

## 5.1: Logistic Regression

Dr. Bean - Stat 5100

### 1 Why Logistic Regression?

Recall the linear regression model

$$Y = \beta_0 + \beta_1 X_1 + \cdots + \beta_{p-1} X_{p-1} + \epsilon \quad (\epsilon \sim N(0, \sigma^2)).$$

What are some properties of the variable  $Y$  that are required for  $\epsilon \sim N(0, \sigma^2)$ .

- $Y$  must be linearly related to  $X_1, \dots, X_{p-1}$ .
- $Y$  must be a **continuous, quantitative** variable

#### 1.1 Why not regression on categorical data?

Consider fitting a regression model where we use age to try and predict whether or not a person has a disease (a 0-1 variable).

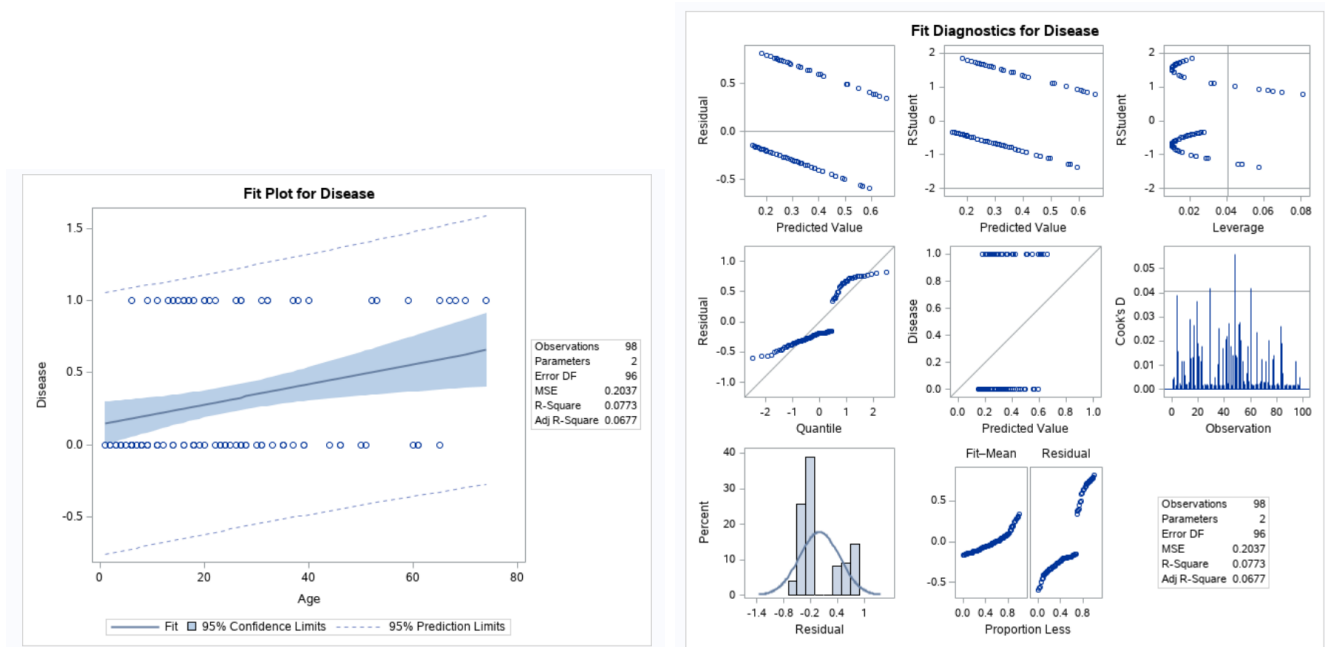


Figure 1: Fit plot and residual diagnostics for regression model that uses age to predict the presence/absence of a disease.

It is for this reason that instead of trying to predict the **value** of a categorical predictor, we should rather try to predict the **probability** of occurrence  $\pi_i$ ,

$$\pi_i = \beta_0 + \beta_1 X_{i,1} + \cdots + \beta_{p-1} X_{i,p-1} + \epsilon_i \quad (\epsilon \sim N(0, \sigma^2)). \quad (1)$$

However, based on the previous example, what are some of the issues with trying to predict the probability using (1)?

- We don't actually know  $\pi_i$ .
- Model can predict negative probabilities or probabilities above 1.
- Residual assumptions never satisfied (impossible for residuals to be normally distributed).

## 2 Transforming Probabilities

Because regression works best with **unconstrained** variables (i.e. variables that can theoretically take on any value). We need to find a transformation that maps  $\pi \in [0, 1]$  to  $f(\pi) \in (-\infty, \infty)$ .

**Solution: log-odds ratio.**

- $\pi \rightarrow [0, 1]$
- $\frac{\pi}{1-\pi} \rightarrow [0, \infty)$
- $L = \log\left(\frac{\pi}{1-\pi}\right) \rightarrow (-\infty, \infty)$

The **probit** function is another common transformation that achieves similar results.

- Probit:  $Q_i = Z_{\pi_i} \rightarrow$  Z score (of a standard normal distribution) associated with the percentile  $\pi_i$ .

Other “S” shape curves exist, which tend to reach similar conclusions.

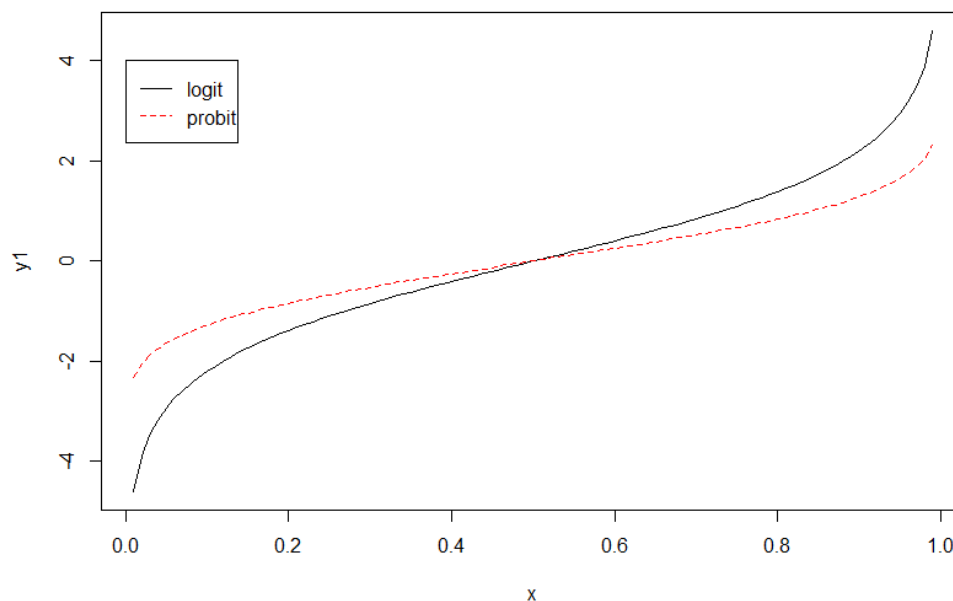


Figure 2: Visualization of logit and probit function for various probabilities.

### 3 Logistic Regression

$$L_i = \beta_0 + \beta_1 X_{i,1} + \cdots + \beta_{p-1} X_{i,p-1} + \epsilon_i$$

- $b_k$  estimates obtained from MLE-based iterative procedure (Newton-Raphson, Fisher)
- Transform estimates  $\hat{L}_i = b_0 + b_1 X_{i,1} + \cdots + b_{p-1} X_{i,p-1}$  back to probability scale.

$$\hat{\pi}_i = \frac{1}{1 + e^{-\hat{L}_i}} \quad Odds_i = e^{\hat{L}_i}$$

#### 3.1 Interpretation of Estimates

- $X_{i,1} = \cdots = X_{i,p-1} = 0 \implies \hat{L}_i = b_0 \implies Odds_i = e^{b_0}$
- Hold  $X_{i,2} = \cdots = X_{i,p-1} = 0$ , increase  $X_{i,1}$  from 0 to 1  

$$\implies \hat{L}_i = b_0 + b_1 \implies Odds_i = e^{b_0+b_1} = e^{b_0} e^{b_1}$$
- Thus, an increase in one unit in  $X_j$  *multiplies the odds* (in favor of  $Y = 1$ ) by a factor of  $e^{b_j}$ .
  - Note that it is the *odds* that are multiplied, **not** the probability.
- Alternative Interpretation: the odds of  $Y = 1$  change by  $100(e^{b_j} - 1)\%$  per unit increase in  $X_j$  while holding other predictors constant.
  - Example (Handout 5.1.1):  $b_j$  for sector is 1.57  $\implies e^{1.57} = 4.83$ .
  - “Holding all other predictors constant, the odds of having disease are  $100(4.83 - 1) = 383\%$  greater in Sector 2 than in Sector 1.
- The “Odds Ratio” for  $X_j$  (odds of  $Y = 1$  when  $X_j + 1$  vs odds of  $Y = 1$  when  $X_j$ )

$$\frac{e^{b_0+b_1X_1+\cdots+b_j(\mathbf{X}_j+1)+\cdots+b_{p-1}X_{p-1}}}{e^{b_0+b_1X_1+\cdots+b_j(\mathbf{X}_j)+\cdots+b_{p-1}X_{p-1}}} = e^{b_j}$$

#### 3.2 Inference with Estimates

- Single Variable Test:
  - $H_0 : \beta_j = 0$  ( $X_j$  has no effect on  $P(Y = 1)$ ).
  - Test statistic:  $t = \frac{b_j}{SE\{b_j\}}$  (standard normal for “large” N).
  - $\implies t^2 \sim \chi_1^2$  (obtain confidence intervals from here)
    - \* This approach is called the “Wald Test”
- Subset variables test:
  - $H_0 : \beta_{p-H} = \cdots = \beta_{p-1} = 0$ 
    - \* reorder the X variables so that the subset we are checking for comes last
  - Let  $L_{full}$  be the likelihood associated with the full model
  - Test statistics:  $\chi^2 = -2 \log \frac{L_{red}}{L_{full}}$
  - Under  $H_0 : \chi^2 \sim \chi_H^2$

- Overall model test:

$$\text{Model}\chi^2 = -2 \log L_{\text{intercept}} + 2 \log L_{\text{int\&covariates}}$$

- Often called the **deviance**,  $DEV$  or  $DEV(X_0, X_1, X_{p-1})$
- Conditional Effect plot: predicted  $\hat{\pi}$  vs one predictor  $X_j$ 
  - While holding all other predictors at some constant level. The default level in SAS is the mean (average) of each variable.

## 4 Goodness of Fit Measures:

- Pseudo R-square:  $\frac{\chi^2}{\chi^2 + n}$  ( $\chi^2$  from model test)
- Hosmer-Lemeshow Goodness of Fit Test
  - $H_0$  : logistic regression response function is appropriate
  - Based on sorted  $\hat{\pi}$  values, group observations into 5-10 roughly equal sized groups.
  - Within each group, look at the total observed numbers of  $Y = 1$  and  $Y = 0$
  - Based on the model fit, calculate the total *expected* numbers of  $Y = 1$  and  $Y = 0$ .
  - Test statistic  $\chi^2$  is sum (across groups) of  $\frac{(\text{observed} - \text{expected})^2}{\text{expected}}$
- “Concordance” - look at all pairs of observations with different  $Y$ 
  - Let  $n_c$  be the # of “concordant” pairs (observed  $Y = 1$  has larger  $\hat{\pi}$ )
  - Let  $n_d$  be the # of “discordant” pairs (observed  $Y = 1$  has smaller  $\hat{\pi}$ )
  - Let  $n_t$  be the # of “tied” paired (observed  $Y = 1$  and  $Y = 0$  have same  $\hat{\pi}$  (likely due to identical X-profiles))
  - Define rank correlation indices (larger is better):

$$\text{Somers' } D = \frac{n_c - n_d}{n_c + n_d + n_t}$$

$$\gamma = \frac{n_c - n_d}{n_c + n_d}$$

$$\text{Tau-a} = \frac{n_c - n_d}{0.5(n-1)n}$$

$$\text{AUC} = \frac{n_c + 0.5n_t}{n_c + n_d + n_t}$$

- ROC (Receiver Operating Characteristic) Curve
  - Sort all observations from the smallest to biggest  $\hat{\pi}$ .
  - At each position in the list:
    - \* Use  $\hat{\pi}$  as threshold for  $\hat{Y} = 1$ , moving cutoff from the standard 0.5 threshold.

- \* Calculate sensitivity: (proportion  $Y_i = 1$  values with  $\hat{Y}_i = 1$ ).
- \* Calculate specificity: (proportion  $Y = 0$  values with  $\hat{Y} = 0$ ).
  - Sensitivity and Specificity - think smoke alarms.
- \* False positive rate (prop  $Y = 0$  values with  $\hat{Y} = 1$ ) =  $1 - \text{specificity}$
- \* Plot false positives against true positive rates (sensitivity)
- \* Calculate the area under the curve.

Given the three ROC curves in Figure 3, which model has the best predictive power and why?

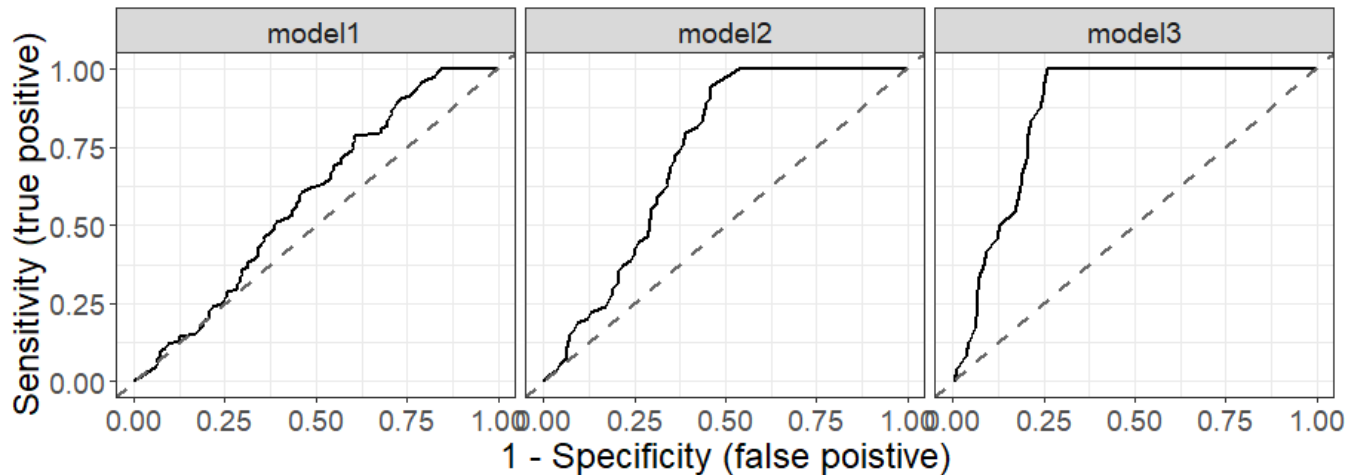


Figure 3: Comparison of three ROC curves.

Model 3 is the most accurate. The model sensitivity increases much faster than the false positive rate.

## 5 Multicollinearity

Recall that multicollinearity occurs when  $X$  variables are highly correlated with each other. It has **nothing** to do with the response variable  $Y$ .

As in OLS, multicollinearity inflates the variance of the  $b_k$  estimates, making them hard to interpret/test for significance.

As in OLS, stepwise selection and all possible regression methods exist to “score” each combination of explanatory variables and select a best model.

## 6 Outliers in Logistic Regression

If  $Y$  can only take on two values (0 or 1), how are outlier values possible?

An outlier is a point for which the observation strongly disagrees with the predicted probability.

- Define “deviance residual” as

$$dev_i = \text{sign}(Y_i - \hat{\pi}_i) \sqrt{-2(Y_i \log \hat{\pi}_i + (1 - Y_i) \log(1 - \hat{\pi}_i))}$$

- The more certain we are (probability near 0 or 1), the more potential we have to be very wrong.
- $DEV(X_0, \dots, X_{p-1}) = \sum_i dev_i^2$
- “Outliers” are values not well represented by the model
- “Half-normal probability plot - observed  $|dev_i|$  vs expected value under normality
  - **However**, since the residuals are not normally distributed, we assess differences from our expectation using simulations based on  $\hat{\pi}_i$ .
    - \* Create 19 simulations by generating a “new” response variable where the values of  $Y_{new,i} \sim \text{Bernoulli}(\hat{\pi}_i)$
  - Simulated envelop (SEE 5.1.1 MACRO ON CANVAS) plots the minimum, maximum, and mean of the 19 simulations
    - \* Why 19 simulations? - Since our observed deviances represent the 20th observation, the probability that our deviances will fall outside the envelope is less than 5% IF the fitted model is appropriate.
    - \* Points falling outside in the envelop in the upper right corner of the plot are evidence of outliers/bad fits.

## 7 Influential Observations

Influential observations have the same effect on model coefficients as they did in OLS.

Diagnostics (similar to Leverage and DFBETAS):

- $\Delta D_i : DEV - DEV_{(i)}$ 
  - Measures decrease in “misfit” when obs.  $i$  is ignored. (essentially measures the “poorness of fit for observation  $i$ ).
  - “large”  $\Delta D_i \implies$  obs.  $i$  overly influences model fit
  - SAS: DIFDEV - one step difference in deviance
- $\Delta B_i$ 
  - Similar to Cook’s distance, measures influence of obs.  $i$  on the estimates  $b_j$
  - SAS: C - confidence interval displacement C
- $\Delta \chi_i^2$ 
  - Similar to  $\Delta D_i$ : “poorness of fit” for obs  $i$
  - SAS: DIFCHISQ - one step difference in Pearson  $\chi^2$

Unlike in OLS, there is no consistent numerical rule of thumbs to determine thresholds for the  $\Delta$  measures.

Instead, we will simply rely on graphical diagnostics.

- $\Delta D_i, \Delta B_i, \Delta X_i^2$  vs Observation Number - look for extreme values
- $\Delta D_i$  vs  $\hat{\pi}_i$  (or  $\Delta X_i^2$  vs  $\hat{\pi}_i$ )
  - Look for points with low  $\hat{\pi}$  but  $Y_i = 1$  (upper left corner) OR high  $\hat{\pi}$  but  $Y = 0$  (upper right corner) which are much different than the overall pattern
  - (Optional) plot different size points where point size is determined by  $\Delta B_i$

## 8 Remedial Measures

Similar to OLS:

- Look for typos in the data
- Consider transformations of the  $X$  variables
- Consider dropping problematic points (only if you have a good argument for removing them).

## 9 Final Thought

If you have a lot of explanatory variables, you should strongly consider classification trees and random forest for classification.