = 1) is restricted to [0, 1].

Predicting Pr(event) or Pr(no event)

- Can we flip the story?



Back to predicting Prob(burst)

We'll use the `glm` function in R, specifying a logistic regression model.

- Instead of predicting $Pr(burst)$, we're predicting $log(odds(burst))$ or $logit(burst)$.

`fit2` for Prob(burst)

```
fit2 <- glm(burst ~ temp, data = orings1,
            family = binomial(link = "logit"))

tidy(fit2, conf.int = TRUE) |> gt() |>
  fmt_number(decimals = 3) |> tab_options(table.font.size = 24)
```

term	estimate	std.error	statistic	p.value	conf.low	conf.high
(Intercept)	15.043	7.379	2.039	0.041	3.331	34.342
temp	−0.232	0.108	−2.145	0.032	−0.515	−0.061

$$\log\left[\frac{P(\widehat{\text{burst} = 1})}{1 - P(\widehat{\text{burst} = 1})}\right] = 15.$$

Understanding `fit2`'s predictions

- For a temperature of 70 F at launch, what is our prediction?
  - log(odds(burst)) = 15.043 - 0.232 (70) = -1.197
  - odds(burst) = exp(-1.197) = 0.302
  - so, we can estimate the probability by

$$Pr(burst) = \frac{0.302}{(0.302+1)} = 0.$$

Prediction from `fit2` for temp = 60

What is the predicted probability of a burst if the temperature is 60 degrees?

- log(odds(burst)) = 15.043 - 0.232 (60) = 1.123
- odds(burst) = exp(1.123) = 3.074
- Pr(burst) = 3.074 / (3.074 + 1) = 0.755

Using predict(fit2)

What is the predicted probability of a burst?

```
temps <- tibble(temp = c(40,50,60,70,80))

predict(fit2, newdata = temps, type = "link") # est. log odds of burst
```

```
        1         2         3         4         5 
 5.756392  3.434764  1.113137 -1.208490 -3.530118 
```

```
predict(fit2, newdata = temps, type = "response") # fitted Pr(burst)
```

```
         1          2          3          4          5 
0.99684747 0.96877352 0.75271348 0.22996826 0.02846733 
```


Will augment do this, as well?

Yes, and it will retain many more decimal places in intermediate calculations…

```
temps <- tibble(temp = c(60,70))

augment(fit2, newdata = temps, type.predict = "link")
```

```
# A tibble: 2 × 2
   temp .fitted
  <dbl>   <dbl>
1    60    1.11
2    70   -1.21
```

```
augment(fit2, newdata = temps, type.predict = "response")
```

```
# A tibble: 2 × 2
   temp .fitted
  <dbl>   <dbl>
1    60   0.753
2    70   0.230
```

A “Simple” Model Plot

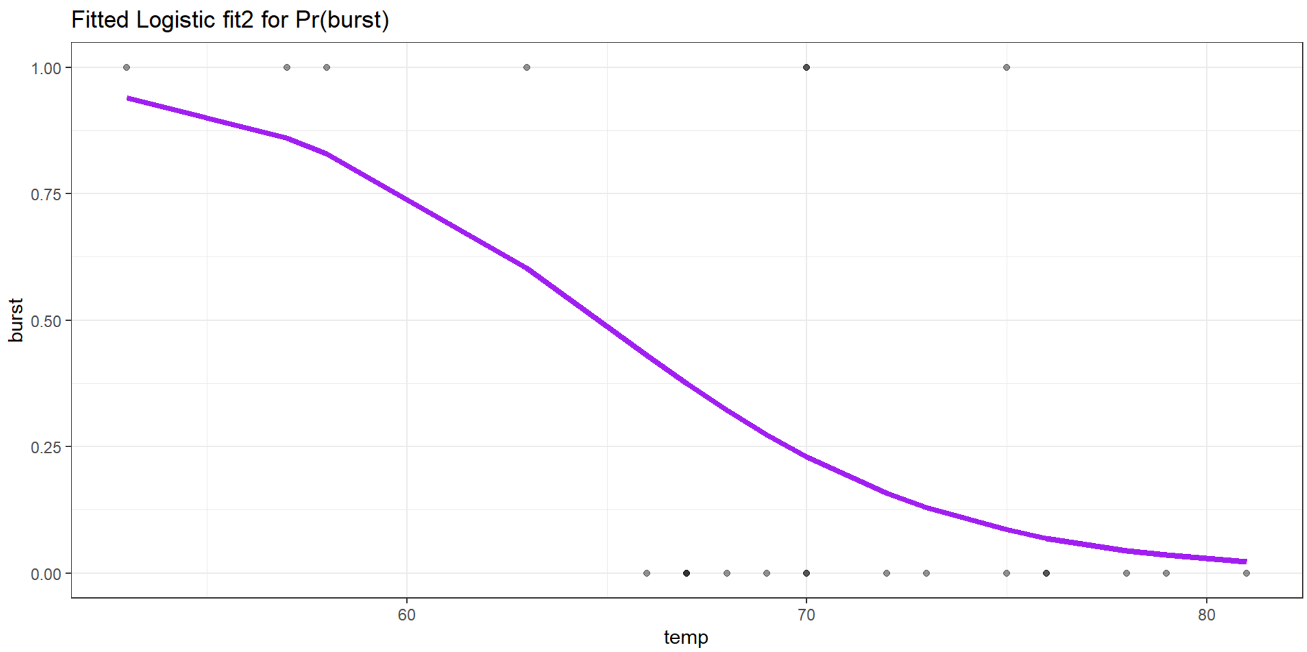
As we’ll see on the next slide, we will use the `augment` function to get the fitted probabilities into the original data, then plot.

- Note that we’re just connecting the predictions made for observed `temp` values with `geom_line`, so the appearance of the function isn’t as smooth as the actual logistic regression model.

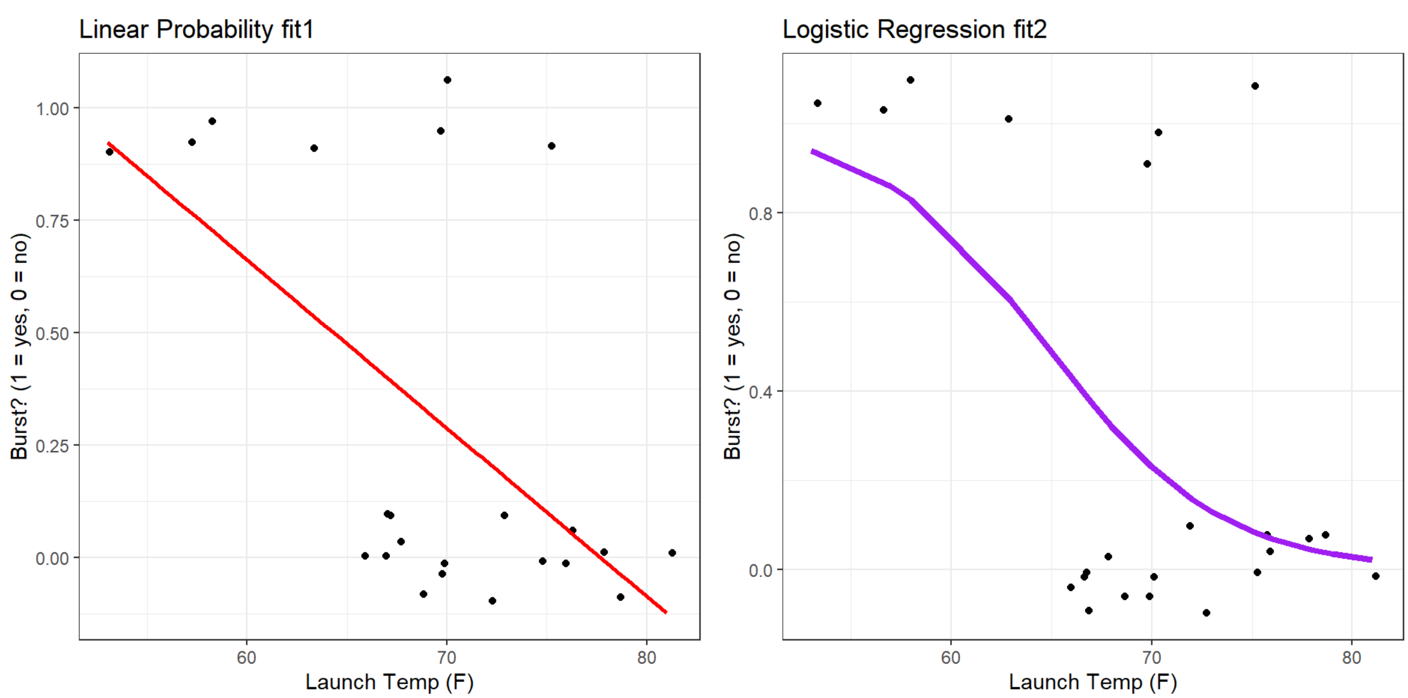
Plot our Model fit2

```
fit2_aug <- augment(fit2, type.predict = "response")

ggplot(fit2_aug, aes(x = temp, y = burst)) +
  geom_point(alpha = 0.4) +
  geom_line(aes(x = temp, y = .fitted),
            col = "purple", size = 1.5) +
  labs(title = "Fitted Logistic fit2 for Pr(burst)")
```

Plot our Model fit2



Comparing fits of `fit1` and `fit2`



Try exponentiating `fit2` coefficients?

How can we interpret the coefficients of the model?

$$logit(burst) = log(odds(burst)$$

Exponentiating the slope is helpful

```
exp(-0.232)
```

```
[1] 0.7929461
```


Exponentiating the slope helps

```
exp(-0.232)
```

```
[1] 0.7929461
```

Suppose Launch A's temperature was one degree higher than Launch B's.

- The **odds** of Launch A having a burst are 0.793 times as large as they are for Launch B.
- Odds Ratio estimate comparing two launches whose `temp` differs by 1 degree is 0.793

Exponentiated and tidied slope `fit2`

```
tidy(fit2, exponentiate = TRUE, conf.int = TRUE, conf.level = 0.90) |>
    filter(term == "temp") |>
    gt() |> fmt_number(decimals = 3) |>
    tab_options(table.font.size = 24)
```

term	estimate	std.error	statistic	p.value	conf.low	conf.high
temp	0.793	0.108	−2.145	0.032	0.632	0.919

- What would it mean if the Odds Ratio for `temp` was 1?
- How about an odds ratio that was greater than 1?

Standing Break

Regression on a Binary Outcome

Linear Probability Model (a linear model)

```
lm(event ~ predictor1 + predictor2 + ..., data = tibblename)
```

- Pr(event) is linear in the predictors

Logistic Regression Model (generalized linear model)

```
glm(event ~ pred1 + pred2 + ..., data = tibblename,
            family = binomial(link = "logit"))
```

- Logistic Regression forces a prediction in (0, 1)
- log(odds(event)) is linear in the predictors

The logistic regression model

$$logit(event) = log\left(\frac{Pr(event)}{1 - Pr(event)}\right)$$

$$odds(event) = \frac{Pr(event)}{1 - Pr(event)}$$

$$Pr(event) = \frac{odds(event)}{odds(event) + 1}$$

$$Pr(event) = \frac{exp(logit(event))}{1 + exp(logit(event))}$$

`model_parameters()` for `fit2`

```
1  model_parameters(fit2, ci = 0.90)
```

```
Parameter   | Log-Odds |   SE |         90% CI |     z |     p
--------------------------------------------------------------
(Intercept) |    15.04 | 7.38 | [ 4.95, 30.48] |  2.04 | 0.041
temp        |    -0.23 | 0.11 | [-0.46, -0.08] | -2.14 | 0.032

Uncertainty intervals (profile-likelihood) and p-values (two-tailed)
  computed using a Wald z-distribution approximation.

The model has a log- or logit-link. Consider using `exponentiate =
  TRUE` to interpret coefficients as ratios.
```

Odds Ratios from `model_parameters()`

```
1  model_parameters(fit2, exponentiate = TRUE, ci = 0.90)
```

```
Parameter   | Odds Ratio |       SE |               90% CI |     z |     p
--------------------------------------------------------------------------
(Intercept) |   3.41e+06 | 2.52e+07 | [141.15, 1.73e+13] |  2.04 | 0.041
temp        |       0.79 |     0.09 | [  0.63,     0.92] | -2.14 | 0.032
```


model `fit2` slope (and CI)

Sample odds ratio for `temp` is 0.79, with 90% CI (0.63, 0.92)

- If launch 1 has a temperature 1 degree colder than launch 2, then our model estimates the odds of a burst to be 0.79 times as large (79% as large) for launch 2 as for launch 1.
- If our sample of launches was a random sample, then our 90% confidence interval suggests that if we generalize to the population of launches, then our data are consistent (at the 90% confidence level) with odds ratios between 0.63 and 0.92, assuming logistic regression assumptions are met.

Compare `fit2` to a null model

- Likelihood Ratio test compares `fit2` to a model with only an intercept term (no `temp` information)

```
anova(fit2, test = "LRT")
```

```
Analysis of Deviance Table

Model: binomial, link: logit

Response: burst

Terms added sequentially (first to last)

     Df Deviance Resid. Df Resid. Dev Pr(>Chi)
NULL                    22     28.267
temp  1    7.952        21     20.315 0.004804 **
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
```


Other ANOVA options

- We can also get Rao's efficient score test (`test = "Rao"`) or Pearson's chi-square test (`test = "Chisq"`)

```
anova(fit2, test = "Rao")
```

```
Analysis of Deviance Table

Model: binomial, link: logit

Response: burst

Terms added sequentially (first to last)

     Df Deviance Resid. Df Resid. Dev    Rao Pr(>Chi)
NULL                    22     28.267
temp  1    7.952        21     20.315 7.2312 0.007165 **
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
```

Evaluating how well a logistic regression model predicts the outcome

AUC and evaluating prediction quality

The Receiver Operating Characteristic (ROC) curve is the first approach we'll discuss today.

- Specifically, we will calculate the Area under this curve (sometimes labeled AUC or just C).

```
performance_roc(fit2)
```

```
AUC: 78.57%
```

- AUC falls between 0 and 1, and we interpret its result using the table on the next slide…

Interpreting the AUC (C statistic)

AUC	Interpretation
0.5	A coin-flip. Model is no better than flipping a coin.
0.6	Still a fairly weak model.
0.7	Low end of an "OK" model fit.
0.8	Pretty good predictive performance.
0.9	Outstanding predictive performance.
1.0	Perfect predictive performance.

Recall that our `fit2` has AUC = 0.7857.

Classification Table (Confusion Matrix)

1. Select a decision rule.
   - We'll predict burst = 1 if `fit2` model predicted probability > 0.5
2. Build a set of predictions, and make them a factor.

```
fit2_preds <- as_factor(ifelse(predict(fit2, type = "response") > 0.5, 1, 0))
```

3. Ensure the factor has "event occurs" first.

```
fit2_preds <- fct_relevel(fit2_preds, "1", "0")
```

Classification Table

4. Obtain the actual "event" status, as a factor

```
fit2_actual <- fct_relevel(as_factor(orings1$burst), "1", "0")
```

5. Build the table

```
fit2_tab <- table(predicted = fit2_preds, actual = fit2_actual)
fit2_tab
```

```
         actual
predicted  1  0
        1  4  0
        0  3 16
```

- Of the 4 launches predicted to have a burst, all 4 did.
- Of the 19 launches predicted to have no burst, 3 actually had a burst.

Confusion Matrix Summaries

```
fit2_tab
```

```
         actual
predicted  1  0
        1  4  0
        0  3 16
```

A more complete Set of Summaries

```
confusionMatrix(fit2_tab)
```

```
Confusion Matrix and Statistics

         actual
predicted  1  0
        1  4  0
        0  3 16

               Accuracy : 0.8696
                 95% CI : (0.6641, 0.9722)
    No Information Rate : 0.6957
    P-Value [Acc > NIR] : 0.04928

                  Kappa : 0.6497
```


Quality of Fit with `glance()` (1/2)

```
glance(fit2)
```

```
# A tibble: 1 × 8
  null.deviance df.null logLik   AIC   BIC deviance df.residual  nobs
          <dbl>   <int>  <dbl> <dbl> <dbl>    <dbl>       <int> <int>
1          28.3      22  -10.2  24.3  26.6     20.3          21    23
```

- `nobs` = we fit `fit2` using 23 observations
- null model (intercept) has 22 residual df (`df.null`) with `null.deviance` of 28.3
- `fit2` (includes `temp`) has 21 residual df (`df.residual`) with `deviance` of 20.3
  - The deviance quantifies what the model **doesn't** explain

Quality of Fit with `glance()` (2/2)

```
glance(fit2) |>
  gt() |>
  fmt_number(columns = c(-df.null, -df.residual, -nobs), decimals = 2) |>
  tab_options(table.font.size = 24)
```

null.deviance	df.null	logLik	AIC	BIC	deviance	df.residual	nobs
28.27	22	−10.16	24.32	26.59	20.32	21	23

- Our `fit2` has `deviance` = -2*log likelihood (`logLik`)
- `AIC` and `BIC` are for comparing models for the same outcome, as in linear regression (smaller values indicate better fits, as usual.)

`model_performance(fit2)` (1/5)

```
model_performance(fit2)
```

```
# Indices of model performance

AIC  | AICc |  BIC | Tjur's R2 |  RMSE | Sigma | Log_loss | Score_log
---------------------------------------------------------------------
24.3 | 24.9 | 26.6 |     0.338 | 0.372 |     1 |    0.442 |    -2.957

AIC  | Score_spherical |   PCP
------------------------------
24.3 |           0.149 | 0.720
```

- `AIC` and `BIC` are Akaike and Bayes information criteria
- `AICc` is a corrected AIC (correction for small sample size)
- `Sigma` is the estimated residual standard deviation
- `RMSE` estimates the root mean squared error

`model_performance(fit2)` (2/5)

$$\text{Tjur's R2} = 0.338 \text{ for fit2}$$

- `Tjur's R2` is Tjur's coefficient of determination. Higher values indicate better fit.
  - Other choices: Cox-Snell R^2, Nagelkerke R^2, McFadden R^2.
  - These pseudo-R^2 measures do **some** of what R^2 does in linear regression are available in logistic regression.
  - Pseudo-R^2 measures don't describe proportionate reduction in error.
- Tjur's R^2 can be calculated as follows:
  - For each level of the dependent variable, find the mean of the predicted probabilities of an event.
  - Take the absolute value of the difference between these means.

`model_performance(fit2)` (3/5)

$$\text{Log\_loss} = 0.442 \text{ for fit2}$$

- `Log_loss` quantifies prediction quality. If y_i is the actual/true value (1 or 0), p_i is the predicted probability, and ln is the natural logarithm, then:

$$\text{Log\_loss}_i = -[y_i ln(p_i) + (1 -$$

- Model `Log_loss` = sum of individual `Log_loss` values.
- **Lower** `Log_loss` values indicate better predictions.

`model_performance()` (4/5)

```
Score_log | Score_spherical
---------------------------
   -2.957 |           0.149
```

- `Score_log` and `Score_spherical` are two other scoring rules for predictive performance in a logistic regression.
- `Score_log` takes values from [-, 0] with values closer to 0 indicating a more accurate model.
- `Score_spherical` takes values from [0, 1] with values closer to 1 indicating a more accurate model.
- See this link for more details.

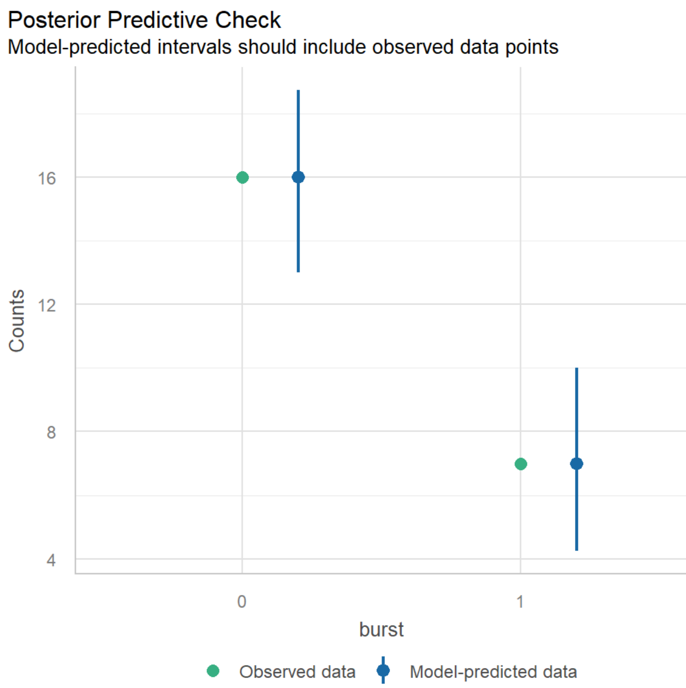
`model_performance()` (5/5)

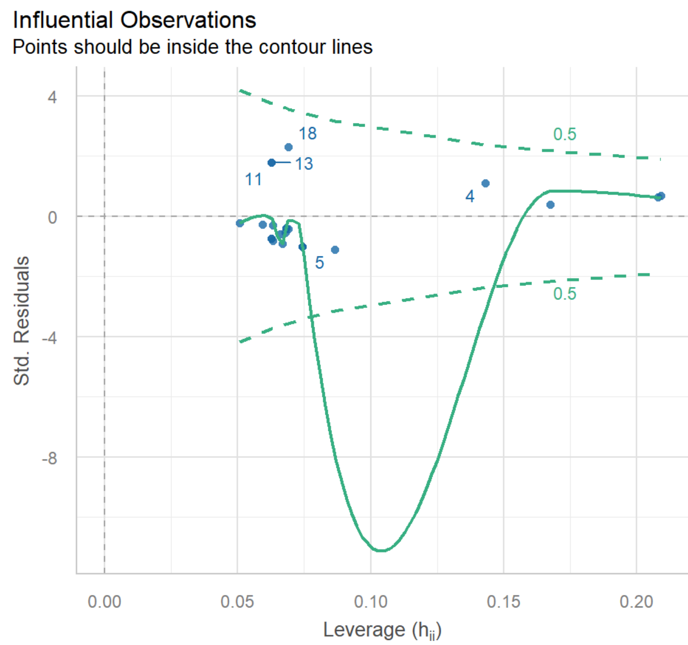
$$\text{PCP} = 0.720 \text{ for fit2}$$

- `PCP` is called the percentage of correct predictions
- `PCP` = sum of predicted probabilities where y=1, plus the sum of 1 - predicted probabilities where y=0, divided by the number of observations
  - `PCP` ranges from 0 (worst) to 1 (best).
  - In general, the PCP should exceed 0.5.
- See this link for more details.

Checking the fit2 model

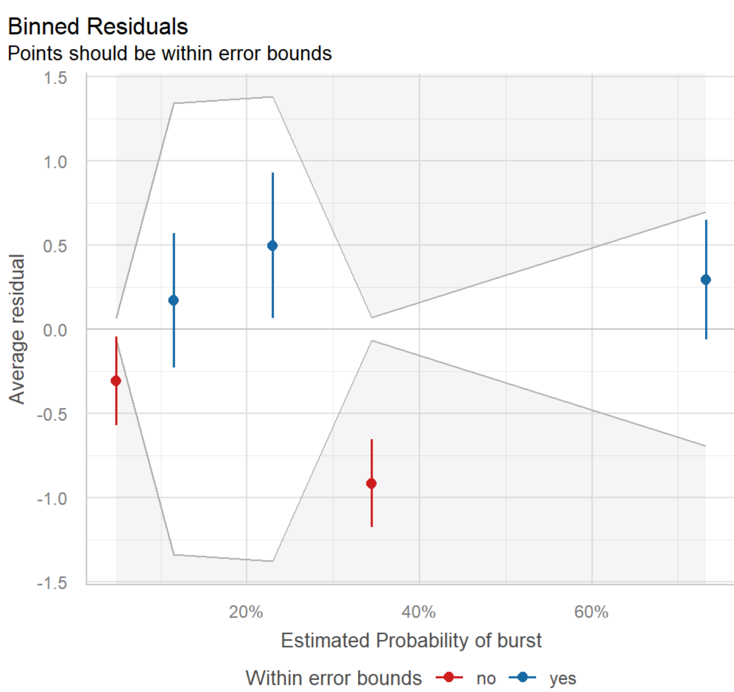
```r
check_model(fit2, check = c("pp_check", "outliers"))
```





Checking the fit2 model

```r
check_model(fit2, check = c("binned_residuals", "qq"))
```



Coming Up…

- The next several classes will be dedicated to providing more examples and more tools for working with linear regression and with logistic regression models.
- You should now have everything you need to do Lab 2.