Overview Logit Transformation Maximum Likelihood Model Outcome Model Comparison: Likelihood Ratio and Pseudo *R*<sup>2</sup>

# **Logistic Regression**

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Quantitative Method for Management

1/44 J. Reboulleau Logistic Regression

### **Outline**

- Overview
- 2 Logit Transformation
- Maximum Likelihood
- **Model Outcome**
- Model Comparison: Likelihood Ratio and Pseudo R<sup>2</sup>

# PART I: LOGISTIC REGRESSION OVERVIEW

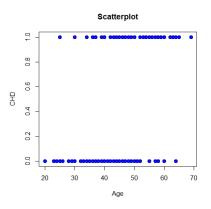
- Overview
  - Overview
  - Specifities of Logistic Regression
- 2 Logit Transformation
- Maximum Likelihood
- Model Outcome
- **6** Model Comparison: Likelihood Ratio and Pseudo  $R^2$

### A specific regression

- The logistic regression is a specific case where the outcome variable is a binary or dichotomous.
- As a result, the methods employed will be very close to the one presented in the linear regression.
- We will use our Regression chapter as a motivation in the logistic regression context.
- We start by highlighting the differences between these 2 types of regression.

- We consider the sample of heart diseases.
- We select 100 subjects (ID) and their age (Age).
- We note the presence or absence of significant coronary heart disease (CHD): 0 if absent, 1 if present.
- We also add an age group variable AGRP.
- The interest of the study is to explore the relationship between the Age and CHD.
- CHD is going to be our response variable.

 Step 1: Scatterplot We start by developing an intuitive analysis of the various relationship:

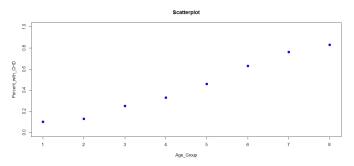


- All points fall into 2 lines: y = 0 and y = 1.
- The structure of the relationship between CHD and Age is not clear.

 To clarify the relationship, we use the AGRP and compute the Average frequence of CHD per age category:

Age Group	AGRP	Absent	Present	Mean Proportion within Age Group
20-29	1	9	1	10%
30-34	2	13	2	13%
35-39	3	9	3	25%
40-44	4	10	5	33%
45-49	5	7	6	46%
50-54	6	3	5	63%
55-59	7	4	13	76%
60-69	8	2	8	83%

 Step 1: Scatterplot The structure of the relationship between CHD and Age Group is now clear.



- What we have done here is to compute the average number of CHD per Age Group, i.e. E[Y|x].
- What we are willing to fit here is

$$E[Y|X] = \beta_0 + \beta_1 \cdot X$$

- However, since our Y variable is binary, E[Y|x] will only take value between 0 and 1 with gradual increase as long as x increase.
- As a result, we need a specific function for E[Y|x] reflecting these 2 properties:
  - Values between 0 and 1
  - Gradual increase

### PART II: LOGIT TRANSFORMATION

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• In order to achieve this, we use the function:

$$E[Y|X] = \pi(X) = \frac{e^{(\beta_0 + \beta_1 X)}}{1 + e^{(\beta_0 + \beta_1 X)}}$$

• We define the *logit transformation* in terms of  $\pi(x)$  as the function g(x):

$$g(x) = \ln(\frac{\pi(x)}{1 - \pi(x)}) = \beta_0 + \beta_1 x$$

In the previous Chapter, we were fitting a model such as

$$y = \beta_0 + \beta_1 x + \epsilon$$

where  $\epsilon$  were normally distributed.

- In our context, this does not make sense as y should take either the value 1 or the value 0.
- We should instead see it the following way

$$y = \beta_0 + \beta_1 x + \epsilon$$

where

If 
$$y=1$$
 then,  $\epsilon=1-g(x)$  with probability  $\pi(x)$   
If  $y=0$  then,  $\epsilon=-g(x)$  with probability  $1-\pi(x)$ 

• As a result, the errors  $\epsilon$  are following a binomial distribution with probability  $\pi(x)$ .

### Logit Transformation: Difference with regression

As a result,

If 
$$y=1$$
 then,  $\epsilon=1-g(x)$  with probability  $\pi(x)$   
If  $y=0$  then,  $\epsilon=-g(x)$  with probability  $1-\pi(x)$ 

$$P(Y = y_i = 1 | x_i) = \pi(x_i)^1 = \pi(x_i)^{y_i}$$

and

$$P(Y = y_i = 0|x_i) = (1 - \pi(x_i))^{1-0} = [1 - \pi(x_i)]^{1-y_i}$$

Finally,

$$P(Y = y_i|x_i) = \pi(x_i)^{y_i}[1 - \pi(x_i)]^{1-y_i}$$

# PART I: MAXIMUM LIKELIHOOD

- Overview
- Logit Transformation
- Maximum Likelihood
  - Fitting the Logistic Regression: MLE Method
- Model Outcome
- **Model Comparison: Likelihood Ratio and Pseudo**  $R^2$

- We recall that the maximum likelihood estimation (MLE) is a method of estimating the parameters of a statistical model given observations.
- The target is to find the parameter values that maximize the likelihood of making the observations given the parameters.
- The likelihood function is mathematically defined as

$$I(\beta) = \prod_{i=1}^n f(y_i|x_i)$$

• We are willing to maximize this likelihood function.

### Fitting the logistic regression: MLE Method

### In our case

- $\beta$  is the vector of parameters we are looking for, i.e.  $\beta = (\beta_0, \beta_1)$ .
- In our case, we have already found the contribution for each data  $f(y_i|x_i)$ , so that

$$I(\beta) = \prod_{i=1}^{n} f(y_i|x_i)$$
$$= \prod_{i=1}^{n} \pi(x_i)^{y_i} [1 - \pi(x_i)]^{1-y_i}$$

• In order to maximize we have to work with the derivatives with respect to  $\beta_0$  and  $\beta_1$ .

Maximizing the likelihood is equivalent to maximizing the log-likelihood, so that we consider  $L(\beta)$ 

$$L(\beta) = \log(I(\beta))$$

$$= \log(\prod_{i=1}^{n} \pi(x_i)^{y_i} [1 - \pi(x_i)]^{1 - y_i})$$

$$= \sum_{i=1}^{n} [y_i \cdot \log(\pi(x_i)) + (1 - y_i) \cdot \log(1 - \pi(x_i))]$$

$$= \sum_{i=1}^{n} [\log(1 - \pi(x_i)) + y_i \cdot \log(\frac{\pi(x_i)}{1 - \pi(x_i)})]$$

$$= \sum_{i=1}^{n} [-\log(1 + e^{\beta_0 + \beta_1 x_i}) + y_i \cdot (\beta_0 + \beta_1 x_i)]$$

### **MLE Method: First parameter**

• Computing the first derivative with respect to the first parameter  $\beta_0$ 

$$\frac{\partial L(\beta)}{\partial \beta_0} = \frac{\partial}{\partial \beta_0} \sum_{i=1}^n \left[ -\log(1 + e^{\beta_0 + \beta_1 x_i}) + y_i(\beta_0 + \beta_1 x_i) \right]$$

$$= \sum_{i=1}^n \left[ -\frac{1}{1 + e^{\beta_0 + \beta_1 x_i}} (e^{\beta_0 + \beta_1 x_i}) + y_i \right]$$

$$= \sum_{i=1}^n \left[ -\pi(x_i) + y_i \right]$$

The first derivative leads to

$$\sum_{i=1}^{n} \left[ -\pi(x_i) + y_i \right] = 0 \Leftrightarrow \sum \widehat{\pi(x_i)} = \sum y_i$$

- However, it is not possible to go further as the equation is not linear.
- We thus need some computer algorithms to solve this problem.
- The equation means that the sum of our predicted values are equal to the sum of our response data.

• Computing the first derivative with respect to the second parameter  $\beta_1$ 

$$\frac{\partial L(\beta)}{\partial \beta_1} = \frac{\partial}{\partial \beta_1} \sum_{i=1}^n \left[ -\log(1 + e^{\beta_0 + \beta_1 x_i}) + y_i(\beta_0 + \beta_1 x_i) \right]$$

$$= \sum_{i=1}^n \left[ -x_i \frac{1}{1 + e^{\beta_0 + \beta_1 x_i}} (e^{\beta_0 + \beta_1 x_i}) + y_i \cdot x_i \right]$$

$$= \sum_{i=1}^n \left[ x_i \cdot (-\pi(x_i) + y_i) \right]$$

### MLE Method. Second parameter

The other derivative leads to

$$\sum_{i=1}^{n} x_i [-\pi(x_i) + y_i] = 0$$

 However, it is not possible to go further as the equation is again not linear.

### **MLE Method: Conclusions**

- A direct algebric equation is not possible when fitting with the MLE method.
- The MLE method expressed in the one dimension case (only one dependant variable x) is easily generalized to multiple cases.

# PART III: MODEL RESULTS

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  - Model outcome
- **5** Model Comparison: Likelihood Ratio and Pseudo  $R^2$

### **Example: Model Outcome**

### We get the following outcome for our model

```
> mymodel <- glm(CHD ~ Age, family=binomial (link='logit'))
> summary(mymodel)
Call:
glm(formula = CHD ~ Age, family = binomial(link = "logit"))
Deviance Residuals:
   Min
            1Q Median
                                      Max
-1.9702 -0.8447 -0.4572 0.8264 2.2866
Coefficients:
           Estimate Std. Error z value Pr(>|z|)
(Intercept) -5.31026 1.13463 -4.680 2.87e-06 ***
           0.11088    0.02407    4.606    4.11e-06 ***
Age
Signif. codes: 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
(Dispersion parameter for binomial family taken to be 1)
   Null deviance: 136.66 on 99 degrees of freedom
Residual deviance: 107.40 on 98 degrees of freedom
AIC: 111.4
Number of Fisher Scoring iterations: 4
```

• The  $\widehat{\pi(x_i)}$  is going to give us the model prediction

$$\widehat{\pi(x_i)} = \frac{e^{\beta_0 + \beta_1 \cdot x_i}}{1 + e^{\beta_0 + \beta_1 \cdot x_i}}$$

$$= \frac{e^{-5.31 + 0.11 \cdot x_i}}{1 + e^{-5.31 + 0.11 \cdot x_i}}$$

For somebody aged 43 years, one gets

$$\widehat{\pi(x_i)}$$
 =  $\frac{e^{-5.31+0.11\cdot 43}}{1+e^{-5.31+0.11\cdot 43}}$   
= 0.367

• Finally, our logit function is given by

$$\widehat{g(x_i)} = -5.31 + 0.11 \cdot x_i = -0.58$$

For somebody aged 43 years, one gets

$$\widehat{\pi(x_i)} = 0.367$$

$$\widehat{g(x_i)} = -0.5$$

- The interpretation of  $g(x_i) = -0.58$  is not clear. It is similar to a score.
- The interpretation of  $\widehat{\pi(x_i)} = 0.367$  is easier because  $\widehat{\pi(x_i)}$  is a probability.
- A low score for  $\widehat{\pi(x_i)}$  will tend to predict a 0 value for our response variable  $\widehat{y_{43}}$ .
- A high score for  $\widehat{\pi(x_i)}$  will tend to predict a 1 for  $\widehat{y_i}$ .
- The threshold level (cutting point) will have to be decided: at which level of  $\widehat{\pi(x_i)}$  do we consider that we predict a 0 or a 1.
- Generally, we decide with the 0.5 level.

Likelihood ratio test

Model comparison: Likelihood

Model comparison: Pseudo-R squared

Prediction Quality: ROC Curve

Executive Summary

### PART IV: LIKELIHOOD RATIO TEST

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  - Likelihood ratio test
  - Model comparison: Likelihood
  - Model comparison: Pseudo-R squared
  - Prediction Quality: ROC Curve
  - Executive Summary

# Testing for the significance of the model

- The idea is the same as in the previous Chapter. We estimate the model quality by comparing our observed data  $y_i$  to predicted data  $\hat{y_i}$
- In our context of likelihood, the tool we are going to use is called the likelihood ratio D:

$$\begin{array}{ll} D & = & -2 \cdot \log[\frac{\text{likelihood of a 1st model}}{\text{likelihood of a 2nd model}}] \\ & = & -2 \cdot (\log[\text{likelihood of a 1st model}] \\ & & -\log[\text{likelihood of a 2nd model}]) \end{array}$$

- The main use of Likelihood ratio is to establish models comparison by comparing their likelihood.
- As a result *D* is often called the deviance from one model to the other.

# Testing for the significance of the model

- The deviance D plays the same role as the SSE is the multiple linear regression context. It is a measure of goodness of fit.
- The value −2 at the beginning of the equation is for fitting with the probability distribution.
- For instance, we can compare any model to the perfect model "saturated model".
- A perfect model will exactly represent each y<sub>i</sub>. This saturated model
  has as many parameters as numbers of data and "makes no mistake".
- In the context of a saturated model, we make no mistake and  $\pi(x_i) = y_i$ .

### Testing for the significance of the model

• Since  $y_i$  takes values either 0 or 1, we get for a saturated model

$$I(\beta) = \prod_{i=1}^{n} \pi(x_i)^{y_i} [1 - \pi(x_i)]^{1 - y_i}$$
$$= \prod_{i=1}^{n} y_i^{y_i} [1 - y_i]^{1 - y_i}$$
$$= 1$$

Our likelihood ratio is reduced to

 $D = -2 \cdot \log[\text{likelihood of the fitted model}]$ 

# **Comparing Model**

- The idea is to find which models offer a better fit.
- Of course, the more we have predictors, the best fit we will get.
- However, the improvements may not be that significant regarding the increase in model complexity.
- Suppose we compare 2 models: Model 1 with more complexity/variables (Alternative Model), Model 2 with fewer variables (Null Model).

 $H_0 :=$  the 2 models are equivalent, we choose Model 2

 $H_1 := Model 1 offers a better fit$ 

Likelihood ratio test Model comparison: Likelihood Model comparison: Pseudo-R squared Prediction Quality: ROC Curve Executive Summary

### **Comparing Model**

 We compare 2 models: Model 1 with more complexity/variables, Model 2 with fewer variables.

> $H_0 := \text{the 2 models are equivalent, we choose Model 2}$  $H_1 := \text{Model 1 offers a better fit}$

We compute

$$\begin{array}{ll} D & = & -2 \cdot \log[\frac{\text{likelihood of Model 2 (Null Model)}}{\text{likelihood of Model 1 (Alternative Model)}}] \\ & = & +2 \cdot \log[\frac{\text{likelihood of Model 1}}{\text{likelihood of Model 2}}] \\ & = & -2 \cdot (\log[\text{likelihood of Model 2}] \\ & -\log[\text{likelihood of Model 1}]) \end{array}$$

 If the difference is significant (p-value criteria), then the model improvement with increasing complexity is of interest and we choose Model 1.

# **Comparing Model**

- We use the German Credit data (62 characteristics and 1000 observations).
- The target is to estimate if a client is a bad consumer (0) or a good consumer (1) according to several characteristics.

```
> ################Loading Data
> library(caret)
> data(GermanCredit)
> ######Defining Complex model: Model 1
> mod fit one <- glm(Class ~ Age + ForeignWorker + Property.RealEstate + Housing.Own +
                      CreditHistory.Critical, data=GermanCredit, family="binomial")
> ######Defining Simpler model: Model 2
> mod fit two <- glm(Class ~ Age + ForeignWorker, data=GermanCredit, family="binomial")
> library(lmtest)
> lrtest(mod_fit_one, mod_fit_two)
Likelihood ratio test
Model 1: Class ~ Age + ForeignWorker + Property.RealEstate + Housing.Own +
   CreditHistory.Critical
Model 2: Class ~ Age + ForeignWorker
 #Df LogLik Df Chisq Pr(>Chisq)
1 6 -575.42
2 3 -602.48 -3 54.124 1.056e-11 ***
Signif. codes: 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
```

• Complex model is significantly better.

### **Pseudo-R Squared**

- In the context of logistic regression, there is no R<sup>2</sup>, meaning no analysis
  of the part of the response variable explained.
- We will work with Pseudo R<sup>2</sup> for which the most famous is the McFadden.
- The McFadden is defined by

$$R_{McF}^2 = 1 - \frac{\log(LM)}{\log(L_0)}$$

where log(LM) is the log likelihood value for the fitted model and  $log(L_0)$  is the log likelihood for the null (constant) model with only an intercept as a predictor.

 R<sup>2</sup><sub>McF</sub> takes values between 0 and 1. Small values (close to 0) present models with few predicting capacity.

Likelihood ratio test Model comparison: Likelihood Model comparison: Pseudo-R squared Prediction Quality: ROC Curve Executive Summary

### **Pseudo-R Squared**

In our example, one gets

 The level of explanation is quite poor. As previously anticipated, the situation is even worst in our second model.

- In order to evaluate the model quality, we simply compare the prediction with the realized data.
- To prevent from overfitting, we usually, start by working on sample data and test the prediction ability on new data.
- After partitioning the data and training the model, we finally get our model predicting quality estimate

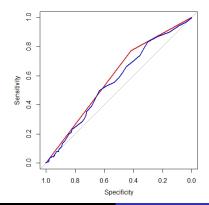
```
> Train <- createDataPerrition(GermanCredit$Class, p=0.6, list=FALSE)
> training <- GermanCredit[ Tain, ]
> testing <- GermanCredit[ -Train, ]
> mod_fit <- train(Class ~ Age + ForeignWorker + Property.RealEstate + Housing.Own + CreditHistory.Critical, da
> pred = predict(mod_fit, newdata=testing)
> accuracy <- table(pred, testing(, "Class"))
> sum(diag(accuracy))/sum(accuracy)
[1] 0.7025
> accuracy

pred Bad Good
Bad 24 23
Good 96 257
```

- After looking at the model ability to predict correctly the response variable y, one might be willing to look at the independant variable individually.
- To achieve this task, a useful tool is the ROC curve. To introduce the ROC curve, we need to define the sensitivity, the specificity and the cut-point.
- The **sensitivity** is the proportion of truly positive observations which is classified as such by the model or test (indicating y = 1 correctly).
- Conversely the **specificity** is the probability of the model predicting 'negative' given that the observation is 'negative' (indicating y = 0 correctly).

- To decide, if we are going to indicate y = 0 or y = 1, we need a decision rule, meaning a **cut-point c**. Generally speaking, the cut-off point is 0.5.
- We classify the observations with a fitted probability above c as positive and those at or below it as negative.
- For this particular cut-off, we can estimate the sensitivity by the proportion of observations with Y=1 which have a predicted probability above c, and similarly we can estimate specificity by the proportion of Y=0 observations with a predicted probability at or below c.
- There is always a trade-off between specificity and sensitivity because if one increases, the other decreases.

- We come to the ROC curve, which is simply a plot of the values of sensitivity against one minus specificity, as the value of the cut-point c is increased from 0 through to 1.
- We can apply this to either the full model or individual variable.



- A perfect model would predict perfectly the (sensitivity), i.e. reaching 100% of correct answer. At the same time, it would make no mistake for predicting negative answers (1-specificity).
- As a result, a perfect model would reach the upper left corner of our ROC graph.
- It means that we can estimate the model quality by computing the area
  of the ROC curve above the purely random model represented by the
  straight line.
- If this area is high, we have a good discrimination level.
- The area takes value between 0.5 and 1. A value above 0.8 would be considered as a good level.

 Individual application with in red the Housing Owned curve and in blue the Age one.

```
> library(pBCC)
> & Compute AUC for predicting Class with the variable CreditHistory.Critical
> f1 = roc(Class - Housing.Own, data=training)
> f2 = roc(Class - Age, data=training)
> f1

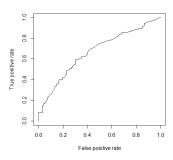
Call:
roc.formula(formula = Class - Housing.Own, data = training)

Data: Housing.Own in 180 controls (Class Bad) < 420 cases (Class Good).
Area under the curve: 0.594
> f2

Call:
roc.formula(formula = Class - Age, data = training)

Data: Age in 180 controls (Class Bad) < 420 cases (Class Good).
Area under the curve: 0.5884
```

• We can develop the same tool for the overall model



And we get the following area

Likelihood ratio test Model comparison: Likelihood Model comparison: Pseudo-R squared Prediction Quality: ROC Curve Executive Summary

### **Executive Summary**

- Logistic Regression specificities: 0 and 1.
- Model fitting through MLE method.
- No diagnostic plot: qqplot does not make sense.
- Model outcome: the score function and interpretation
- Model comparison and selection: the likelihood ratio test
- Prediction quality analysis: Pseudo R<sup>2</sup>, Overall prediction, ROC curve.