# PM 592 Regression Analysis for Public Health Data Science

Week 9

**Logistic Regression II** 

# Logistic Regression II

**Assessing Assumptions** 

**Goodness of Fit** 

**Model Diagnostics** 

**Model Selection** 

# **Lecture Objectives**

- > Determine whether a logistic regression model is well-fit.
- > Identify outliers in logistic regression.
- > Explain and assess the assumptions of logistic regression.
- ➤ Describe the advantages and disadvantages of automated selection procedures.

- ✓ Three ways to measure the effect on a binary outcome
- ✓ 2x2 contingency tables, odds, the odds ratio
- ✓ The concept of a "link" function
- ✓ The logit link computing an odds ratio
- ✓ The logit link computing predicted probabilities

# **Example**

In a study of 508 adults, vital characteristics (e.g. blood pressure, height, weight) and presence of coronary calcium (a measure of blockage in the arteries of the heart) was assessed.

What is the relationship between age and SBP with presence of coronary calcium?

```
> corcalc %>%
   select(age, sbp, cor_calcium) %>%
   psych::describe()
                          sd median trimmed mad min max range skew kurtosis
                   mean
                                                        56 -0.15
            1 506 60.76 9.94
                                    60.98 10.38 32 88
                                                                  -0.47 0.44
age
sbp
       2 506 129.64 16.86
                               128 128.73 17.79 90 200 110 0.57 0.61 0.75
                                     0.43 0.00 0 1 1 0.24
                                                                  -1.95 0.02
cor calcium 3 506 0.44 0.50 0
```

sbp

```
Call:
glm(formula = cor_calcium ~ sbp, family = binomial, data = corcalc)

Deviance Residuals:
    Min    1Q    Median    3Q    Max
-1.4240   -1.0778   -0.9876    1.2592    1.4615

Coefficients:
```

0.00537 2.126 0.0335 \*

Estimate Std. Error z value Pr(>|z|)

0.01142

We know this is a logistic regression because we specified "family = binomial".

SBP is significantly related to coronary calcium. The odds ratio associated with a 1-unit increase in SBP is exp(0.01142) = 1.011. Since this is a small odds ratio, it might help to instead interpret the odds ratio for a 10-unit increase in SBP. This odds ratio would be exp(10\* 0.01142) = 1.12.

"A 10-unit increase in SBP is associated with 1.12 times the odds of coronary calcium."

"A 10-unit increase in SBP increases the likelihood of coronary calcium by 12%."

age

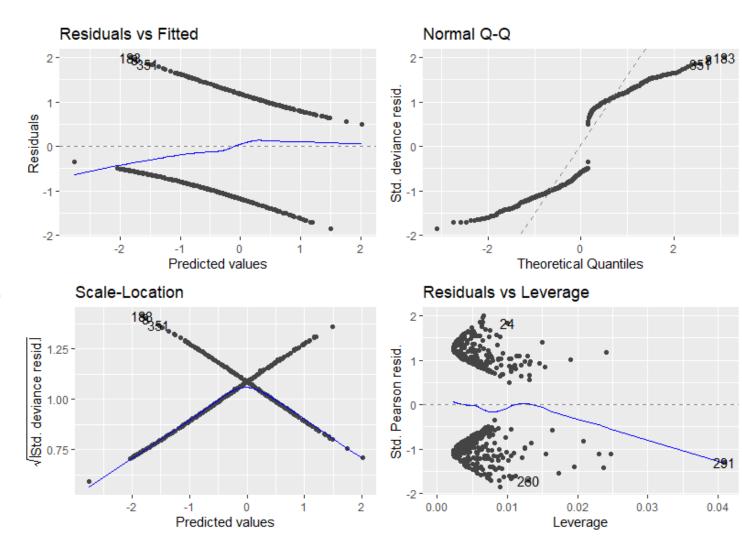
```
Call:
glm(formula = cor calcium ~ sbp, family = binomial, data = corcalc)
Deviance Residuals:
   Min
          1Q Median
                         3Q
                               Max
-1.4240 -1.0778 -0.9876 1.2592
                            1.4615
Coefficients:
         Estimate Std. Error z value Pr(>|z|)
sbp
          0.01142 0.00537 2.126 0.0335 *
Call:
glm(formula = cor_calcium ~ sbp + age, family = binomial,
data = corcalc)
Deviance Residuals:
   Min
          10 Median
                         3Q
                               Max
-1.8395 -1.0011 -0.5806 1.0914
                             1.9891
Coefficients:
          Estimate Std. Error z value Pr(>|z|)
-0.003940 0.005965 -0.661
                                  0.509
sbp
```

After adjusting for age, SBP does not appear to be related to presence of coronary calcium (p=.51).

#### How do the residuals look?

Because we are comparing observed values of Y (that can only take on the values of 0 and 1) with predicted probabilities  $\hat{\pi}$ , our residuals are going to look a lot weirder than usual.

In fact, the assumptions of OLS (ordinary least squares) regression do not apply for this type of modeling.



Here, we will go over the usual assumptions of linear regression and see how they apply to logistic regression.

- **Linearity** X and Y cannot be linearly related if Y is binary. However we <u>do</u> assume linearity *in the logit*.
- Independence we do assume all X are independent of each other.
- Normality we do not assume that the residuals are normally distributed.
- **Equal Variances** we <u>do not</u> assume that the residuals have constant variance over all X values.

That said, the primary assumption we need to check is that of linearity. In logistic regression it is slightly more difficult to do because:

- Due to the binary nature of the outcome, we can not directly observe a linear effect.
- We assume linearity in the logit instead of linearity in Y.

There are 3 methods of assessing the linearity assumption on the logit scale:

- 1. Grouped Smooth
- 2. Lowess Smoothing
- 3. Fractional Polynomials

```
> glm(cor calcium ~ age,
     data = corcalc,
     family = binomial) %>%
   summary()
Call:
glm(formula = cor_calcium ~ age, family = binomial, data = corcalc)
Deviance Residuals:
                                   Max
   Min
            10 Median
                            3Q
-1.8281 -1.0034 -0.5915 1.0805
                                1.9844
Coefficients:
          Estimate Std. Error z value Pr(>|z|)
0.08203
                     0.01085 7.562 3.96e-14 ***
age
Signif. codes: 0 '*** 0.001 '** 0.01 '* 0.05 '.' 0.1 ' '1
(Dispersion parameter for binomial family taken to be 1)
   Null deviance: 694.33 on 505 degrees of freedom
Residual deviance: 625.93 on 504 degrees of freedom
AIC: 629.93
Number of Fisher Scoring iterations: 4
```

A 1-year increase in age is associated with exp(0.082) = 1.085 times the odds of coronary calcium (p<.001).

This model assumes a linear effect of age – the effect of age on odds of coronary calcium is the same across all values of age.

# **Grouped Smooth**

Strategy: Group the x observations by quantiles, then see if the quantile groupings are linearly related to the logit.

- 1. Create a dummy variable set that indicates which quantile the individual's observation belongs to.
- 2. Fit the model, getting a beta term for each quantile indicator relative to quantile 1.
- 3. Assign the midpoint value to the quantile and plot the beta coefficients vs. the midpoint values.
- 4. Re-parameterize x as the plot suggests (e.g.,  $x^2$ ).

First, let's create and verify age quartiles.

```
corcalc <-
  corcalc %>%
 mutate(age.q4 =
          cut(age,
               breaks = quantile(age, probs = 0:4/4),
               include.lowest = T))
> corcalc %>%
   group_by(age.q4) %>%
    summarise(
     mean = mean(age, na.rm=T),
     min = min(age, na.rm=T),
     max = max(age, na.rm=T),
          = n())
     n
`summarise()` ungrouping output (override with `.groups` argument)
# A tibble: 4 x 5
                 min
  age.q4
          mean
                       max
                               n
 <fct> <dbl> <dbl> <dbl> <int>
1 [32,54] 47.9
                  32
                        54
                             131
2 (54,61] 58.0
                  55
                      61
                             126
3 (61,68] 64.6
                  62
                      68
                             125
4 (68,88]
         73.4
                  69
                        88
                             124
```

> glm(cor calcium ~ age.q4,

# Then, regress coronary calcium on age quartile.

```
data = corcalc,
     family = binomial) %>%
   summary()
Call:
glm(formula = cor calcium ~ age.q4, family = binomial, data = corcalc)
Deviance Residuals:
                                       Max
   Min
             10 Median
                               30
-1.4395 -0.9400 -0.7212
                           1.1035
                                    1.7170
Coefficients:
             Estimate Std. Error z value Pr(>|z|)
(Intercept)
              -1.2139
                          0.2079 -5.838 5.28e-09 ***
age.q4(54,61] 0.6261 0.2789 2.245
                                           0.0248 *
age.q4(61,68]
                          0.2747
                                   5.061 4.18e-07 ***
               1.3904
                                   6.468 9.93e-11 ***
age.q4(68,88]
               1.8118
                          0.2801
```

These coefficients reflect the change in the logit compared to the reference group.

Compared to the lowest quartile, those in the second age quantile have  $\exp(0.626) = 1.87$  times the odds of coronary calcium (p=.025).

The global test (Likelihood Ratio vs. the null model) shows us that these variables, as a set, are related to coronary calcium.

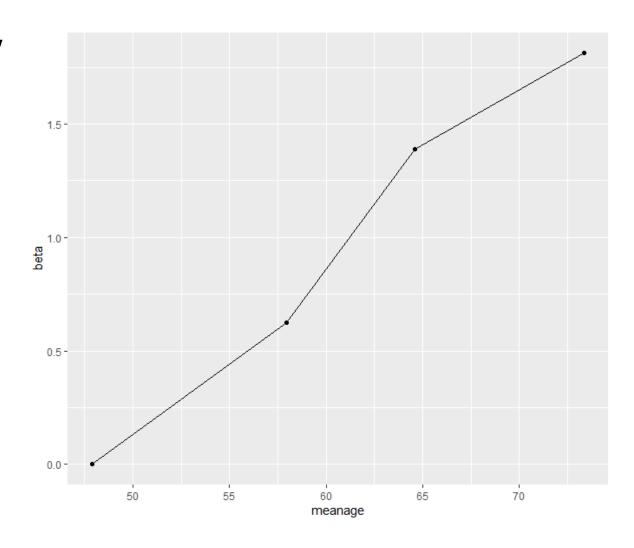
```
> glm(cor calcium ~ age.q4,
     data = corcalc,
     family = binomial) %>%
   anova(test = "LRT")
Analysis of Deviance Table
Model: binomial, link: logit
Response: cor calcium
Terms added sequentially (first to last)
      Df Deviance Resid. Df Resid. Dev Pr(>Chi)
                                694.33
NULL
                        505
age.q4 3 55.501
                        502 638.83 5.368e-12 ***
Signif. codes: 0 '*** 0.001 '** 0.01 '* 0.05 '.' 0.1 ' ' 1---
```

When we use dummy predictor variables, we allow for modeling **flexibility** because we don't assume a linear relationship across all X values.

If we plot the logit and see that the relationship between X and the logit appears linear, then we know we can be more restrictive in our modeling approach.

The relationship between the logit and age quartile isn't perfectly linear, but it seems like a pretty good approximation!

In this approach, we allow flexibility in the estimation of the logit among age quartiles.



The logit is estimated as a function of the dummy variables for age quartile.

$$logit(\hat{\pi}) = \beta_0 + \beta_1 X_{age,q2} + \beta_2 X_{age,q3} + \beta_3 X_{age,q4}$$

If a linear approach is good enough, though, then we could fit this relationship with a straight line.

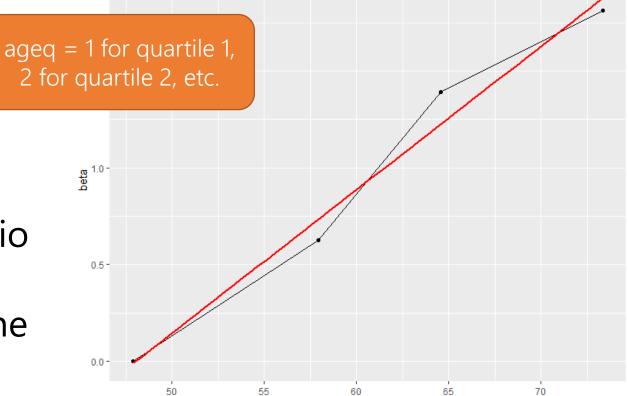
The equation for the red line is simpler but imposes more constraints.

$$logit(\hat{\pi}) = \beta_0 + \beta_1 X_{ageg}$$

The dummy variable scheme is more flexible in comparison to the linear model. We can use the likelihood ratio test to see if this flexibility improves model fit, or if we should stay with the more parsimonious linear model.

```
> anova(agequantlin.m, agequant.m, test = "LRT")
Analysis of Deviance Table
```

```
Model 1: cor_calcium ~ as.integer(age.q4)
Model 2: cor_calcium ~ age.q4
Resid. Df Resid. Dev Df Deviance Pr(>Chi)
1 504 639.49
2 502 638.83 2 0.66029 0.7188
```



meanage

This suggests that there is no appreciable departure from linearity!

#### **Extra Practice**

- Examine the grouped smooth approach for SBP.
- ☐ Regress coronary calcium on the 4 quartiles of SBP.
- ☐ Do the beta estimates for the slopes appear to be increasing linearly?
- ☐ Plot the change in logit corresponding to each of the quartiles, vs. the mean of the values in each quartile.

# **LOESS (Locally-Estimated) Smoothing**

Strategy: Similar to grouped smooth, but instead of using discrete categories, use a moving window/band.

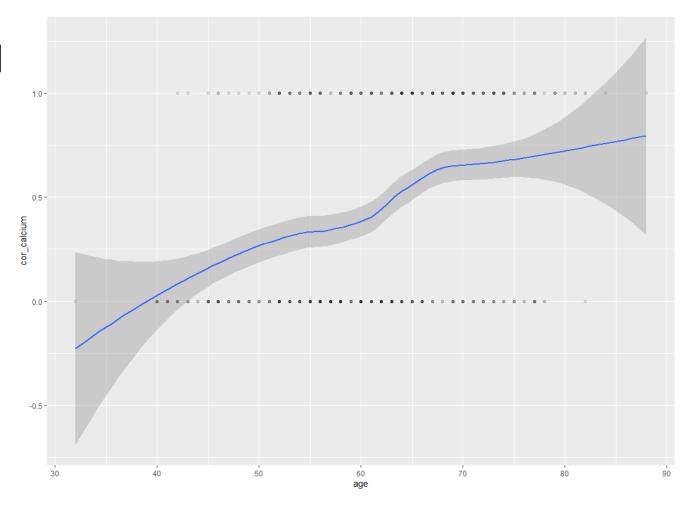
• Calculate the logit( $\hat{\pi}$ ) for each point in the dataset, using a weighted average regression of adjacent points (weighted by distance from the current point).

This is a graph of the relationship between age and predicted probability of coronary calcium, using the LOESS smoother.

This assesses the relationship between **age and the predicted probability of cor\_calcium**.

Therefore...



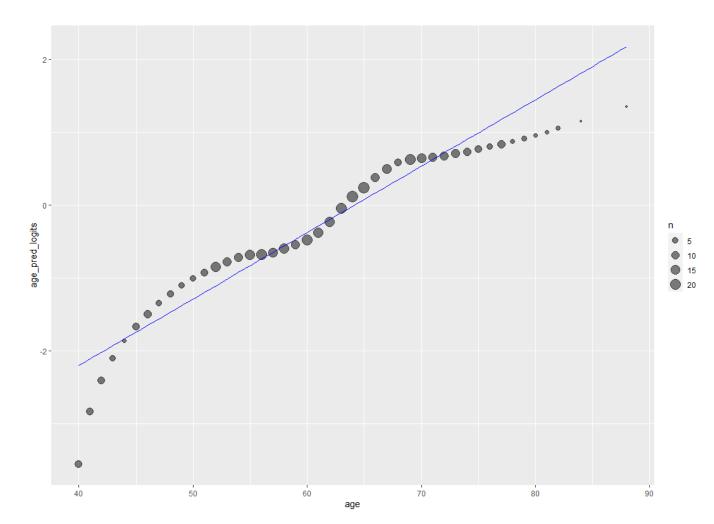


Instead, we want to examine the relationship between age and the <u>logit</u> of the probability of coronary calcium.

Note that this tells you the predicted logit across X values.

The LOESS smoother can be sensitive to the actual data. Therefore, it may pick up small departures from linearity.

This relationship between age and the logit of coronary calcium appears relatively linear.



#### **Extra Practice**

Examine the LOESS approach for SBP.

- ☐ Find the predicted probabilities and logits of coronary calcium over the values of SBP.
- ☐ Plot the predicted logit over the values of SBP.

# **Fractional Polynomials**

Strategy: Find a transformation of X (e.g., log(X),  $X^2$ ) that fits the data best.

 We have learned about fractional polynomials in Week 7, and the approach can be used here to examine the linearity assumption.

Here we see that there is no transformation to age would improve the model fit.

```
> mfp(cor calcium ~ fp(age), data = corcalc, family = binomial)
Deviance table:
                  Resid. Dev
Null model
                  694.3336
Linear model
                 625,9316
Final model
                 625.9316
Fractional polynomials:
   df.initial select alpha df.final power1 power2
                  1 0.05 1 1
age 4
Transformations of covariates:
          formula
age I((age/100)^1)
Rescaled coefficients:
Intercept
             age.1
 -5.26382 0.08203
Degrees of Freedom: 505 Total (i.e. Null); 504 Residual
Null Deviance:
Residual Deviance: 625.9 AIC: 629.9
```

If we specify "verbose = T" then we can see the best one-term and two-term polynomial transformations. The mfp() procedure automatically chooses the best one for you, though.

For the linear model, DF = 1. For the one-term polynomial, DF=2. For the two-term polynomial, DF=4.

We can use the chi-square test on the difference in deviance scores and DFs to compare models.

E.g., For the difference between the two-term and one-term polynomial models,  $\chi_2^2 = 0.248$ , p=0.88.

#### **Extra Practice**

- Examine the fractional polynomials approach for SBP.
- ☐ Write out the linear predictor for the 1-term and 2-term models.
- ☐ Does the 2-term model significantly differ from the 1-term model? From the linear model?
- ☐ Test whether the 1-term model differs from the linear model.
- ☐ Considering the grouped smooth, loess, and fractional polynomial results, how should we model SBP?

# Recap

- Logistic regression models assume linearity between x and the logit.
- We can check for linearity through:
  - Grouped smooth
  - LOESS plot
  - Fractional polynomials

# Recap

Implement the three methods described in this section to assess linearity assumption for a continuous predictor.

#### **Test Yourself**

Suppose we examine patients that are seen at the burn unit at LAC+USC hospital. We want to know if age is related to having an inhalation injury.

Based on the grouped smooth approach, is age linearly related to the logit of the probability of inhalation injury?

```
> anova(agequantlin.m, agequant.m, test = "LRT")
Analysis of Deviance Table
Model 1: inhal ~ as.integer(age.q5)
Model 2: inhal ~ age.q5
  Resid. Df Resid. Dev Df Deviance Pr(>Chi)
        132
                 181.40
        129
                 177.67 3
                              3.7334
                                       0.2917
 -0.5
beta
 -1.0
                                   meanage
```

#### **Test Yourself**

Suppose we examine patients that are seen at the burn unit at LAC+USC hospital. We want to know if age is related to having an inhalation injury.

Based on the grouped smooth approach, is age linearly related to the logit of the probability of inhalation injury?

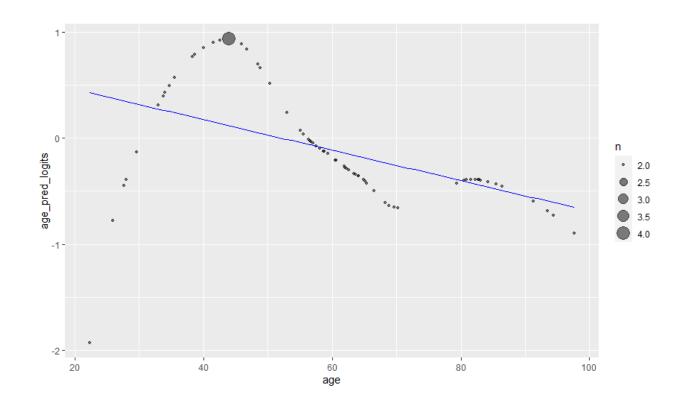
Yes. The grouped smooth approach shows that a single line is sufficient to describe the relationship between age and the logit.

```
> anova(agequantlin.m, agequant.m, test = "LRT")
Analysis of Deviance Table
Model 1: inhal ~ as.integer(age.q5)
Model 2: inhal ~ age.q5
  Resid. Df Resid. Dev Df Deviance Pr(>Chi)
        132
                 181.40
        129
                 177.67 3
                              3.7334
                                       0.2917
 -0.5
beta
 -1.0
                                   meanage
```

#### **Test Yourself**

Suppose we examine patients that are seen at the burn unit at LAC+USC hospital. We want to know if age is related to having an inhalation injury.

Based on the LOESS approach, is age linearly related to the logit of the probability of inhalation injury?

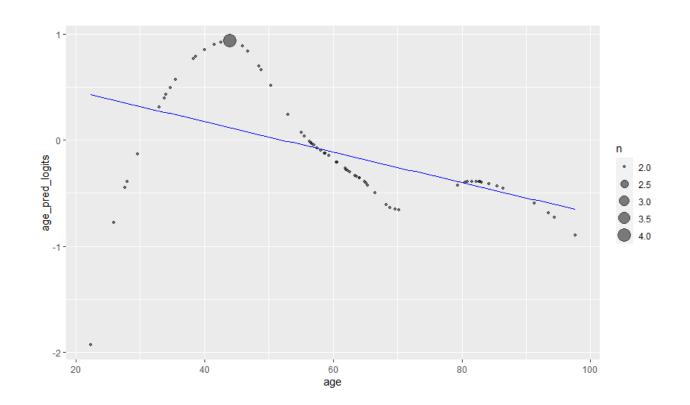


#### **Test Yourself**

Suppose we examine patients that are seen at the burn unit at LAC+USC hospital. We want to know if age is related to having an inhalation injury.

Based on the LOESS approach, is age linearly related to the logit of the probability of inhalation injury?

Probably not. It looks like inhalation injury is higher around 35-50 years of age, and then drops off at higher ages.



#### **Test Yourself**

Suppose we examine patients that are seen at the burn unit at LAC+USC hospital. We want to know if age is related to having an inhalation injury.

Based on the fractional polynomials approach, is age linearly related to the logit of the probability of inhalation injury?

	Variable	Deviance	Power(s)
Cycle 1	 L		
-	age		
	_	185.734	
		183.221	1
		182.661	3
		173.052	-2 -2
	rmation ift scale 0 100		
Fractional polynomials df.initial select alpha df.final power1 power2 age 4 1 0.05 4 -2 -2			
Transformations of covariates:			
age I((age/100)^-2)+I((age/100)^-2*log((age/100)))			

### 2. Assessing Assumptions

### **Test Yourself**

Suppose we examine patients that are seen at the burn unit at LAC+USC hospital. We want to know if age is related to having an inhalation injury.

Based on the fractional polynomials approach, is age linearly related to the logit of the probability of inhalation injury?

No. The FP approach has found a good 2-parameter solution for the form of age.

	Variable	Deviance	Power(s)
Cycle 1	age		
	age	185.734 183.221 182.661 173.052	1 3 -2 -2

Tansformation shift scale age 0 100

Fractional polynomials

df.initial select alpha df.final power1 power2

age 4 1 0.05 4 -2 -2

Transformations of covariates:

formula age I((age/100)^-2)+I((age/100)^-2\*log((age/100)))

# Some things to look for when model building

- Does our model contain the correct main effects?
- Are the continuous independent variables modeled according to the correct functional form?
- Have all sensible interactions been considered?
- [Model of association] Have all potential confounders been examined?
- [Prediction model] Have all predictive variables been considered appropriately, and does the model only include these predictive variables?

Even though we relaxed some of the modeling assumptions for logistic regression (vs OLS), we still want to see if the model fits the data well. Similar to linear regression, the model fits well if:

- the distance between observed Y and predicted  $\widehat{Y}$  is small (low error)
- each individual makes a small, unsystematic contribution (no observations making undue influence)

#### To test the fit we:

- Examine overall goodness-of-fit
- Examine lack-of-fit by specific departures from the model

## **Summary Measures**

To obtain summary measures, the observed and expected values are enumerated for each **covariate pattern**.

For example, if we have a model with gender (dichotomous) and race/ethnicity (black/Hispanic vs. otherwise), we will have 4 covariate patterns:

```
> corcalc %>%
   count(gender.f, bl hisp.f)
# A tibble: 4 x 3
 gender.f bl_hisp.f
  <fct> <fct>
                             <int>
1 Female Not Black/Hispanic
                               139
2 Female
         Black/Hispanic
                                58
3 Male
          Not Black/Hispanic
                               237
          Black/Hispanic
4 Male
                                72
```

Suppose we have n subjects (i = 1, ..., n)

and J covariate patterns (X<sub>1</sub>,...,X<sub>J</sub>; J≤n)

# of people with Y=1 among those with covariate pattern j.

We can create a 2xJ table:

	j=1	j=2	•••	j=J	
Y=1	$Y_1$	Y <sub>2</sub>		Yi	$n_1$
Y=0				,	$n_0$
	$m_1$	$m_2$		m <sub>i</sub>	n

# of people with covariate pattern j

The **residuals** of logistic regression are the difference between observed and expected values, for **each covariate pattern**.

Predicted probability of outcome for covariate pattern j.

$$-\hat{\pi}_{j} = \frac{\exp(\hat{\beta}x)}{1 + \exp(\hat{\beta}x)}$$

$$\widehat{Y}_j = m_j \widehat{\pi}_j$$

The **expected** number with Y=1 in covariate pattern j is the total number that have covariate pattern j multiplied by the probability of outcome for this group.

	j=1	j=2	•••	j=J	
Y=1	Y <sub>1</sub>	Y <sub>2</sub>		Y <sub>i</sub>	n <sub>1</sub>
Y=0				,	$n_0$
	$m_1$	$m_2$		m <sub>i</sub>	n

The Pearson residuals are given as:

Observed - expected 
$$r_j = \frac{y_j - m_j \hat{\pi}_j}{\sqrt{m_j \hat{\pi}_j (1 - \hat{\pi}_j)}}$$
 A measure of variation

And the corresponding GOF summary statistic is:

$$\sum r_i^2 \sim \chi^2(df = J - (p+1))$$
 (p = # of variables in the model)

H<sub>0</sub>: The model fits the data (the observed matches what we expected)

H<sub>A</sub>: The model departs from good fit

# **Example**

```
> summary(gender race.m)
Call:
glm(formula = cor calcium ~ gender.f + bl hisp.f, family = binomial,
   data = corcalc)
Deviance Residuals:
   Min
            1Q Median
                           3Q
                                  Max
-1.3714 -0.9591 -0.5614 0.9951
                               1.9625
Coefficients:
                    Estimate Std. Error z value Pr(>|z|)
                               0.1702 -4.613 3.98e-06 ***
(Intercept)
                     -0.7849
gender.fMale
                    1.2302 0.2017 6.100 1.06e-09 ***
Signif. codes: 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
> DescTools::PseudoR2(gender race.m)
 McFadden
0.08850083
```

Male gender is associated with increased odds of CC (p<.001).

Black/Hispanic is associated with lower odds of CC (p<.001).

These variables explain approximately 9% of the variation in CC.

### Here we examine some fit statistics for each covariate pattern.

```
> dx(gender race.m)
   (Intercept) gender.fMale bl_hisp.fBlack/Hispanic
                                                                            yhat
                                                                                         Pr
                                                  0 149 0.6095166 237 144.455437
1:
                                                                                 0.6050955
                                                     39 0.3132702 139 43.544563 \ 0.8310598
2:
                                                     22 0.3686745 72 26.544563 -1.1101399
3:
4:
                                                    13 Ø.1457834 58 8.455437 1.6909865
           dr
                        h
                                 sPr
                                            sdr
                                                   dCh⁄isq
                                                               dDev
                                                                          dBhat
   0.6069678 0.003919350
                          0.6062848
                                     0.6081607 0.3675813 0.3698595 0.001446348
   -0.8394792 0.006229179 -0.8336603 -0.8421061 0.6949895 0.7091427 0.004356351
3: -1.1254453 0.010564361 -1.1160507 -1.1314377/1.2455691 1.2801512 0.013299139
   1.5889396 0.007665932 1.6975054 1.5950652 2.8815247 2.5442329 0.022260218
```

Observed # with Y=1

Predicted P(Y=1)

N with pattern

Predicted # with Y=1

The Pearson GOF test can be obtained as follows. Note that p=0.023 means we reject  $H_0$ ; the model does indicate departure from goodness of fit.

```
Setting levels: control = 0, case = 1
Setting direction: controls < cases
$ct
           y1hat y1
                       y0hat y0
     n
1: 237 144.455437 149 92.54456 88
2: 139
       43.544563 39 95.45544 100
   72 26.544563 22 45.45544 50
       8.455437 13 49.54456 45
   58
$chiSq
  test
            chiSq df
                              pVal
   PrI 514.653478 503 3.498981e-01
    drI 632.884462 503 6.996823e-05
3:
   PrG
         5.148647
                   1 2.326450e-02
         4.864491
                    1 2.741488e-02
    drG
                    1 2.326450e-02
5: PrCT
         5.148647
                    1 2.741488e-02
6: drCT
         4.864491
```

> gof(gender race.m, g=4, plotROC = F) %>% unclass()

PrG: Pearson Residual (Group) on the covariate patterns

The Pearson chi-square GOF requires m-asymptotics.

This means that the total sample size isn't as important as the number of observations within each covariate pattern.

Therefore when the number of covariate patterns approaches the sample size (J≈n), the chi-square approximation does not hold for this test.

This is especially a problem with continuous variables! When we add age to the regression, we start to get *a lot* of covariate patterns.

```
> corcalc %>%
    count(gender.f, bl_hisp.f, age)
# A tibble: 138 x 4
   gender.f bl_hisp.f
                                 age
                                         n
   <fct>
            <fct>
                               <dbl> <int>
           Not Black/Hispanic
 1 Female
                                  45
 2 Female
           Not Black/Hispanic
                                  46
            Not Black/Hispanic
                                  48
 3 Female
 4 Female
            Not Black/Hispanic
                                  49
 5 Female
            Not Black/Hispanic
                                  50
 6 Female
            Not Black/Hispanic
                                  51
 7 Female
            Not Black/Hispanic
                                  52
            Not Black/Hispanic
 8 Female
                                  53
            Not Black/Hispanic
 9 Female
                                  54
10 Female
            Not Black/Hispanic
                                  55
# ... with 128 more rows
```

There are 138 covariate patterns for 506 individuals.

#### **Hosmer-Lemeshow GOF Test**

An alternative to the Pearson GOF test that "fixes" the problem of having too many covariate patterns.

#### How?

- Collapse the J covariate patterns into g groups (g<J, and fix g<<n). Then calculate the observed and expected frequencies.
- 2. Obtain the predicted probabilities,  $\hat{\pi}_i$ , for each covariate pattern j.
- Order the j columns (covariate patterns) from lowest to highest predicted probabilities.
- 4. Collapse the J columns into deciles of risk (g=10)
- 5. Calculate expected values for each of the 10 categories (sum over all subjects in the cells with Y=1 or in cells with Y=0).
- 6. Perform chi-square test and compare to a  $\chi^2$  with g-2 degrees of freedom.

(0.821, 0.967] 9 39 5.800773 42.199227

```
> hoslem.test(gender_race_age.m$y, fitted(gender_race_age.m), g=10)
         Hosmer and Lemeshow goodness of fit (GOF) test
                                                              There is no evidence of lack of fit (p=0.61).
data: gender_race_age.m$y, fitted(gender_race_age.m)
X-squared = 6.3405, df = 8, p-value = 0.6092
> hoslem.test(gender_race_age.m$y, fitted(gender_race_age.m), g=10) %>%
  {cbind(.$observed, .$expected)}
             y0 y1 yhat0
                                yhat1
[0.031,0.115] 47 4 46.695674 4.304326
(0.115,0.181] 43 8 43.233451 7.766549
                                           The range of predicted probabilities is split into 10 quantiles.
(0.181,0.25] 44 11 42.914692 12.085308
                                          Within each quantile, we calculate how many observations with
(0.25, 0.312] 38 13 36.245566 14.754434
                                           Y=0 and with Y=1 we expect, and compare that to how many
(0.312,0.416] 29 16 28.553477 16.446523
                                             we would observe. You can see that the observed closely
(0.416, 0.496] 25 29 29.565518 24.434482
                                                              matches the expected.
(0.496,0.609] 25 24 21.706068 27.293932
(0.609, 0.713] 14 39 17.400573 35.599427
(0.713,0.821) 9 40 10.884210 38.115790
```

This kind of test can be used to make sure that prediction models are calibrated correctly.

## Forecast calibration for FiveThirtyEight "polls-only" forecast

WIN PROBABILITY RANGE	FORECASTS	EXPECTED WINNERS	ACTUAL WINNERS
95-100%	31	30.5	30
75-94%	15	12.4	13
50-74%	11	6.9	9
25-49%	12	4.0	2
5-24%	22	2.4	1
0-4%	89	0.9	1



**Cole Fitzpatrick** @colefitzpatrick · May 11, 2016 Replying to @NateSilver538 @NateSilver538 Ah, the Hosmer-Lemeshow test.

# **Comparative Model Fit**

Information Criteria are derived from the model log-likelihood (-2LL) and can be used to compare models when making decisions about which is better.

Unlike the likelihood ratio test, the AIC and BIC can be used to compare models with different independent variables.

AIC – Akaike's Information Criterion: -2LL + 2k (k = # of model parameters estimated)

BIC - Bayesian Information Criterion: -2LL + kln(N) (N = sample size)

Smaller values indicate comparatively better model fit.

The BIC imposes a penalty for having more model parameters.

# Recap

- Pearson's Goodness-of-Fit test allows us to examine whether the model departs from good fit.
- Models that fit well will have, within each covariate pattern, an observed number of individuals with Y=1 approximately equal to the expected number.
- When there are many covariate patterns, we can instead rely on the Hosmer-Lemeshow test.

## Recap

- ➤ Implement the Pearson's and Hosmer-Lemeshow GOF tests.
- Interpret the results of these tests with respect to model fit.

### **Test Yourself**

In the previous model examining the relationship between age and probability of inhalation injury, which GOF statistic would be more appropriate: Pearson's or Hosmer-Lemeshow?

### **Test Yourself**

In the previous model examining the relationship between age and probability of inhalation injury, which GOF statistic would be more appropriate: Pearson's or Hosmer-Lemeshow?

Hosmer-Lemeshow, since age is continuous and therefore the number of covariate patterns would be quite large.

# **Diagnostics**

As with linear regression, we need to check:

- Collinearity
- Leverage
- Influence

# **Collinearity**

We can check for collinearity as we normally would with OLS regression.

```
> DescTools::VIF(gender_race_age.m)
gender.f bl_hisp.f age
1.160517 1.003035 1.163754
```

There is no evidence of collinearity. The largest VIF is 1.16, far below 10.

## Leverage

Recall, leverage indicates observations that have the potential to be influential because they are far from the average value of a covariate.

In linear regression, leverage values are obtained from the hat matrix: H = X(X'X)-1X'.

In logistic regression, H = V1/2 X(X'VX)-1X'V1/2 , where V is a JxJ diagonal matrix with element  $v_j = m_j \hat{\pi}(x_j)(1 - \hat{\pi}(x_j))$ .

H is the leverage; the distance of covariate pattern  $X_i$  from the mean.

## 4. Diagnostics

### Influence

An observation is influential when it has a high **residual** and a large value of **leverage**.

Influence is assessed by estimating the effect of deleting all subjects with a particular covariate pattern J.

We can see how this affects:

- The estimated coefficients (betas)
- The summary GOF measures

### Influence

We typically want to see the following plots:

- $\Delta \chi_j^2$  vs  $\hat{\pi}_j$  (Change in Pearson GOF)
- $\Delta D_i$  vs  $\hat{\pi}_i$  (Change in Deviance GOF)
- $\Delta \hat{\beta}_i$  vs  $\hat{\pi}_i$  (Change in Cook's Distance)

# These values can be produced either:

- For each covariate pattern
- For each individual

```
dx(gender_race_age.m)
dx(gender_race_age.m, bycov = F)
```

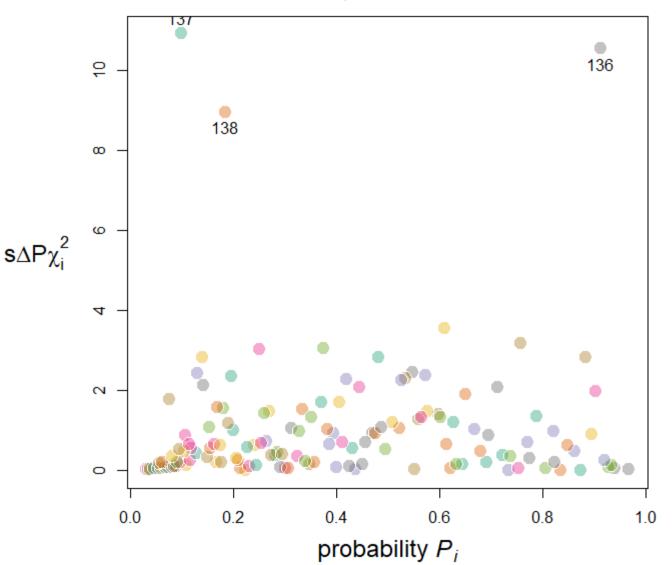
 $\Delta\chi_j^2$  vs  $\hat{\pi}_j$ 

Poorly fit points will lie in the upper corners.

Assuming m-asymptotics, 4 is a crude approximation of the upper 95<sup>th</sup> percentile of the distribution of  $\Delta \chi_i^2$ .

Probability  $P_i \times \text{scaled change in Pearson chi-sq s}\Delta P$ 

$$Pr_i = \frac{y_i - \mu_y}{\sigma_y}$$
,  $s\Delta P\chi_i^2 = \frac{Pr_i}{\sqrt{1 - h_i}}$ 

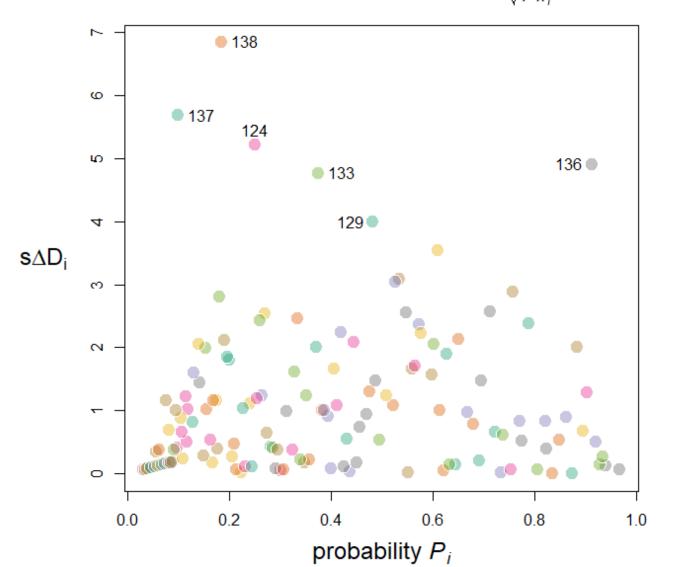


 $\Delta D_j$  vs  $\hat{\pi}_j$ 

Poorly fit points will lie in the upper corners.

Assuming m-asymptotics, 4 is a crude approximation of the upper 95<sup>th</sup> percentile of the distribution of  $\Delta D_i$ .

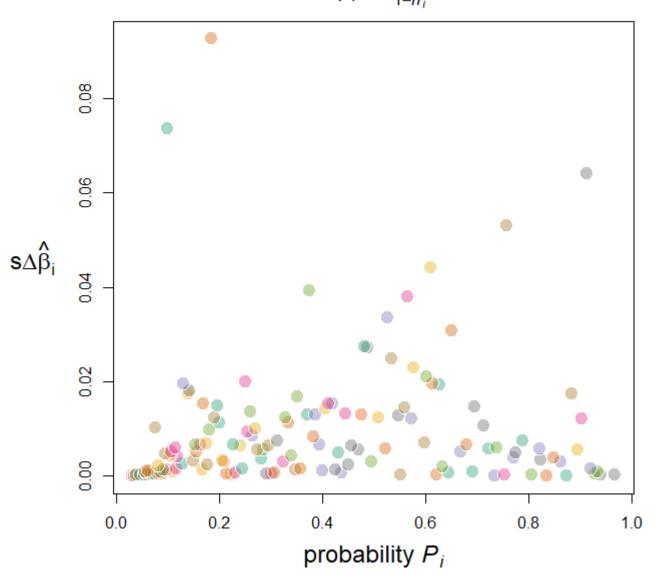
Probability  $P_i \times \text{scaled change in deviance } \Delta D_i$  $dr_i = \text{sign}(y_i - \hat{y}_i) \sqrt{d_i}, \text{ s} \Delta D_i = \frac{dr_i}{\sqrt{1 - h_i}}$ 



 $\Delta eta_j$  vs  $\hat{\pi}_j$ 

Values above 1.0 indicate removal of the covariate pattern is associated with considerable changes to the parameter estimates.

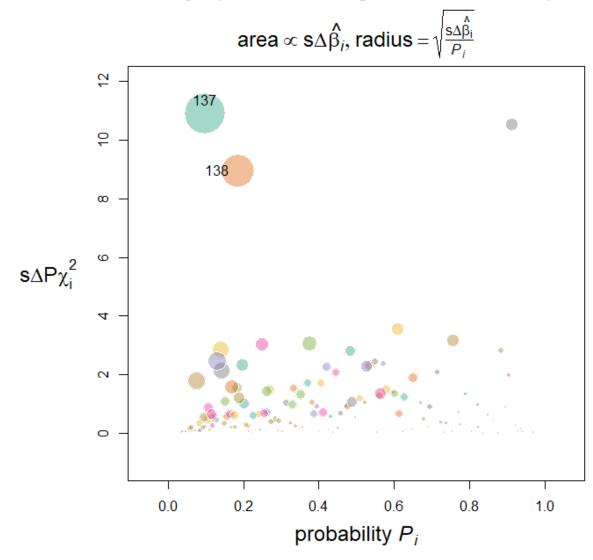
Probability  $P_i \times \text{scaled change in coefficients } s\Delta \hat{\beta}_i$  $s\Delta \hat{\beta}_i = \frac{sPr_i^2h_i}{1-h_i}$ 



# Plotting with symbol size proportional to dbeta

This will show us which covariate patterns affect the chi-square the most, while also affecting the dbeta value the most.

Probability  $P_i \times \text{scaled change in Pearson chi-sq s}\Delta F$ 



### 4. Diagnostics

# Why are covariate patterns 137 and 138 so poorly fit?

```
> dx(gender_race_age.m, bycov = F)
     (Intercept) gender.fMale bl_hisp.fBlack/Hispanic age y
                                                                      Ρn
                                                        74 7 0.87407292 8 6.99258334
  1:
  2:
                                                       71 5 0.83603556 6 5.01621336
  3:
                                                       65 6 0.73343936 8 5.86751491
  4:
                                                       46 0 0.03099609 1 0.03099609
  5:
                            0
                                                       47 0 0.03423756 1 0.03423756
134:
                                                       77 1 0.60909298 5 3.04546489
135:
                                                     1 73 0 0.75693416 1 0.75693416
136:
                                                    0 78 0 0.91283188 1 0.91283188
137:
                                                       58 2 0.09897633 3 0.29692898
                            0
                                                       65 2 0.18407797 2 0.36815594
138:
```

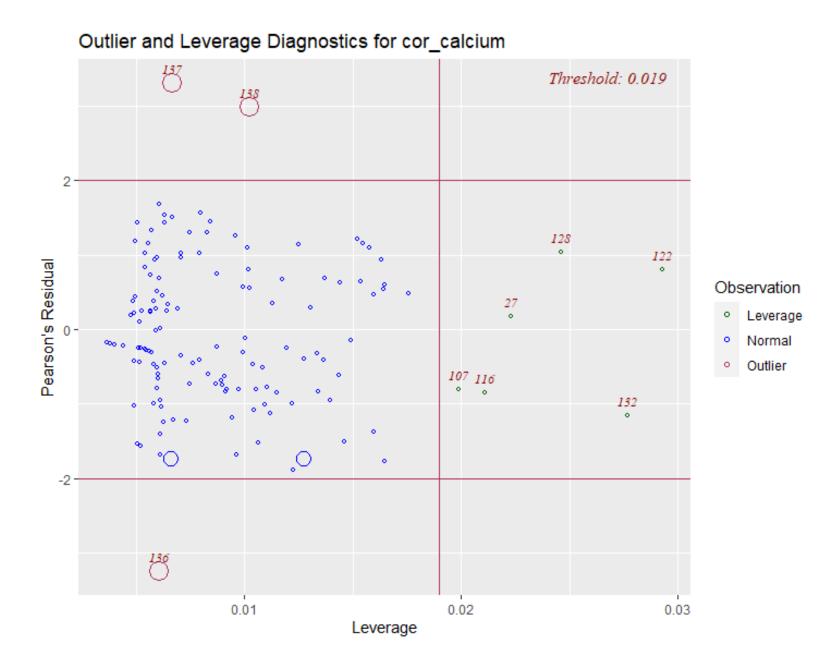
In this package, covariate patterns with higher index numbers are more poorly fit.

Of the 2 people with covariate pattern 138, 100% had Y=1. However, our model only expects them to have an 18% chance of outcome.

## 4. Diagnostics

I wrote a crude function that aligns with olsrr's residual/leverage plot.

(See plot\_resid\_lev\_logistic.R)



# What happens when we find problematic observations?

List the covariate pattern to see why the observation is influential.

You can delete these patterns and refit the model to determine the true effect of these observations on your  $\hat{\beta}$  of interest.

#### Then decide:

- What is the reason for the outliers? If you delete them, you must have a valid reason to do so.
- Are the outlying patterns reasonable? Or are they due to a mistake?
- Is there a variable or set of variables you didn't include that would fix the model?

# What if there are multiple suspect patterns?

# Check the following:

- Did you use the correct link?
- Did you omit an important predictor or interaction?
- Are the covariates on the proper scale?
- Is there "extra-binomial variation"? (more or less variation in predicted probabilities than expected under the binomial model; can occur when observations are clustered)

## 4. Diagnostics

## Recap

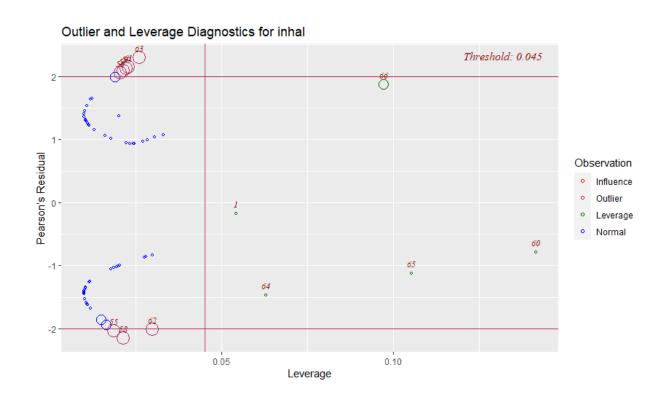
• An examination of the change in Pearson's GOF, Deviance GOF, and betas can help identify covariate patterns that are poorly fit.

## Recap

- ➤ Use the diagnostic measures discussed in this section to determine the most influential observations.
- ➤ Decide, based on these metrics, whether these observations pose a problem.
- > Determine how to proceed when faced with problematic observations.

### **Test Yourself**

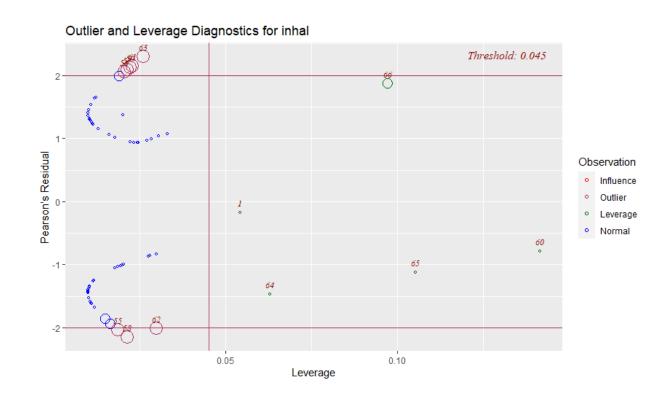
In the inhalation injury example, the following diagnostics plot was produced. Which covariate pattern should we check for further investigation?



### **Test Yourself**

In the inhalation injury example, the following diagnostics plot was produced. Which covariate pattern should we check for further investigation?

Maybe pattern 66.



# Recall the two goals of regression analysis

- Determine the most accurate association between X and Y (model of association)
- 2. Find the best model to predict Y (prediction model).

#### 5. Variable Selection

Until now we have generally focused on models of association.

However, logistic regression models are especially important when it comes to prediction:

- Is this patient at risk for heart attack?
- Is this particular growth malignant cancer?
- Does this test indicate infection with COVID-19?

### **Example**

Can we use characteristics of the mother in order to predict low birth weight?

```
> 1bw %>%
    select(LOW, AGE, LWT, RACE, SMOKE, PTL, HT, UI, FTV) %>%
    psych::describe()
                         sd median trimmed
                                            mad min max range skew kurtosis
      vars
                 mean
LOW*
         1 189
                 1.31
                       0.46
                                      1.27
                                            0.00
                                                             1 0.80
                                                                       -1.36 0.03
AGE
         2 189
                23.24
                       5.30
                                     22.90
                                            5.93
                                                 14 45
                                                            31 0.71
                                                                      0.53 0.39
LWT
         3 189 129.81 30.58
                               121
                                    126.07 20.76 80 250
                                                           170 1.38
                                                                      2.25 2.22
         4 189
                                      1.81 0.00
RACE*
                 1.85 0.92
                                                             2 0.31
                                                                       -1.75 0.07
SMOKE*
         5 189
                 1.39
                       0.49
                                      1.37
                                            0.00
                                                             1 0.44
                                                                       -1.82 0.04
PTL
         6 189
                                                                      8.17 0.04
                 0.20 0.49
                                      0.08
                                            0.00
                                                             3 2.76
HT*
         7 189
                 1.06 0.24
                                      1.00
                                            0.00
                                                  1 2
                                                            1 3.55
                                                                      10.67 0.02
         8 189
                 1.15 0.36
UI*
                                      1.07
                                            0.00
                                                             1 1.97
                                                                       1.87 0.03
         9 189
FTV
                 0.79 1.06
                                      0.62
                                            0.00
                                                             6 1.56
                                                                       3.00 0.08
```

When faced with several possible predictive variables, it can be cumbersome to manually arrive at a good model.

**Automatic selection procedures** (while criticized for being too "hands-off") provide a way to assess which variables may be important.

### **Selection Algorithms**

- Best Subsets
- Backward Elimination
- Forward Selection
- Stepwise Selection

#### 5. Variable Selection

Traditionally, these selection algorithms were based on p-values.

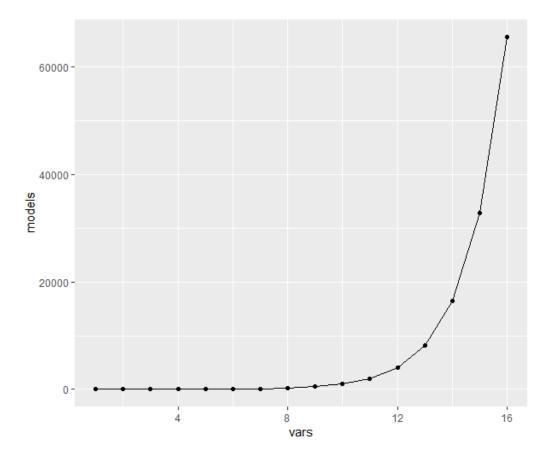
i.e., add the most significant variables to the model according to their p-value until they're no longer significant.

Recently, there has been a push to stop using p-values as a criterion for model inclusion/exclusion and instead turn to other measures, such as R<sup>2</sup> or the information criteria (AIC/BIC/etc.).

#### **Best Subsets**

For K variates under consideration, assess the fit of all models with k=1, 2, 3, ..., K variables included in the model.

- The best subset is chosen using <u>some</u> criteria (Information Criterion, R<sup>2</sup>, Mallow's C<sub>p</sub>, etc.)
- This approach is computationally intensive, as it requires fitting 2<sup>K</sup>-1 models.



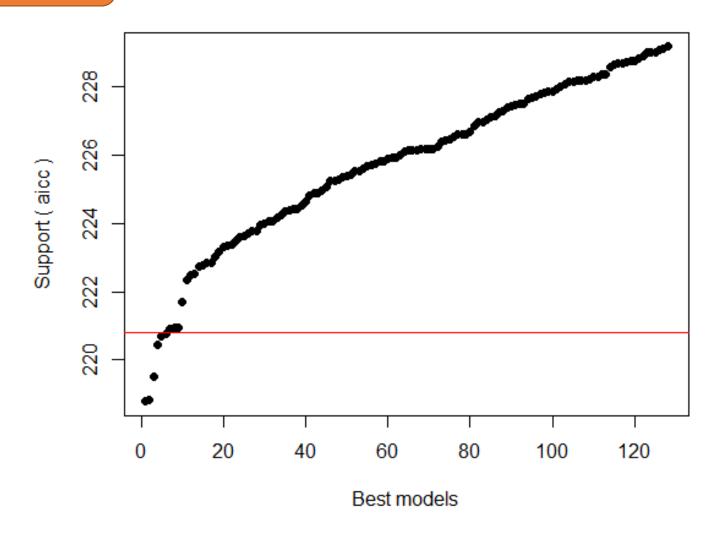
# Finding the best subset of predictors

```
best subset low <-
glmulti(LOW ~ AGE + LWT + RACE + SMOKE + PTL + HT + UI + FTV, data=lbw,
        level=1, family = binomial, crit="aicc", confsetsize=128)
> print(best subset low)
glmulti.analysis
Method: h / Fitting: glm / IC used: aicc
Level: 1 / Marginality: FALSE
From 128 models:
Best IC: 218.785587197454
Best model:
[1] "LOW \sim 1 + RACE + SMOKE + HT + UI + LWT + PTL"
Evidence weight: 0.103340083255988
Worst IC: 229,190066247819
6 models within 2 IC units.
80 models to reach 95% of evidence weight.
```

Level=1 considers main effects. Interactions can be considered by specifying level=2.

The best model has the lowest AICC (218.79). 6 models are within 2 units of the best model.

#### IC profile



### Let's print the top 6 models.

"Weights" are the Akaike weights for each model. Think of these as the probability that each given model is the best model out of all models considered.

#### Here's the "best" model.

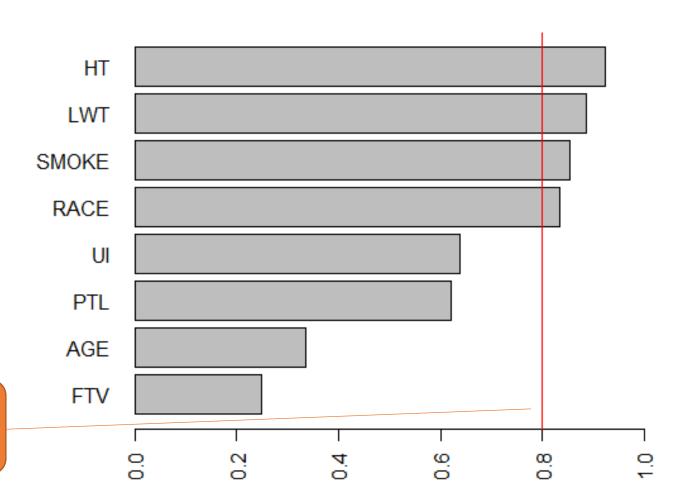
```
> best_subset_low@objects[[1]] %>% summary()
Call:
fitfunc(formula = as.formula(x), family = ...1, data = data)
Deviance Residuals:
   Min
             1Q Median
                             3Q
                                     Max
-1.9049 -0.8124 -0.5241 0.9483 2.1812
Coefficients:
            Estimate Std. Error z value Pr(>|z|)
(Intercept) -0.086550
                    0.951760 -0.091 0.92754
RACEblack
           1.325719 0.522243 2.539 0.01113 *
RACEother 0.897078 0.433881 2.068
                                      0.03868 *
SMOKEyes 0.938727 0.398717 2.354 0.01855 *
           1.855042 0.695118 2.669 0.00762 **
HTyes
           0.785698 0.456441 1.721
                                      0.08519 .
UIyes
           -0.015905 0.006855 -2.320
                                       0.02033 *
LWT
PTL
           0.503215  0.341231  1.475  0.14029
Signif. codes: 0 '*** 0.001 '** 0.01 '* 0.05 '.' 0.1 ' ' 1
   Null deviance: 234.67 on 188 degrees of freedom
Residual deviance: 201.99 on 181 degrees of freedom
AIC: 217.99
```

#### Here's the "second best" model.

```
> best_subset_low@objects[[2]] %>% summary()
Call:
fitfunc(formula = as.formula(x), family = ...1, data = data)
Deviance Residuals:
   Min
            1Q Median
                             3Q
                                     Max
-1.7396 -0.8322 -0.5359 0.9873 2.1692
Coefficients:
            Estimate Std. Error z value Pr(>|z|)
(Intercept)
           0.056276
                     0.937853
                                0.060 0.95215
RACEblack
           1.324562 0.521464 2.540 0.01108 *
RACEother 0.926197 0.430386 2.152 0.03140 *
SMOKEyes 1.035831 0.392558 2.639
                                      0.00832 **
HTyes
          1.871416 0.690902 2.709
                                      0.00676 **
UIyes 0.904974 0.447553 2.022
                                      0.04317 *
           -0.016732
                     0.006803 -2.459
                                      0.01392 *
LWT
Signif. codes: 0 '*** 0.001 '** 0.01 '* 0.05 '.' 0.1 ' ' 1
   Null deviance: 234.67 on 188 degrees of freedom
Residual deviance: 204.22 on 182 degrees of freedom
AIC: 218.22
Number of Fisher Scoring iterations: 4
```

We can also look at the relative importance of all predictors, averaged across all the models. This is the sum of the weights for all models containing that variable.

#### Model-averaged importance of terms



0.8 is a somewhat arbitrary cutoff used for determining importance in the model.

### **Sequential Selection**

**Backward.** Start with a "full" model and sequentially remove variables that do not contribute to model fit.

**Forward.** Start with an empty model and sequentially add variables that contribute to model fit.

**Stepwise.** A mix of adding and deleting variables at each step.

### **Forward Selection**

```
forward low <-
 MASS::stepAIC(
    glm(LOW \sim 1,
        data=lbw, family = binomial),
    scope = list(upper = ~AGE + LWT + RACE + SMOKE + PTL + HT + UI + FTV,
                 lower = \sim 1),
    direction = "forward"
> forward low %>% summary()
Call:
glm(formula = LOW ~ PTL + LWT + HT + RACE + SMOKE + UI, family = binomial,
    data = 1bw)
Coefficients:
             Estimate Std. Error z value Pr(>|z|)
(Intercept) -0.086550
                       0.951760 -0.091 0.92754
PTL
            0.503215
                     0.341231
                                 1.475 0.14029
LWT
            -0.015905
                       0.006855
                                 -2.320
                                          0.02033 *
HTyes
            1.855042
                       0.695118
                                 2.669
                                          0.00762 **
RACEblack
            1.325719
                      0.522243
                                 2.539
                                          0.01113 *
                                         0.03868 *
RACEother
            0.897078
                       0.433881
                                   2.068
SMOKEyes
            0.938727
                        0.398717
                                   2.354
                                         0.01855 *
UIyes
            0.785698
                       0.456441
                                 1.721
                                         0.08519 .
```

Start with an empty model, then specify the scope of all variables you want to consider.

#### 5. Variable Selection

### **Backward Selection**

```
backward low <-
 MASS::stepAIC(
    glm(LOW ~ AGE + LWT + RACE + SMOKE + PTL + HT + UI + FTV,
        data=lbw, family = binomial),
    scope = list(upper = ~AGE + LWT + RACE + SMOKE + PTL + HT + UI + FTV,
                 lower = \sim 1),
    direction = "backward"
> stepwise low %>% summary()
Call:
glm(formula = LOW ~ PTL + LWT + HT + RACE + SMOKE + UI, family = binomial,
    data = 1bw)
Coefficients:
             Estimate Std. Error z value Pr(>|z|)
(Intercept) -0.086550
                        0.951760 -0.091 0.92754
PTL
            0.503215
                      0.341231
                                 1.475 0.14029
            -0.015905
                        0.006855
                                          0.02033 *
LWT
                                 -2.320
            1.855042
                        0.695118
                                   2.669
                                          0.00762 **
HTyes
RACEblack
            1.325719
                      0.522243
                                 2.539
                                          0.01113 *
RACEother
            0.897078
                        0.433881
                                   2.068
                                          0.03868 *
SMOKEyes
            0.938727
                        0.398717
                                   2.354
                                          0.01855 *
UIyes
             0.785698
                        0.456441
                                   1.721
                                         0.08519 .
```

Start with a full model, then specify the scope of how sparse of a model you want.

# Stepwise Selection

```
stepwise low <-
 MASS::stepAIC(
    glm(LOW \sim 1,
        data=lbw, family = binomial),
    scope = list(upper = ~AGE + LWT + RACE + SMOKE + PTL + HT + UI + FTV,
                 lower = \sim 1),
    direction = "both"
> stepwise low %>% summary()
Call:
glm(formula = LOW ~ PTL + LWT + HT + RACE + SMOKE + UI, family = binomial,
    data = 1bw)
Coefficients:
             Estimate Std. Error z value Pr(>|z|)
(Intercept) -0.086550
                       0.951760 -0.091 0.92754
PTL
            0.503215
                     0.341231
                                 1.475 0.14029
LWT
            -0.015905
                       0.006855
                                 -2.320
                                          0.02033 *
            1.855042
                       0.695118
                                 2.669
                                          0.00762 **
HTyes
RACEblack
            1.325719
                      0.522243
                                 2.539
                                          0.01113 *
RACEother
            0.897078
                       0.433881
                                   2.068
                                          0.03868 *
SMOKEyes
            0.938727
                        0.398717
                                   2.354
                                         0.01855 *
UIyes
            0.785698
                        0.456441
                                  1.721
                                         0.08519 .
```

Start with any model (full or empty) and then sequentially add and remove variables.

### Recap

- Automatic selection procedures have been criticized for being too data-driven and for removing the input from the analyst
- Conventional approaches include backward, forward, and stepwise selection
- With the advent of increased computing power, it is feasible to perform a best-possible-subset regression
- Higher-order terms (e.g., polynomial) need to be added manually
- Diagnostics still need to be examined

### Recap

➤ When faced with a model-building problem, implement a selection procedure to find the most important variables.

- **Linearity** is the only regression assumption that needs to be checked for logistic regression, but it is considerably more difficult to do so.
- **Goodness of fit** tests are a way to describe how well your logistic regression model fits your data; <u>not</u> rejecting  $H_0$  (p>.05) indicates acceptable fit.
- **Diagnostics** are performed similarly to linear regression, but on covariate patterns. Influence is still a combination of being an outlier with high leverage.

### **Additional Reading**

 Now that you know stepwise regression, why you shouldn't use it: <a href="https://towardsdatascience.com/stopping-stepwise-why-stepwise-selection-is-bad-and-what-you-should-use-instead-90818b3f52df">https://towardsdatascience.com/stopping-stepwise-why-stepwise-selection-is-bad-and-what-you-should-use-instead-90818b3f52df</a>

# **Packages and Functions**

```
psych::logit()
LogisticDx::dx()
LogisticDx::OR
LogisticDx::gof()
ResourceSelection::hoslem.test()
glmulti::glmulti()
MASS::stepAIC()
```