# **Module 6: Linear Models for Classification**

ISE-529

Content based on ISLR Chapter 4.1 - 4.3

### **Outline**

- Classification Basic Theory
  - Logistic regression basic theory
  - Parameter estimation
  - Confounding
  - Classification from logistic regression models
- Assessment
  - Misclassification Rate
  - Sensitivity/Specificity
  - Receiver Operating Characteristics (ROC) Charts and optimizing the classification threshold
  - Lift and Lift Curves

# **Data Mining Techniques Overview**

Classification Analysis

The process of predicting the "class" (or label or group membership) of newly encountered entities based on analyzing known class membership of other similar types of entities.

- Belongs to the group of techniques referred to as "supervised" learning
- If classes are binary (pass/fail, purchase/no purchase, fraudulent/not fraudulent, it is referred to as "binary classification"

We will only be addressing binary classification in this module

**Credit Scoring** 

Can credit score and home ownership predict load default?

#### **Predictor Variables:**

- Credit Score: 300–850
- Home Ownership: Yes/No/Rent



### Response Variable:

Loan Default: Yes/No



**Biostatistics** 

Are alcohol and smoking related to heart disease?

#### **Predictor Variables:**

- Alcohol: ounces per day
- Smoking: cigarettes per day



### Response Variable:

• Heart Disease: 1/0



Campaign Marketing

Does a customer make a purchase based on past behavior?

#### **Predictor Variables:**

- Purchases: total spent in past 90 days
- Age Group: four levels
- Gender: M/F



#### Response Variable:

• Campaign: Yes/No



### Classification

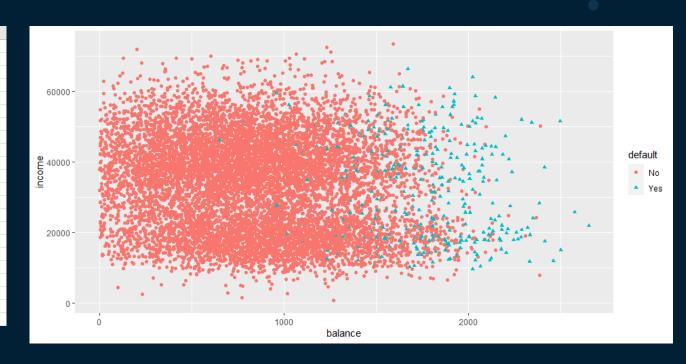
- Similar to regression, objective is to develop a mathematical model of the relationship of one or more independent variables (or predictors or regressors or explanatory variables) to one dependent variable (or response variable).
- However, in classification problems the dependent variable is a categorical attribute.
- Common special case is where the dependent variable takes one of two possible values (true/false, pass/fail, sick/healthy, etc.) – referred to as binary classification
- Generally, we are more interested in estimating the probabilities that the output belongs into each category level.
  - For example, it is more valuable to have an estimate of the probability that an insurance claim is fraudulent than just a classification of "Fraudulent"

### Credit Card Default

4	Α	В	С		D		Е	F
1		default	student	balance		inco	me	
2	1	No	No	\$	729.53	\$	44,361.63	
3	2	No	Yes	\$	817.18	\$	12,106.13	
4	3	No	No	\$	1,073.55	\$	31,767.14	
5	4	No	No	\$	529.25	\$	35,704.49	
6	5	No	No	\$	785.66	\$	38,463.50	
7	6	No	Yes	\$	919.59	\$	7,491.56	
8	7	No	No	\$	825.51	\$	24,905.23	
9	8	No	Yes	\$	808.67	\$	17,600.45	
10	9	No	No	\$	1,161.06	\$	37,468.53	
11	10	No	No	\$	-	\$	29,275.27	
12	11	No	Yes	\$	-	\$	21,871.07	
13	12	No	Yes	\$	1,220.58	\$	13,268.56	
14	13	No	No	\$	237.05	\$	28,251.70	
15	14	No	No	\$	606.74	\$	44,994.56	
16	15	No	No	\$	1,112.97	\$	23,810.17	
17	16	No	No	\$	286.23	\$	45,042.41	
18	17	No	No	\$	-	\$	50,265.31	
19	18	No	Yes	\$	527.54	\$	17,636.54	
20	19	No	No	\$	485.94	\$	61,566.11	
21	20	No	No	\$	1,095.07	\$	26,464.63	
22	21	No	No	\$	228.95	\$	50,500.18	
23	22	No	No	\$	954.26	\$	32,457.51	
24	23	No	No	\$	1,055.96	\$	51,317.88	
25	24	No	No	\$	641.98	\$	30,466.10	
26	25	No	No	\$	773.21	\$	34,353.31	
27	26	No	No	\$	855.01	\$	25,211.33	
28	27	No	No	\$	643.00	\$	41,473.51	
29	28	No	No	\$	1,454.86	\$	32,189.09	
ВО	29	No	No	\$	615.70	\$	39,376.39	
81	30	No	Yes	\$	1,119.57	\$	16,556.07	
32	31	No	No	\$	494.82	\$	54,384.78	
33	32	No	Yes	\$	448.88	\$	15,799.47	
34	33	No	Yes	\$	584.90	\$	22,429.94	
3.0	24	No	No	Ċ	012 50	Ċ	46 007 22	

Credit Card Default Data.csv

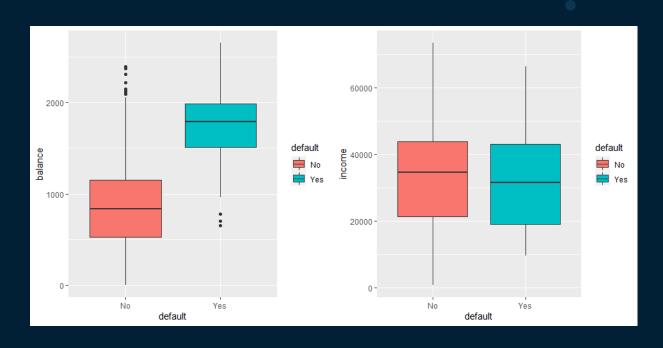
						ı
1	Α	В	С	D	E	
		default	student	balance	income	
	1	No	No	\$729.53	\$44,361.63	
	2	No	Yes	\$817.18	\$12,106.13	
	3	No	No	\$1,073.55	\$31,767.14	
	4	No	No	\$529.25	\$35,704.49	
	5	No	No	\$785.66	\$38,463.50	
	6	No	Yes	\$919.59	\$7,491.56	
	7	No	No	\$825.51	\$24,905.23	
	8	No	Yes	\$808.67	\$17,600.45	
	9	No	No	\$1,161.06	\$37,468.53	
	10	No	No	\$-	\$29,275.27	
	11	No	Yes	\$-	\$21,871.07	
	12	No	Yes	\$1,220.58	\$13,268.56	
	13	No	No	\$237.05	\$28,251.70	
	14	No	No	\$606.74	\$44,994.56	
	15	No	No	\$1,112.97	\$23,810.17	
,	16	No	No	\$286.23	\$45,042.41	
	17	No	No	\$-	\$50,265.31	
	18	No	Yes	\$527.54	\$17,636.54	
	19	No	No	\$485.94	\$61,566.11	
	20	No	No	\$1,095.07	\$26,464.63	
	21	No	No	\$228.95	\$50,500.18	



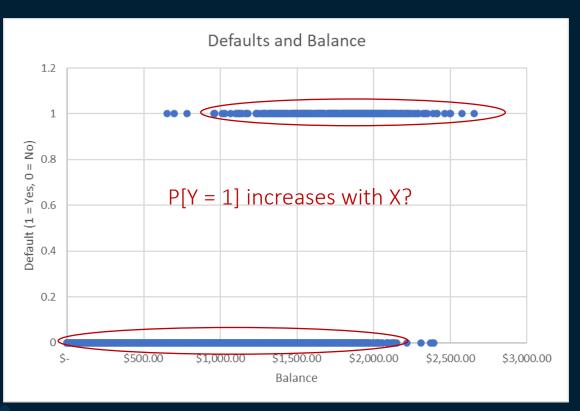
Which factor (balance or income) has the stronger relation to default?

Credit Card Default Data.csv

1	Α	В	С	D	E	
		default	student	balance	income	
	1	No	No	\$729.53	\$44,361.63	
	2	No	Yes	\$817.18	\$12,106.13	
	3	No	No	\$1,073.55	\$31,767.14	
	4	No	No	\$529.25	\$35,704.49	
	5	No	No	\$785.66	\$38,463.50	
	6	No	Yes	\$919.59	\$7,491.56	
	7	No	No	\$825.51	\$24,905.23	
	8	No	Yes	\$808.67	\$17,600.45	
	9	No	No	\$1,161.06	\$37,468.53	
	10	No	No	\$-	\$29,275.27	
	11	No	Yes	\$-	\$21,871.07	
	12	No	Yes	\$1,220.58	\$13,268.56	
Ŀ	13	No	No	\$237.05	\$28,251.70	
	14	No	No	\$606.74	\$44,994.56	
	15	No	No	\$1,112.97	\$23,810.17	
	16	No	No	\$286.23	\$45,042.41	
	17	No	No	\$-	\$50,265.31	
	18	No	Yes	\$527.54	\$17,636.54	
	19	No	No	\$485.94	\$61,566.11	
	20	No	No	\$1,095.07	\$26,464.63	
	21	No	No	\$228.95	\$50,500.18	



Scatterplot



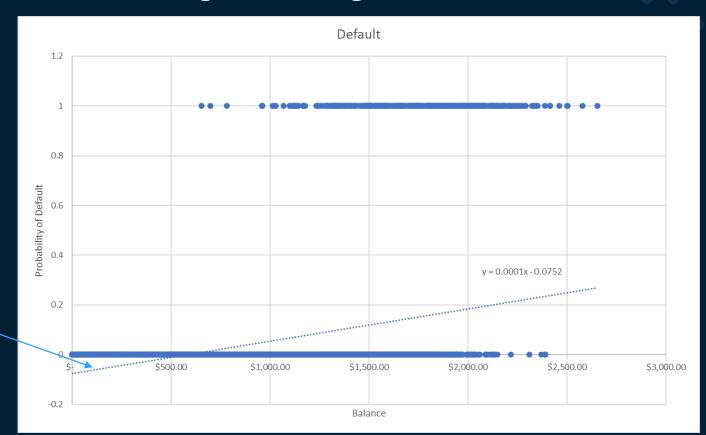
# Can't We Just Use Linear Regression?

• Suppose we code the dependent variable for an insurance claim as fraudulent as follows:

$$Y = \begin{cases} 0 & if \ No \\ 1 & if \ Yes \end{cases}$$

• Can't we simply perform a linear regression of Y on X and classify as Yes if  $\hat{Y} > 0.5$ ?

# **Issues With Using Linear Regression For Classification**

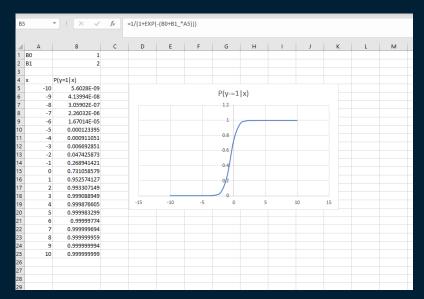


Negative probability of default is meaningless!

# The Logistic Regression Model

 Logistic regression is based on the assumption that a good mathematical model for a binary variable (with a single regressor) is:

$$p(X) \equiv P(Y = 1|X) = \frac{1}{1 + e^{-(\beta_0 + \beta_1 X)}} = \frac{e^{(\beta_0 + \beta_1 X)}}{1 + e^{(\beta_0 + \beta_1 X)}}$$



### The Logistic Regression Model

• A bit of re-arrangement of p(X) yields the log odds or logit function:

$$\log\left(\frac{p(X)}{1-p(X)}\right) = \beta_0 + \beta_1 X$$
Logit Function

The logit function is referred to as the link function for logistic regressions.

### The Logistic Regression Model

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$$\log\left(\frac{p(X)}{1-p(X)}\right) = \beta_0 + \beta_1 X$$
Logit Function

The logit function is referred to as the link function for logistic regressions.

• Recall that for linear regression, we estimated the parameters based on minimizing the residuals sum of squares:

$$RSS = \sum_{i=1}^{n} \epsilon_i^2 = \sum_{i=1}^{n} (y_i - \hat{\beta}_0 - \hat{\beta}_1 x_i)^2$$

- However, we cannot use that method for estimating the parameters of many models, including for logistic regressions
  - WHY???
  - Hint: remember that for linear regression, we are modeling the actual value of the output attribute. What are we modeling for logistic regression?

- In logistic regression, we are not modeling the value of an output attribute, we are modeling the probability that the output attribute takes on one of two possible states.
  - If we have enough data, we could observe the actual probabilities by counting the percentage of states for each given value of X
- In practice, we generally use an alternate technique called Maximum Likelihood Estimation (MLE)

#### Maximum Likelihood Estimation

- In OLS (Ordinary Least Squares), we are trying to find the parameters of a line (or curve) that minimizes the sum of the squares of the differences between the estimation (given by the regression equation) and the actual data.
- In MLE, we are trying to find the parameters of an equation that maximizes the probability of having actually observed the data that we observe (our training data)

### **Maximum Likelihood Estimation**

- Parameter estimation is performed by Maximum Likelihood Estimation
  - Calculate the probability of observing the data given estimated parameters
  - Find the parameter estimates that maximize that probability

$$\ell(\beta_0, \beta_1, \dots) \equiv p(\beta_0, \beta_1, \dots | X) = \prod_{i: y_i = 1} p(x_i) \prod_{i: y_i = 0} (1 - p(x_i))$$

 For computational efficiency, we generally maximize the logarithm of this likelihood (referred to as the log-likelihood)

$$ll(\beta_0, \beta_1, ...) = \sum_{i:y_i=1} \ln(p(x_i)) \sum_{i:y_i=0} \ln(1-p(x_i))$$

# **Maximum Likelihood Estimation**

=1/(1+EXP(-(B0+B1	_*D6)))	=IF(B6="Y	es",F6,(1-F6)
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	Α	В	С	D	E	F	G	н і
1	В0	-10.65						
2	B1	0.005499						
3	II(B0, B1)	-798.23						
4								
5		default	student	balance	income	p(Y=1 X)	likelihood(X)	II(X)
6	1	No	No	\$ 729.53	\$ 44,361.63	0.001307	0.998692505	-0.00130835
7	2	No	Yes	\$ 817.18	\$ 12,106.13	0.002116	0.997884455	-0.00211779
8	3	No	No	\$ 1,073.55	\$ 31,767.14	0.008607	0.991393153	-0.0086441
9	4	No	No	\$ 529.25	\$ 35,704.49	0.000435	0.999564966	-0.00043513
10	5	No	No	\$ 785.66	\$ 38,463.50	0.001779	0.998220565	-0.00178102
11	6	No	Yes	\$ 919.59	\$ 7,491.56	0.003709	0.996290651	-0.00371625
12	7	No	No	\$ 825.51	\$ 24,905.23	0.002215	0.997785479	-0.00221698
13	8	No	Yes	\$ 808.67	\$ 17,600.45	0.002019	0.997981011	-0.00202103
14	9	No	No	\$ 1,161.06	\$ 37,468.53	0.013852	0.986147536	-0.0139493
15	10	No	No	\$ -	\$ 29,275.27	0.000024	0.9999763	-2.3701E-05
16	11	No	Yes	\$ -	\$ 21,871.07	0.000024	0.9999763	-2.3701E-05
17	12	No	Yes	\$ 1,220.58	\$ 13,268.56	0.019114	0.980885527	-0.01929952
18	13	No	No	\$ 237.05	\$ 28,251.70	0.000087	0.999912736	-8.7267E-05
19	14	No	No	\$ 606.74	\$ 44,994.56	0.000666	0.999333979	-0.00066624
20	15	No	No	\$ 1,112.97	\$ 23,810.17	0.010668	0.989332057	-0.01072525
21	16	No	No	\$ 286.23	\$ 45,042.41	0.000114	0.999885636	-0.00011437
22	17	No	No	\$ -	\$ 50,265.31	0.000024	0.9999763	-2.3701E-05
23	18	No	Yes	\$ 527.54	\$ 17,636.54	0.000431	0.999569037	-0.00043106
24	19	No	No	\$ 485.94	\$ 61,566.11	0.000343	0.999657136	-0.00034292
25	20	No	No	\$ 1,095.07	\$ 26,464.63	0.009678	0.990322193	-0.00972494
26	21	No	No	\$ 228,95	\$ 50,500,18	0.000083	0.999916534	-8 3469F-05

### **Maximum Likelihood Estimation**

	Coefficient	Std. Error	Z-statistic	P-value
Intercept	-10.6513	0.3612	-29.5	< 0.0001
balance	0.0055	0.0002	24.9	< 0.0001

#### Interpreting standard regression coefficient statistics:

- Std. Error sample standard deviation (adjusted for sample size)
  - Roughly 95% of the observations fall within 2 Standard Errors of the estimated value
- Z-statistic Coefficient divided by the Std. Error
  - Number of standard errors the coefficient is away from zero
  - Looking for a number greater than 2 or 3 for significance of the coefficient
- P-value probability that the true coefficient is zero
  - Looking for a value less than 0.05 or 0.01

### **Making Predictions**

 Once the parameters have been estimated, it is straightforward to make a prediction on a new case by plugging the values of the parameters and independent variable(s) into the logistic regression equation:

$$p(X) \equiv P(Y = 1|X) = \frac{e^{(\beta_0 + \beta_1 X)}}{1 + e^{(\beta_0 + \beta_1 X)}}$$

### Scikit-Learn Logistic Regression

```
In [154]: import numpy as np
          import pandas as pd
          from sklearn.linear_model import LogisticRegression
          import sklearn.metrics as metrics
In [57]: credit default data = pd.read csv("Credit Card Default Data.csv")
In [95]: credit_default_data
Out[95]:
                default student income balance
                           Yes 9663.79 2024.66
                           Yes 10155.32 1681.48
                           Yes 10470.64 2066.70
                           Yes 10591.72 1707.91
                   Yes
                           Yes 11054.07 1492.96
                            No 70700.65 1067.84
           9496
           9497
                            No 71238.55 1253.18
           9498
                            No 71878.77 201.81
           9499
                            No 72461.30 1233.71
                            No 73554.23 1593.43
          9501 rows × 4 columns
```

### Scikit-Learn Logistic Regression

Consider the example of predicting loan defaults based on loan balance:

```
y = credit_default_data['default']
X = credit_default_data[['balance']]

model1 = LogisticRegression().fit(X,y)

model1.intercept_
array([-10.64979227])

model1.coef_
array([[0.005498]])
```

$$p(X) = \frac{e^{(-10.65+0.0055X)}}{1+e^{(-10.65+0.0055X)}}$$

 What is the estimated probability of default for someone with a balance of \$1000?

$$p(X) \frac{e^{(-10.65+0.0055*1000)}}{1+e^{(-10.65+0.0055*1000)}} = 0.006$$

 What is the estimated probability of default for someone with a balance of \$2000?

$$p(X) \frac{e^{(-10.65+0.005*2000)}}{1+e^{(-10.65+0.005*2000)}} = 0.586$$

### Scikit-Learn Logistic Regression

Consider the example of predicting loan defaults based on student status:

```
Create simple logistic regression model with student as predictor

y = credit_default_data['default']
dummy_vars = pd.get_dummies(credit_default_data['student'])
X = dummy_vars[['Yes']]

model2 = LogisticRegression().fit(X,y)

model2.intercept_
array([-3.43705617])

model2.coef_
array([[0.35856645]])
```

$$p(X) = \frac{e^{(-3.44 + 0.359X)}}{1 + e^{(-3.44 + 0.359X)}}$$

# **Default Example**

### Using Student as Predictor

$$P(default \mid student = Yes) = 0.044$$
  
 $P(default \mid student = No) = 0.031$ 

# **Interpreting Coefficients**

# **Interpreting Coefficients**

Understanding Odds and Odds Ratios

$$\log\left(\frac{p(Y)}{1-p(Y)}\right) = \beta_0 + \beta_1 X$$
Logit Function

### **Odds Ratios**

- ullet A random event may be observed with probability  $\pi$
- The odds ratio (or just "odds") is an expression of how much more likely an event is to occur than not occur
  - Closely tied with gambling where payoffs are based on odds ratios

### **Odds Ratios**

Mathematically:

$$Odds[A] = \frac{\pi}{1 - \pi}$$

- Example, polls indicate:
  - There is a 2/3 chance of candidate A winning
  - There is a 1/3 chance of candidate B winning
- The odds of candidate A winning are "two to one", or 2:1

# **Interpreting Coefficients**

#### Odds Ratios

An odds ratio quantifies that strength of the association between two events and is defined as the ratio of the odds of Y in the presence of X to the odds of Y in the absence of X:

$$odds \ ratio = \frac{odds(Y = 1|X = 1)}{odds(Y = 1|X = 0)}$$

Thus, if the odds ratio is 2, it is twice as likely that Y=1 when X=1 than when X=0.

Why do we care??

# **Interpreting Coefficients**

### Binary Factor Variable X

Some basic algebraic manipulations indicate that the coefficient  $\beta_j$  in the logistic regression is the log of the odds ratio for  $X_i$ :

$$\frac{odds(\beta_0 + \dots + \beta_j(X_j) + \dots + \beta_p X_p)}{odds(\beta_0 + \dots + \beta_j(X_j) + \dots + \beta_p X_p)} = \frac{e^{(\beta_0 + \dots + \beta_j * 1 + \dots + \beta_p X_p)}}{e^{(\beta_0 + \dots + \beta_j * 0 + \dots + \beta_p X_p)}} = e^{\beta_j}$$

Thus, the coefficient  $\beta_i$  in the logistic regression is the log of the odds ratio for  $X_i$ :

$$\left(\frac{odds(X_j=1)}{odds(X_i=0)}\right) = e^{\beta_j}$$

### **Odds and Odds Ratios**

English Language Usage – Odds Ratios

- Consider the odds ratio of the odds of default if student status = 1:
  - If it were 1.5, we would simply say that the odds of default are 1.5 times higher
    if the borrower is a student than if the borrow is not

### **Interpreting the Regression Coefficient**

Student Status as Predictor

$$p(X) = \frac{e^{(-3.44 + 0.359X)}}{1 + e^{(-3.44 + 0.359X)}}$$

Recall:

$$\log(\frac{odds(X_j=1)}{odds(X_j=0)}) = \beta_j = 0.359$$

$$\frac{odds(X_j = 1)}{odds(X_i = 0)} = e^{0.359} = 1.43$$

The odds of the result (default) are 1.43 times higher if the borrower is a student than if not

### **Interpreting Coefficients**

Continuous Variable  $X_i$ 

Similarly, for a continuous variable  $X_j$  if the value of  $X_j$  increases by 1:

$$\frac{odds(\beta_0 + \beta_j(X_j + 1) + \dots + \beta_p X_p)}{odds(\beta_0 + \beta_j X_j + \dots + \beta_p X_p)} = \frac{e^{\beta_0 + \beta_j(X_j + 1) + \dots + \beta_p X_p}}{e^{\beta_0 + \beta_j X_j + \dots + \beta_p X_p}} = e^{\beta_j}$$

Thus, the coefficient  $\beta_j$  in the logistic regression is the log of the odds ratio for an increase by 1 for the value  $X_i$ :

$$\frac{odds(X_j+1)}{odds(X_i)} = e^{\beta_j}$$

### **Multiple Logistic Regression**

 Making a model for loan default based on balance, income, and student status:

Create and Assess multiple logistic model									
	y3 = credit_default_data['default'].copy() X3 = credit_default_data.drop('default', 1).copy()								
	<pre>dummy_vars = pd.get_dummies(credit_default_data['student']) X3['student'] = dummy_vars['Yes'] X3</pre>								
		student	income	balance					
	0	1	9663.79	2024.66					
	1	1	10155.32	1681.48					
	2	1	10470.64	2066.70					
	3	1	10591.72	1707.91					
	4	1	11054.07	1492.96					
	9496	0	70700.65	1067.84					
	9497	0	71238.55	1253.18					
	9498	0	71878.77	201.81					
	9499	0	72461.30	1233.71					
	9500	0	73554.23	1593.43					
9501 rows × 3 columns									

### **Multiple Logistic Regression**

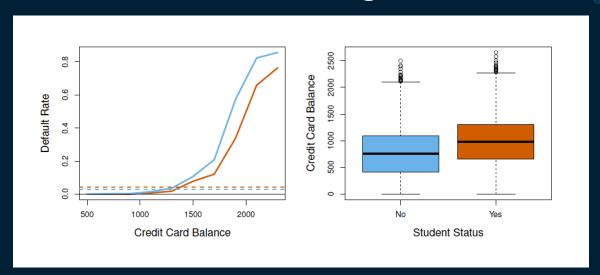
• Making a model for loan default based on balance, income, and student status:

Why is the parameter on student negative here when it was positive as part of a Simple Logistic Regression??

```
Split dataset into training and test
from sklearn.model selection import train test split
X train, X test, y train, y test = train test split(X3, y3, test size = 0.25, random state = 1)
model3 = LogisticRegression().fit(X train, y train)
model3.intercept
array([-2.95293691])
pd.DataFrame(model3.coef .T, columns = ['Coefficients'], index = X.columns)
         Coefficients
           -3.911981
           -0.000135
 income
            0.004101
 balance
```

- This is an example of confounding
  - Combining factors that are correlated in such a way as to distort the true relationship.

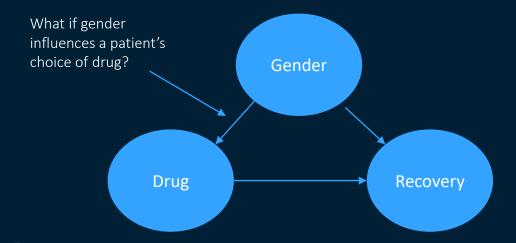
- In this example, student status is confounded with balance levels
  - Without considering other factors, students have higher chance of default
  - Considering balance as an additional factor, students have lower chance of default compared with non-students who hold the same balance
  - Generally, students hold a higher balance and consequently overall higher chance of default. In other words, balance and student status are positively correlated



Left: Default rates are shown for students (orange) and non-students (blue). The solid lines display default rate as a function of balance, while the horizontal broken lines display the overall default rates.

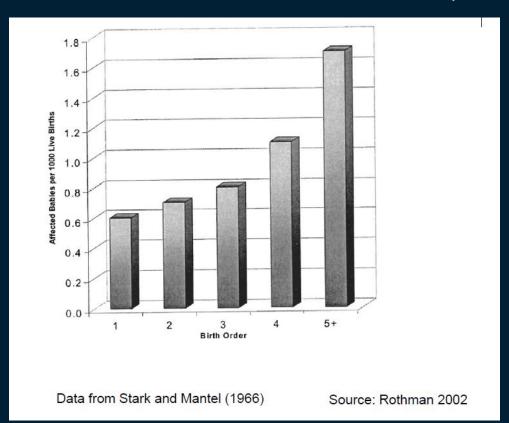
Right: Boxplots of balance for students (orange) and non-students (blue) are shown.

- Confounding occurs when one predictor variable influences both another predictor variable and the response variable
- Example: predicting drug effectiveness



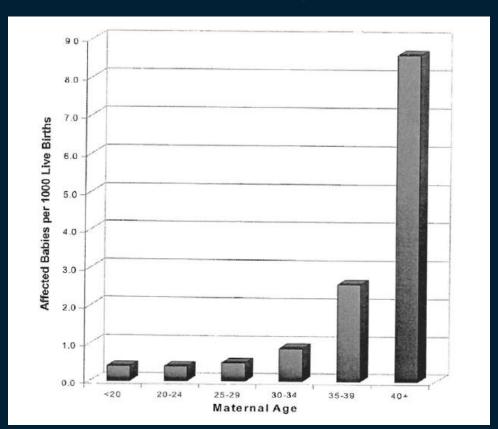
## **Confounding Example**

#### Association Between Birth Order and Down Syndrome



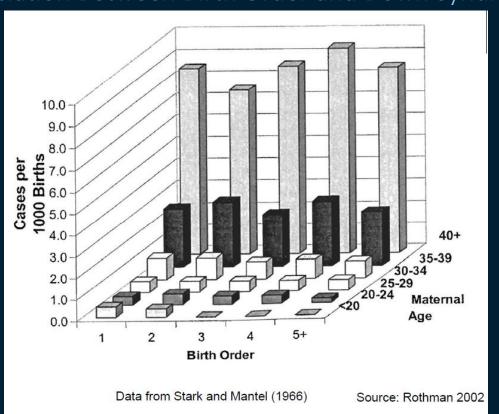
### **Confounding Example**

Association Between Maternal Age and Down Syndrome



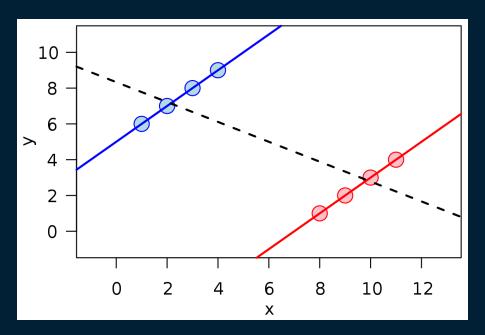
## **Confounding Example**

Association Between Birth Order and Down Syndrome



### Simpson's Paradox

 A trend observed in an overall dataset disappears or reverses when the trend is observed by groups



- "Confounding, the situation in which an apparent effect of an exposure on risk is explained by its association with other factors, is probably the most important cause of spurious associations in observational epidemiology"
  - BMJ Editorial: "The Scandal of Poor Epidemiological Research", 16 October 2004
- Randomized clinical trials (RCTs) attempt to avoid or minimize confounding through randomization and matching techniques
  - As opposed to "observational studies"

# **Model Assessment**

### **Assessment Measures (Fit Statistics)**

**Binary Targets** 

The techniques that are used to model fit assessment for regression models do not apply for classification models (why?)

Three types of assessment measures for binary classification models:

- Classification accuracy: Accuracy in predicting the actual category result (0/1, True/False, Churn/No Churn, etc.)
- Ranking predictions: Accuracy of the rankings of the likelihood of the event
- Estimate predictions: Accuracy of the actual probability predictions

#### **Model Assessment Overview**

#### Classification Accuracy

- Focus is on "misclassification rate" what percentage of our predictions are wrong?
- Key statistics
  - "Confusion matrix"
  - Sensitivity/specificity
- Key assessment graphs
  - Receiver Operating Characteristics (ROC) curves
  - Lift curves

### **Classification Predictions**

#### **Confusion Matrix**

		Actual Classification		
		Negative	Positive	Totals
Predicted	Negative	<b>TN</b> (# true negatives)	<b>FN</b> (# false negatives)	<b>N</b> (# true negatives)
Classification	Positive	<b>FP</b> (# false positives)	<b>TP</b> (# true positives)	P (# true positives)

Sensitivity = 
$$\frac{TP}{TP + FN}$$

Specificity = 
$$\frac{TN}{TN + FP}$$

#### **Classification Predictions**

- Sensitivity: what percentage of the positive outcomes do we correctly identify?
  - Does the classifier capture most of the important events?
- Specificity: what percentage of the negative outcomes do we correctly identify?
  - Does the classifier "weed out" most of the unimportant events?

### **Classification – Assessment Techniques**

#### Confusion Matrix

```
Generate Confustion Matrix
 1 y_hat = model3.predict(X_test)
 2 cnf_matrix = metrics.confusion_matrix(y_test, y_hat)
 3 cnf_matrix
array([[2270,
                13]], dtype=int64)
   metrics.ConfusionMatrixDisplay(cnf_matrix).plot()
<sklearn.metrics._plot.confusion_matrix.ConfusionMatrixDisplay at 0x291b54d8cd0>
                                   2000
                                   1500
             Predicted label
```

### **Classification – Assessment Techniques**

#### Metrics

```
TN = cnf_matrix[0,0]
 2 FP = cnf_matrix[0,1]
   FN = cnf_matrix[1,0]
   TP = cnf_matrix[1,1]
   print('True Negatives:', TN)
 6 print('False Positives:', FP)
   print('False Negatives:', FN)
   print('True Positives:', TP)
True Negatives: 2270
False Positives: 20
False Negatives: 73
True Positives: 13
   Sensitivity = TP/(TP+FN)
   Specificity = TN/(TN + FP)
   print('Sensitivity:', Sensitivity)
   print('Specificity:', Specificity)
Sensitivity: 0.1511627906976744
Specificity: 0.9912663755458515
```

Is this good performance?

- There is generally a tradeoff between sensitivity and specificity
- After modeling the probability of an event, we must decide on the "discrimination threshold" we will use
  - Typically, 50% is used
  - Why would we want to use anything else?
- Adjusting the discrimination threshold allows the data scientist to fine tune the model to get the desired balance between sensitivity and specificity

#### Looking at Prediction Probabilities

```
y_probs = model3.predict_proba(X_test)[:,1]
 2 y_probs
array([0.05459464, 0.00301417, 0.00049685, ..., 0.05420965, 0.00601634,
       0.00354868])
   sns.histplot(y_probs)
<AxesSubplot:ylabel='Count'>
  1000
   400
   200
               0.2
                       0.4
                               0.6
                                        0.8
```

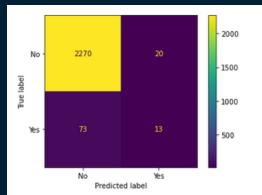
#### Adjusting Discrimination Threshold

 Sklearn does not have a built-in parameter to specify a discrimination threshold, but it is easy to implement:

```
threshold = 0.5
    preds = np.where(y_probs > threshold, 'Yes', 'No')
    cnf_matrix = metrics.confusion_matrix(y_test, preds)
    metrics.ConfusionMatrixDisplay(cnf_matrix, display labels = ["No", "Yes"]).plot()
<sklearn.metrics. plot.confusion matrix.ConfusionMatrixDisplay at 0x291b5d48730>
           2270
                                    - 1500
              Predicted label
```

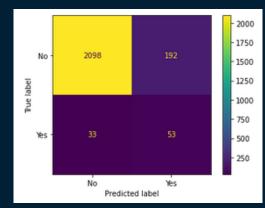
- There is generally a tradeoff between sensitivity and specificity
- Adjusting the discrimination threshold allows the data scientist to fine tune the model to get the desired balance between sensitivity and specificity

Threshold = 0.5



With a 0.5 classification threshold, we "miss" 73 true positives

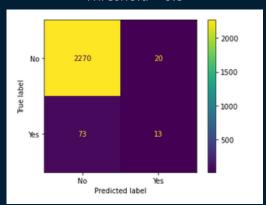
Threshold = 0.1



With a 0.1 classification threshold, we capture an additional 40 true positives, but at the cost of having to look at 192 false positives

### Comparing Thresholds

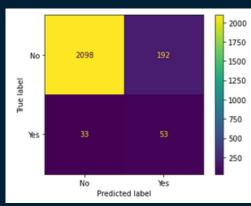
Threshold = 0.5



With a 0.5 classification threshold, we "miss" 73 true positives

Sensitivity: 0.1511627906976744 Specificity: 0.9912663755458515

Threshold = 0.1



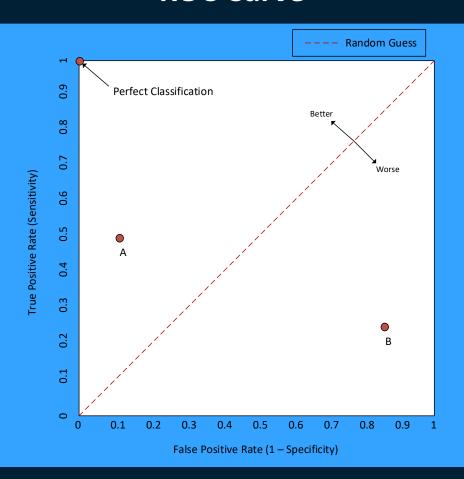
With a 0.1 classification threshold, we capture an additional 40 true positives, but at the cost of having to look at 192 false positives

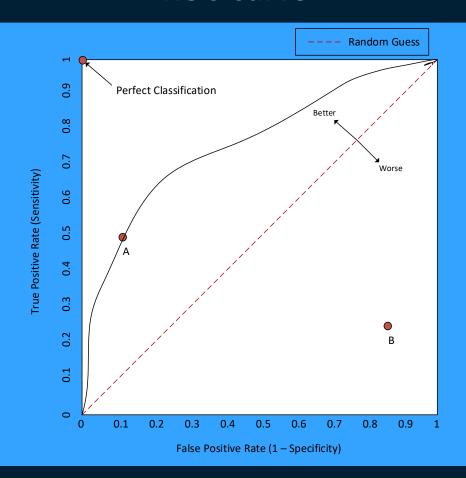
Sensitivity: 0.6162790697674418 Specificity: 0.9161572052401746

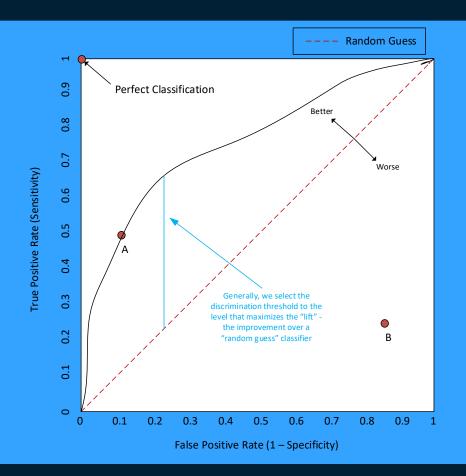
#### **Classification Assessment Visualizations**

#### **ROC Chart**

- Graphical plot to assist in optimizing the sensitivity/specificity tradeoff
- Plots the True Positive Rate (sensitivity) against the False Positive Rate (1-specificity) at each possible value of the discrimination threshold.





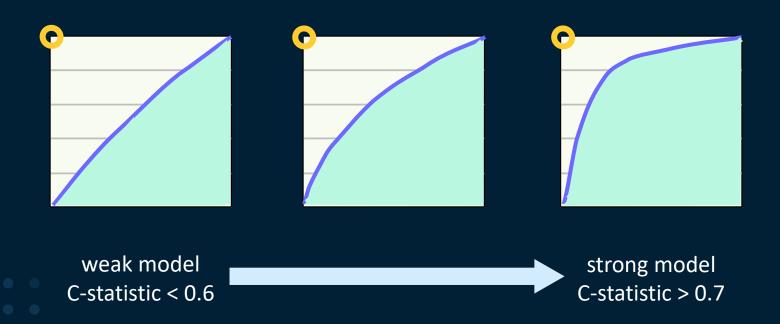


#### Loan Default Example

```
fpr, tpr, thresholds = metrics.roc_curve(y_test, y_probs, pos_label = 'Yes')
   roc_auc = metrics.auc(fpr, tpr)
   display = metrics.RocCurveDisplay(fpr=fpr, tpr=tpr, roc_auc=roc_auc).plot()
  1.0
  0.8
Fue Positive Rate
  0.2
                                          AUC = 0.90
  0.0
      0.0
              0.2
                               0.6
                                        0.8
                                                1.0
                      False Positive Rate
```

## Ranking Predictions

ROC Index / C Statistic



#### Lift

- Background: many classification applications involve looking for relatively low probability, but important events, for example:
  - Fraudulent tax returns
  - Diseases
  - People likely to default on a loan
- We want to identify a group of cases for more in-depth investigation, but we are limited in our ability to perform a large number of investigations. Therefore, we want our classifier to select a group with a high number of "true positive" outcomes

#### **Model Lift**

 Another measure of the performance of a classification model (or an association rule model) that measures the "lift" or "improvement" a model provides over randomly selecting observations.

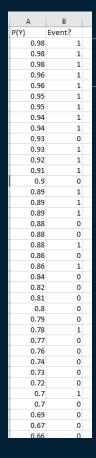
#### • Example:

- Your dataset of 1000 cases has 100 "true positives"
- Randomly selecting 100 cases could thus be expected to return 10 positives
- If your classifier takes its 100 "highest probability" cases and returns 40 positives,
   the lift would be 4.
- Lift curves display a curve of the performance of a classifier for increasing size "bins" your top 5%, 10%, of cases, etc.

#### **Lift Curve – Model Lift**

Event? 100 0.08 Number of observations: 25 0 Number of events: 0.06 0.88 0.13 0.53 0.47 0.89 0.15 0.17 0.02 0.22 0.74 0.41 0.25 0.66 0.49 0.21 0.11 0.66 0.64 0.42 0.7 0.27 0.6 0.51 0.16 0.02 0.84 0.11 0.81 0.95 0.89 0.38 0.45 0.76 0.8 0.7

Sort by decreasing model probability



# of events in top 5% high probability observations: 5

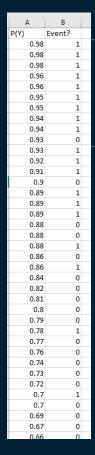
# of events (on average) in a random sample of 5% of observations? 1.25

Model lift at 5%: 5/1.25 = 4

#### **Lift Curve – Model Lift**

Event? 100 0.08 Number of observations: 25 0 Number of events: 0.06 0.88 0.13 0.53 0.47 0.89 0.15 0.17 0.02 0.22 0.74 0.41 0.25 0.66 0.49 0.21 0.11 0.66 0.64 0.42 0.7 0.27 0.6 0.51 0.16 0.02 0.84 0.11 0.81 0.95 0.89 0.38 0.45 0.76 0.8 0.7

Sort by decreasing model probability



# of events in top 10% high probability observations: 9

# of events (on average) in a random sample of 5% of observations? 2.5

Model lift at 5%: 9/2.5 = 3.6

#### "Best" Lift

• Performs the same calculation, as model lift except that it is calculated as though a sorting by probability ends up with all the positives (1s) on the top and all the negatives (0s) on the bottom

# **Lift Curve – Best Lift**

A	А	В	С	
-	P(Y)	Event?	Best Model	
	0.98	1	1	
	0.98	1	1	
	0.98	1	1	
	0.96	1	1	
,	0.96	1	1	
,	0.95	1	1	
	0.95	1	1	
	0.94	1	1	
0	0.94	1	1	
1	0.93	0	1	
2	0.93	1	1	
3	0.92	1	1	
4	0.91	1	1	
5	0.9	0	1	
6 7	0.89	1	1	
7	0.89	1	1	
8	0.89	1	1	
9 0 1	0.88	0	1	
0	0.88	0	1	
1	0.88	1	1	
2	0.86	0	1	
3	0.86	1	1	
4 5 6 7	0.84	0	1	
5	0.82	0	1	
6	0.81	0	1	
	0.8	0	0	
8	0.79	0	0	
8 9 0	0.78	1	0	
0	0.77	0	0	
_	0.76	0	0	
2	0.74	0	0	
3	0.73	0	0	
4	0.72	0	0	
5	0.7	1	0	
	0.7	0	0	
7	0.69	0	0	

# of events in first 5% observations: 5

# of events (on average) in a random sample of 5% of observations? 1.25

Best lift at 5%: 5/1.25 = 4

# **Lift Curve – Best Lift**

4	А	В	С	
	P(Y)	Event?	Best Model	
	0.98	1	1	
	0.98	1	1	
L	0.98	1	1	
,	0.96	1	1	
	0.96	1	1	
	0.95	1	1	
	0.95	1	1	
	0.94	1	1	
0	0.94	1	1	
1	0.93	0	1	
2	0.93	1	1	
3	0.92	1	1	
4	0.91	1	1	
5	0.9	0	1	
6	0.89	1	1	
4 5 6 7	0.89	1	1	
	0.89	1	1	
8 9 0	0.88	0	1	
0	0.88	0	1	
1	0.88	1	1	
2	0.86	0	1	
3	0.86	1	1	
4	0.84	0	1	
5	0.82	0	1	
6	0.81	0	1	
2 3 4 5 7	0.8	0	0	
8	0.79	0	0	
9	0.78	1	0	
9 0 1	0.77	0	0	
1	0.76	0	0	
2	0.74	0	0	
2 4 5 7	0.73	0	0	
4	0.72	0	0	
5	0.7	1	0	
6	0.7	0	0	
7	0.69	0	0	
8	0.67	0	0	

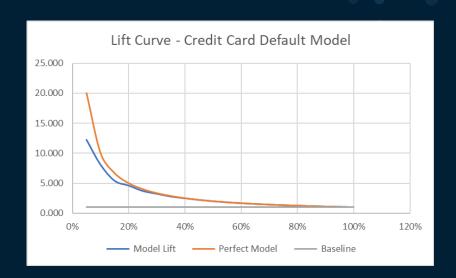
# of events in first 10% observations: 10

# of events (on average) in a random sample of 10% of observations? 2.5

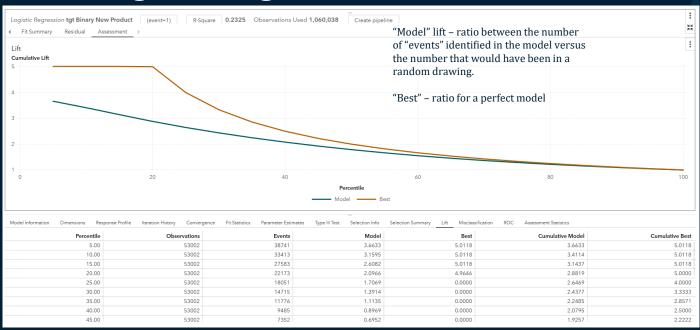
Best lift at 10%: 10/2.5 = 4

# **Lift Curve – Credit Card Default Model**

Percentile	Random	Model	Model Lift	Perfect Model	Baseline
5%	16.65	204	12.252	20	1
10%	33.3	269	8.078	10	1
15%	49.95	270	5.405	6.666666667	1
20%	66.6	307	4.610	5	1
25%	83.25	308	3.700	4	1
30%	99.9	323	3.233	3.333333333	1
35%	116.55	323	2.771	2.857142857	1
40%	133.2	330	2.477	2.5	1
45%	149.85	330	2.202	2.22222222	1
50%	166.5	330	1.982	2	1
55%	183.15	330	1.802	1.818181818	1
60%	199.8	332	1.662	1.666666667	1
65%	216.45	332	1.534	1.538461538	1
70%	233.1	333	1.429	1.428571429	1
75%	249.75	333	1.333	1.333333333	1
80%	266.4	333	1.250	1.25	1
85%	283.05	333	1.176	1.176470588	1
90%	299.7	333	1.111	1.111111111	1
95%	316.35	333	1.053	1.052631579	1
100%	333	333	1.000	1	1



# **Logistic Regression Results: Lift**



In this example in the first bin of 53002 observations which the model assigned the highest probability to:

- 38,741 of the 53,002 observations contained the event
- In a random draw of 53,002 observations, 10,575 observations would have contained the event (based

In the second bin (10%) of 53002 observations which the model assigned the highest probability to:

- 33,413 of the 53,002 observations contained the event
- Thus, in the first two bins cumulatively, 72,154 observations would have contained the event

# Other Classification Model Assessment Statistics

# **Assessment Measures (Fit Statistics)**

Binary Targets

**Prediction Type** 

Fit Statistic

Decisions

Accuracy/Misclassification KS Youden

Maximum distance from ROC curve to diagonal

Rankings

ROC Index
Gini Coefficient

Area under ROC curve Concordance statistic

Estimates

Average Squared Error RMSE/SBC/AIC/Likelihood

# **Ranking Predictions**

Concordance Statistic / Gini Index

- Essentially a correlation coefficient between the predicted and actual order
  - Not always able to determine the actual order

#### **Estimate Prediction**

Average Squared Error

$$ASE_{cat} = \sum_{i=1}^{N} \sum_{j=1}^{J} \frac{(\delta_{ij} - \hat{p}_{ij})^2}{JN}$$

J: Number of target values (classes)

 $\delta_{ij}$ : Equals 1 if value j occurs in observation i, 0 if not

 $\hat{p}_{ij}$ : Predicted probability of nominal target value j for

observation i

# Which Assessment Measure Should You Use?

Inputs Target Predictions



# **Evaluation of Model Performance**

Assessment measures and statistical graphics of performance





#### **Business** needs

- Speed of training
- Speed of scoring
- Feasibility of deployment
- Noise tolerance
- Interpretability



#### Classification Models

Λ	CCI	ıro	$\sim$
	CCL	па	LV

A measure of how many observations are correctly classified for each value of the response variable. It is the number of event and non-event cases classified correctly, divided by all cases.

# Area under the curve (C statistic)

A measure of goodness of fit for binary outcome. It is the concordance rate and it is calculated as the area under the curve.

#### Average squared error

The sum of squared errors (SSE) divided by the number of observations.

#### Captured response

The number of events in each bin divided by the total number of events.

#### Classification Models

Cumulative	captured
response	

The cumulative value of the captured response rate.

**Cumulative lift** 

Cumulative lift up to and including the specified percentile bin of the data, sorted in descending order of the predicted event probabilities.

F1 score

The weighted average of precision (positive predicted value) and recall (sensitivity). It is also known as the *F-score* or *F-measure*.

False discovery rate

The expected proportion of type error I – incorrectly reject the null hypothesis (false positive rate).

False positive rate

The number of positive cases misclassified (as negative).

# Classification Models

Gain	Similar to a lift chart. It equals the expected response rate using the predictive model divided by the expected response rate from using no model at all.
Gini	A measure of the quality of the model. It has values between -1 and 1. Closer to 1 is better. It is also known as Somer's D.
Kolmogorov-Smirnov statistic (KS)	A goodness-of-fit statistic that represents the maximum separation between the model ROC curve and the baseline ROC curve.
KS (Youden)	A goodness-of-fit index that represents the maximum separation between the model ROC curve and the baseline ROC curve.
Lift	A measure of the advantage (or lift) of using a predictive model to improve on the target response versus not using a model. It is a measure of the effectiveness of a predictive model calculated as the ratio between the results obtained with and without the predictive model. The higher the lift in the lower percentiles of the chart, the better the model is.

#### Classification Models

Misclassification (Event)	Considers only the classification of the event level versus all other levels. Thus, a non-event level classified as another non-event level does not count in the misclassification. For binary targets, these two measures are the same. It is computed in the context of the ROC report. That is, at each cutoff value, this measure is calculated.
Misclassification (MCE)	A measure of how many observations are incorrectly classified for each value of the response variable. This is the true misclassification rate. That is, every observation where the observed target level is predicted to be a different level counts in the misclassification rate.
Multiclass log loss	The loss function applied to multinomial target. It is the negative log-likelihood of the true labels given a probabilistic classifier's prediction.
ROC separation	The area under the ROC curve is the accuracy. The ROC separation enables you to change the ROC-based cutoff and evaluate the model's performance under different ranges of accuracy.

Root average squared error

It is the square root of the average differences between the prediction and the actual observation.

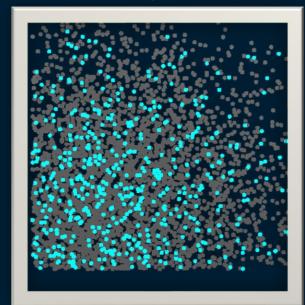
# **Dataset Partitioning Considerations**

- Special handling is required when the target of interest is a rare event relative to the total number of samples
  - For example, detecting fraudulent activity
- "Fitting a model without accounting for the extreme imbalance in the occurrence of the event gives you a model that is extremely accurate at telling you absolutely nothing of value"

- A common practice is to build models from a sample with a primary outcome proportion different from the true population ("Event-Based Sampling")
- It can be shown that you can obtain a model of similar predictive power with a smaller overall case count
  - The amount of information in a data set with a categorical outcome is determined not by the total number of cases in the data set, but by the number of cases in the rarest outcome category

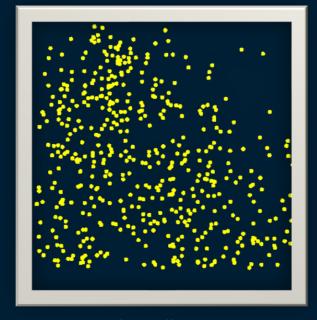
**Event-Based Sampling** 

Secondary Outcome



Select some cases

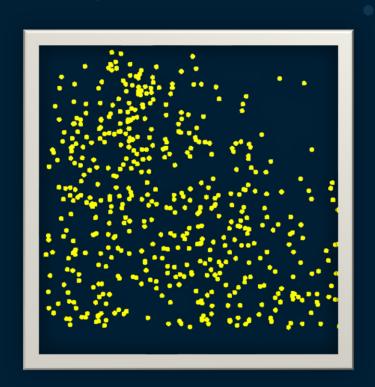
Primary Outcome



Select all cases

**Event-Based Sampling** 

- Similar predictive power with smaller case count
- Must adjust assessment measures and graphics
- Must adjust prediction estimates for bias
- Model Studio automatically adjusts for event-based sampling



## **Dataset Partition Strategies**

- Partition data / address rare events
  - Stratified sampling: ensure partitions have same percentages (of a category) as the overall population
  - Event-based sampling: Over/under sample to get specified percentages of each category of observations in each partition

# **Multinomial Logistic Regression**

# **Multinomial Logistic Regression**

#### Overview

- Extension of logistic regression for multiple categories
- Select a single class to serve as the baseline (here, we select K):

$$P(Y = k | X = x) = \frac{e^{(\beta_{k0} + \beta_{k1} x_1 + \dots + \beta_{kp} x_p)}}{1 + e^{(\beta_{k0} + \beta_{k1} x_1 + \dots + \beta_{kp} x_p)}}$$

for k = 1, ..., K-1, and

$$P(Y = K | X = x) = \frac{1}{1 + e^{(\beta_{k0} + \beta_{k1}x_1 + \dots + \beta_{kp}x_p)}}$$

# **Module 7**

Generalized Linear Models

Overview

Covers cases where the response variable Y is neither qualitative or quantitative

For example, count variables

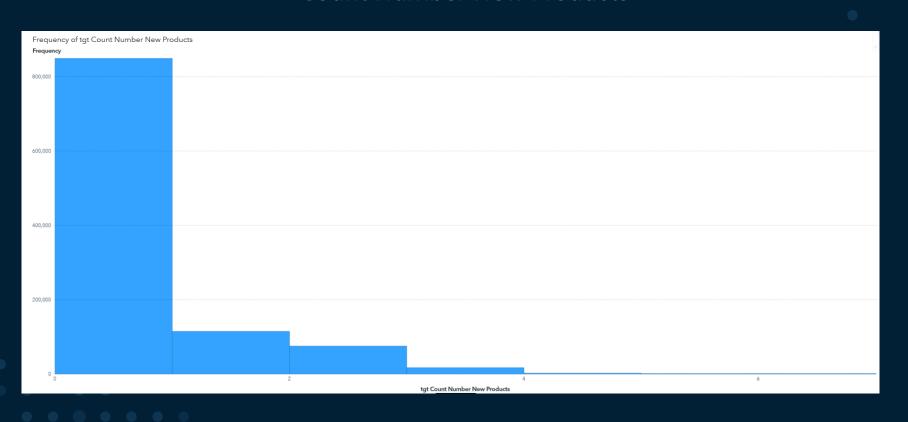
# Example

# VS\_Bank Campaign Response Data

Account ID	category 1 Account Activity Level	category 2 Customer Value Level	logi_rfm1 Average Sales Past 3 Years	logi_rfm10 Count Total Promos Past Year	logi_rfm11 Count Direct Promos Past Year	logi_rfm12 Customer Tenure	logi_rfm2 Average Sales Lifetime	tgt Count Number New Products
00000001	×	A	1.903598951	3.0445224377	2.302585093	4.5325994932	1.8500283774	
00020117	Z	В	2.7725887222	2.3978952728	1.6094379124	2.8903717579	2.7725887222	0
00008192	×	В	2.6390573296	2.3978952728	1.6094379124	3.4011973817	2.6390573296	C
00022680	Z	A	3.258096538	2.5649493575	1.7917594692	2.8332133441	3.258096538	0
00020744	X	A	3.258096538	2.6390573296	1.9459101491	4.7874917428	2.6581594315	0
00020118	Z	В	3.0445224377	2.5649493575	1.7917594692	3.3322045102	3.0445224377	0
00004096	×	A	2.8332133441	2.7080502011	1.9459101491	3.8286413965	2.6946271808	0
00023030	×	A	2.4570214463	3.0910424534	1.9459101491	4.7449321284	2.5160822673	0
00022390	x	A	3.258096538	2.6390573296	1.9459101491	4.4067192473	2.2159372863	0
00021590	×	A	2.9704144656	2.7725887222	2.0794415417	4.3820266347	2.7245795031	.0
00021018	×	A	2.7568403653	2.6390573296	1.9459101491	4.3820266347	2.4484155412	0
00020745	x	A	3.7534960972	2.5649493575	2.0794415417	4.5432947823	3.4397768636	0
00010217	z	A	3.0445224377	2.3978952728	1.6094379124	3.0910424534	3.0445224377	0
00020119	z	В	3.258096538	2.4849066498	1.7917594692	2.8332133441	3.258096538	0
00026873	×	С	2.7725887222	1.9459101491	1.3862943611	4.2046926194	2.5257286443	0
00023692	x	A	2.7725887222	2.4849066498	1.6094379124	4.7361984484	2.1882959466	0
00023368	×	A	2.6026896854	2.3978952728	1.6094379124	3.4965075615	2.6026896854	0
00023031	×	A	4.6151205168	3.0445224377	1.9459101491	4.248495242	4.189654742	0
00022715	Z	A	3.258096538	2.6390573296	1.9459101491	3.1780538303	3.258096538	0
00011128	×	D	2.4423470354	2.1972245773	1.6094379124	4.8040210447	2.0055258587	0
00021914	x	A	3.0445224377	2.6390573296	1.7917594692	4.4998096703	3.1023420086	0
00021591	x	A	3.6571307558	2.7080502011	2.0794415417	4.8283137373	2.8903717579	0
00021294	×	A	3.5115454388	2.7080502011	2.0794415417	4.6728288345	2.9871959425	0
00021019	X	A	3.295836866	2.4849066498	1.9459101491	4.4067192473	2.8390784635	0
00020880	x	A	2.6026896854	2.5649493575	1.7917594692	4.189654742	2.2407096893	0
00010373	×	D	2.6390573296	2.4849066498	1.7917594692	3.7612001157	2.427454075	0
00020593	×	A	2.76000994	2.7080502011	1.9459101491	3.7376696183	2.6511270537	0
100020435	v	۸	2 8332133441	2.7080502011	1 0/50101/01	4.248405242	2 7020321288	

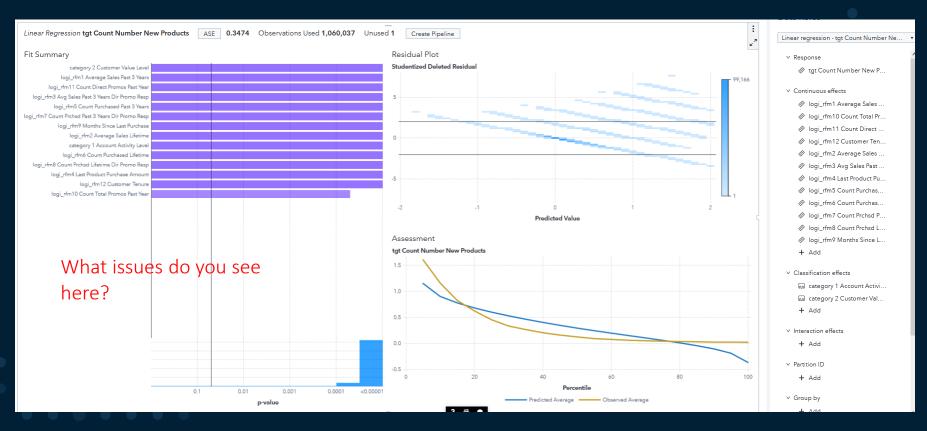
# Example

## **Count Number New Products**



# **Example**

## Linear Model



 Extends the linear regression model by incorporating a "link function" and associated probability distribution to change the distribution of the response variable:

$$g(E(Y|X) = \beta_0 + \beta_1 X_1 + \beta_2 X_2 + \dots + \beta_p X_p + \varepsilon$$

• where  $g(\cdot)$  can be a variety of functions with a variety of probability distributions

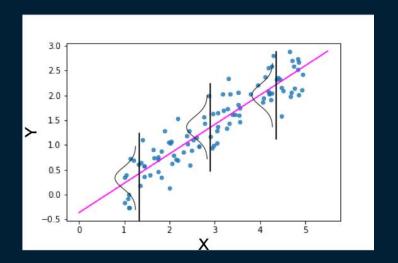
 One way of dealing with response variables that are not normally distributed with respect to the predictors

Linear Regression

Models the mean of a continuous response variable Y

•  $g(\cdot)$  is distributed normally with an identity link function:

$$Y = \beta_0 + \beta_1 X_1 + \beta_2 X_2 + \dots + \beta_p X_p$$



Binary Logistic Regression

Models the odds of "success" for a binary response variable Y

•  $g(\cdot)$  is the logit function with a binomial distribution:

$$logit(\pi_i) = \log\left(\frac{\pi_i}{1 - \pi_i}\right) = \beta_0 + \beta_1 X_1 + \beta_2 X_2 + \dots + \beta_p X_p$$

Poisson Regression

Models the mean of a discrete (count) response variable Y

•  $g(\cdot)$  is the log link function with a Poisson distribution:

$$log\lambda_i = \beta_0 + \beta_1 X_1 + \beta_2 X_2 + \dots + \beta_p X_p$$

#### Common Linear Distributions

Distribution	Available Link Functions (default listed first)		
Beta	Logit, Probit, Log-log, C-log-log		
Binary	Logit, Probit, Log-log, C-log-log		
Exponential	Log, Identity		
Gamma	Log, Identity, Reciprocal		
Geometric	Log, Identity		
Inverse Gaussian	Power(-2), Log, Identity		
Negative Binomial	Log, Identity		
Normal (default)	Identity, Log		
Poisson	Log, Identity		
Tweedie	Identity, Log		

# **Examples of Popular GLMs**

Response Variable	Distribution	Link Function	Variance Function
Continuous	Normal	Identity	$\sigma^2$
Binary	Binomial	Logit	$\mu(1-\mu)$
Count	Poisson	Log	μ