



# **CS430/910: Foundations of Data Analytics**

**Regression | Dr Greg Watson**



# Objectives

- Understand the principle of regression to predict values.
- See how simple linear regression works.
- Extend simple linear regression to multiple linear regression.
- Understand non-linear regression by transformation of variables.
- Apply logistic regression for categoric values.

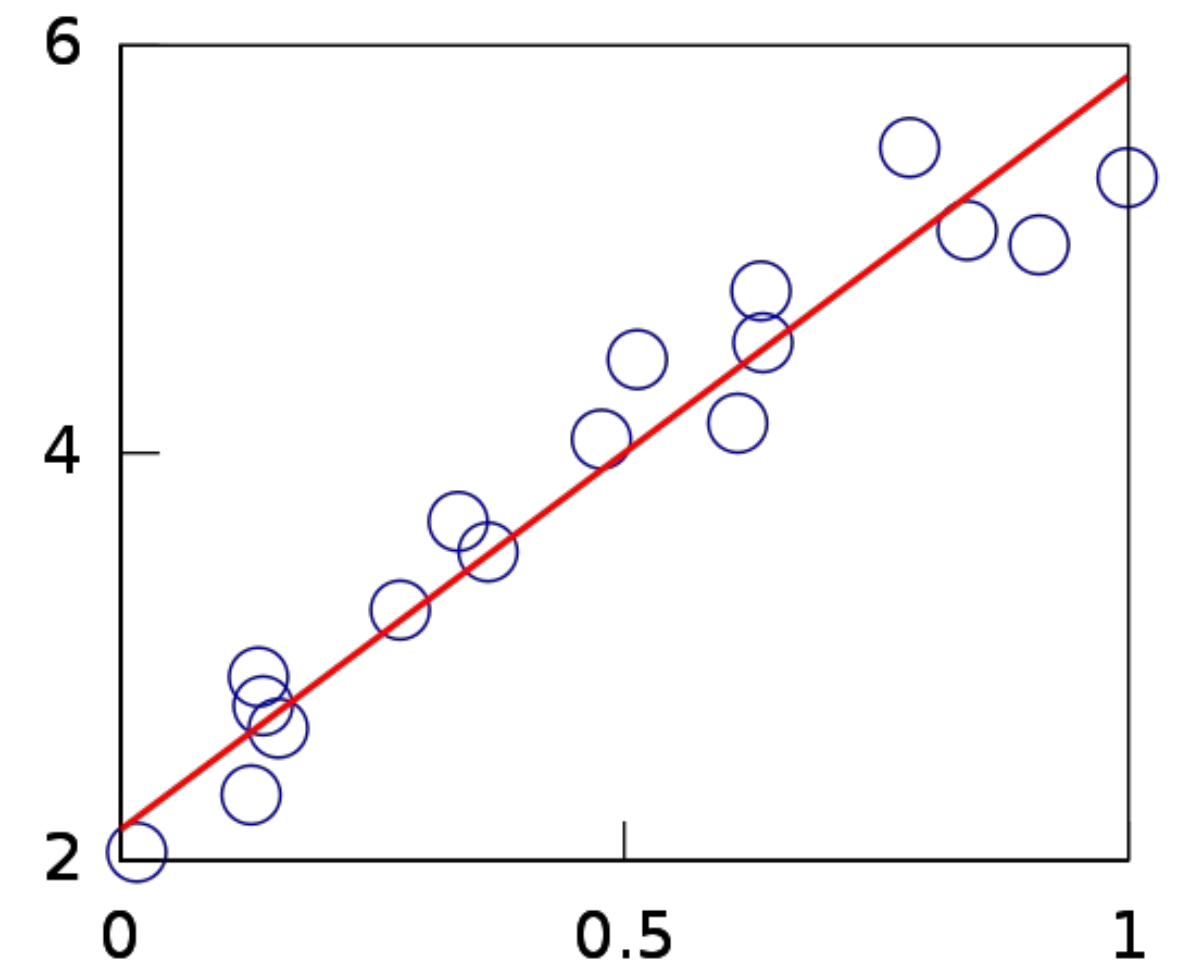
# Part A: Simple Linear Regression

# Supervised and Unsupervised Methods

- *Supervised* methods in data analytics:
  - **Classification:** predict a class (categorical) value given other values.
  - **Regression:** predict a numeric value given other values.
- *Unsupervised* methods in data analytics:
  - **Clustering:** identify groups/clusters of similar records.
- *In-between: Semi-supervised* methods:
  - Use a mixture of labeled and unlabelled data to infer labels.

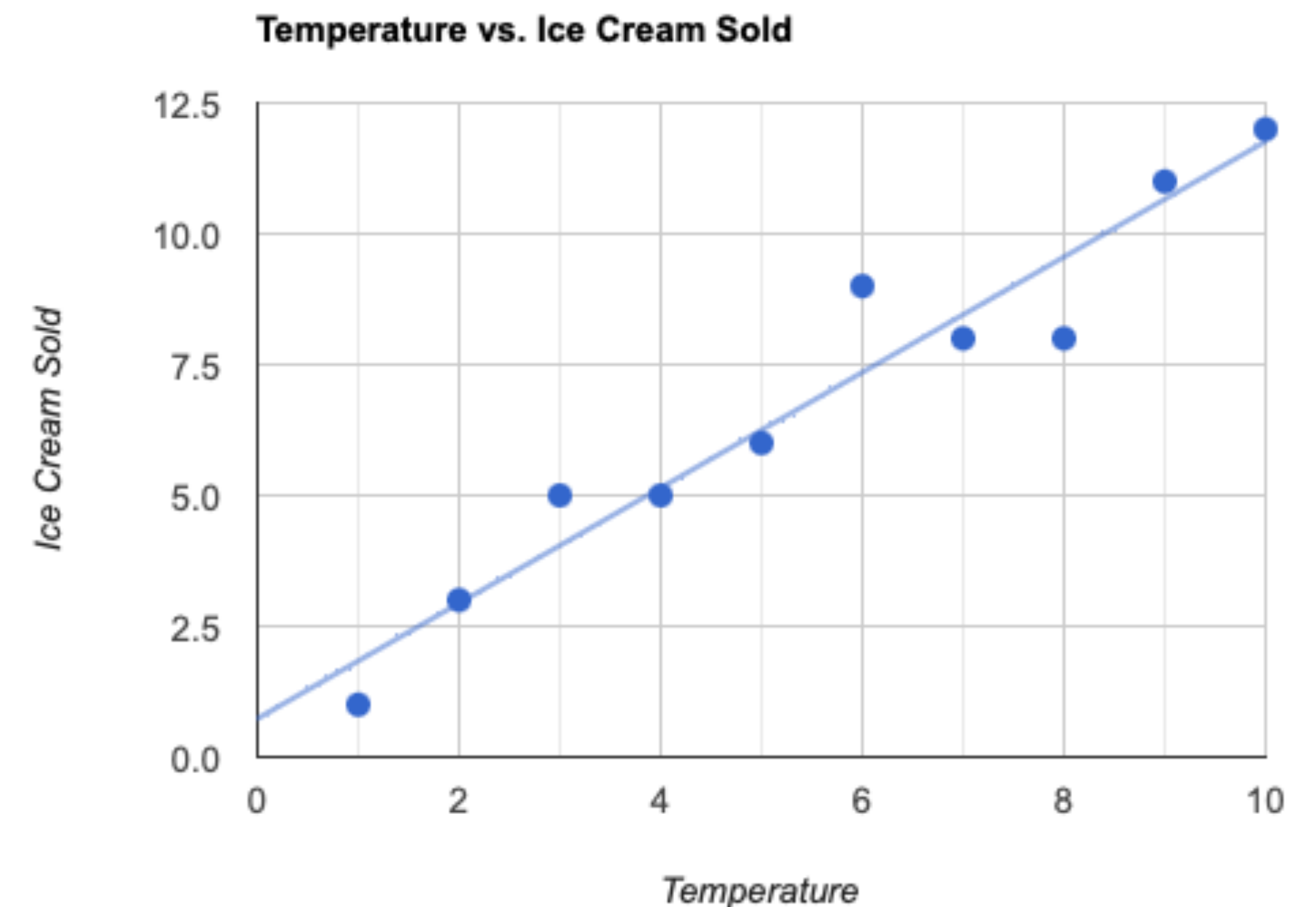
# Overview

- Regression lets us predict a value for a numeric attribute:
  - We fit a model to the data, and use the model to predict.
- Linear regression is the most familiar example:
  - A linear function of the explanatory variables.
  - Predicts a value for the dependent variable.
- Based on the principle of least squares:
  - Minimise the sum of squared differences between data and model.



# Applications

- Consider a shop worker working in a store.
- They suspect that the number of ice cream sold is related to the temperature.
- Get information from  $x$  stores, plot on a scatter diagram:
  - This clearly suggests a straight-line relationship.



# Applications

- Let  $y$  represent the number of ice cream sold, and  $x$  represent the temperature. Our regression model takes the form:

$$y_i = \beta_0 + \beta_1 x_i + \varepsilon_i$$

- $\beta_0$  is known as the *intercept*, and  $\beta_1$  is known as the *slope* or the *coefficient on the explanatory variable*.
- Note: Not all data points fall on the straight line!
  - We can denote the difference between the observed value  $y_i$  and the predicted point  $\beta_0 + \beta_1 x_i$  as the *error*  $\varepsilon_i$ .

# Definitions

- $y_i = \beta_0 + \beta_1 x_i + \varepsilon$  is called a *Simple Linear Regression model*.
- $x$  is called the *explanatory variable*, the *independent variable*, the *predictor*, or the *regressor*.
- $y$  is called the *dependent variable*, or the *response variable*.
- If a model only involves a single regressor variable ( $x$ ), it is known as a *simple linear regression model*.
- The  $\beta$ s are known as *regression coefficients*.

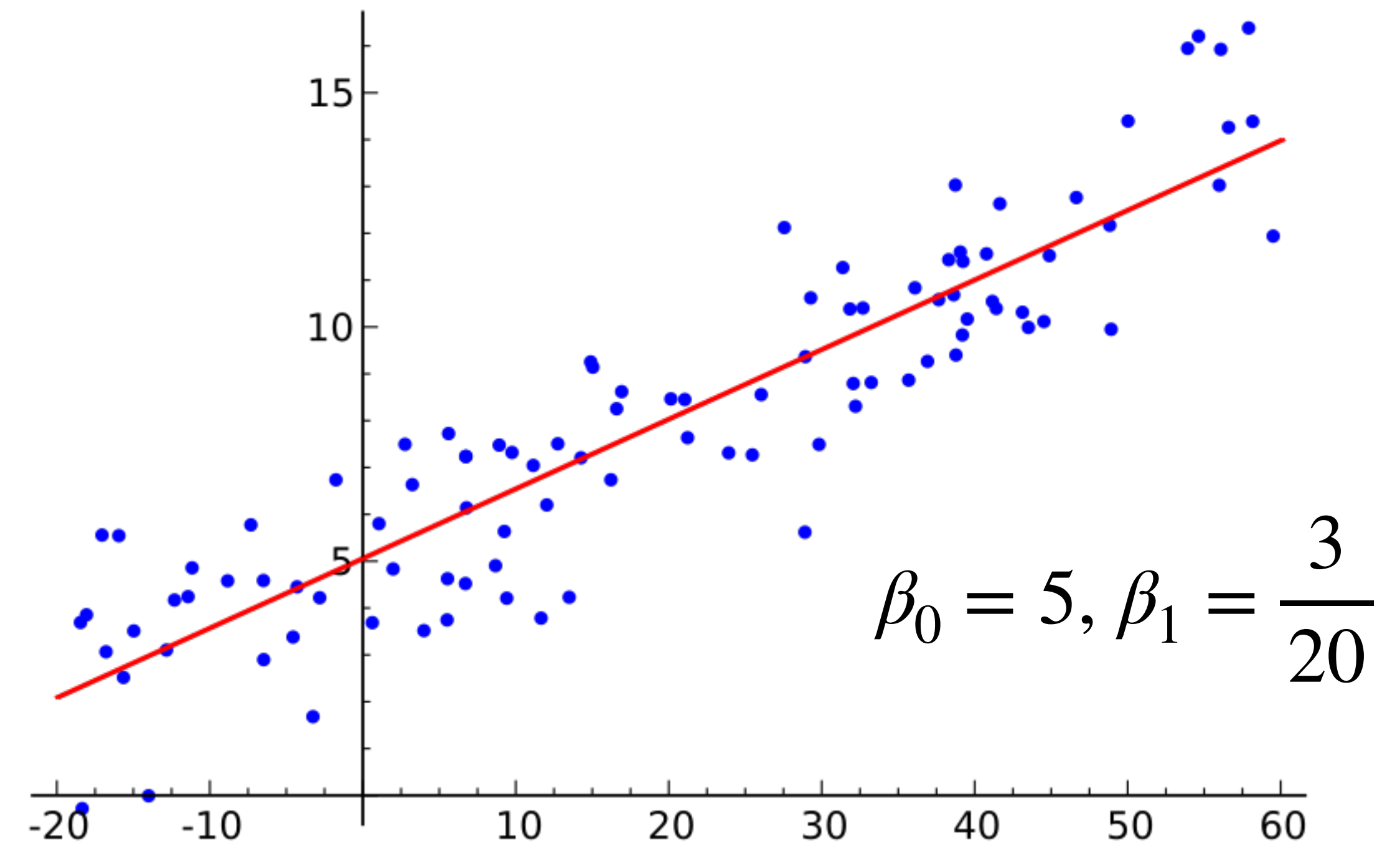


# Example

- Let  $x$  (our explanatory variable) be the number of years a person has spent in education, and  $y$  (our dependent variable) be their income.
- We can build a regression model to predict income, based on years in education.
- $x_m$  = Number of years of education for individual  $m$ .
- $y_m$  = Income for individual  $m$ .
- $\varepsilon_m$  = The error for individual  $m$ .
- Therefore, the income of individual  $m$  can be described by:
  - $y_m = \beta_0 + \beta_1 x_m + \varepsilon_m$

# The Coefficients $\beta_0$ and $\beta_1$

- $\beta_0$  = The  $y$ -intercept.
- $\beta_1$  = The slope of the line.
- Interpretation:
  - If  $x_i = 0$ , then  $y_i = \beta_0 + (\beta_1 \times 0)$ .
  - If  $x_i = 1$ , then  $y_i = \beta_0 + (\beta_1 \times 1)$ .
  - If  $x_i = 2$ , then  $y_i = \beta_0 + (\beta_1 \times 2)$
  - ...





# The Error Term $\varepsilon$

- The error term is the difference between the actual  $y$  value and the predicted  $y$  value. There are three main components of the error term:
  1. Influence of variables not included in the regression (age, background, motivation).
  2. Errors in the labelling.
  3. Randomness affecting the outcome (sudden unexpected promotion).
- The error term  $\varepsilon$  corresponds to the true population error, rather than what the error associated with the sample data.

# True vs. Estimated Regression

- The equation:

$$y_i = \beta_0 + \beta_1 x_i + \varepsilon_i$$

is considered the *theoretical* or *true regression equation*.

- However, we can **never know** what the true regression equation is, due to the **randomness** involved with **sampling** from the population, as well as due to **random events influencing** the outcome.
- Thus, with the data which we do have, we produce the *estimated regression equation*:

$$y_i = \hat{\beta}_0 + \hat{\beta}_1 x_i + \hat{\varepsilon}_i$$

$$\hat{y}_i = \hat{\beta}_0 + \hat{\beta}_1 x_i$$



# True vs. Estimated Regression

- The *estimated regression equation* is:

$$y_i = \hat{\beta}_0 + \hat{\beta}_1 x_i + \hat{\varepsilon}_i$$

$$\hat{y}_i = \hat{\beta}_0 + \hat{\beta}_1 x_i$$

- The hats ( $\hat{\phantom{x}}$ ) over  $y$ ,  $\beta_0$ ,  $\beta_1$  and  $\varepsilon$  dictate that these values are **predicted** or **estimated**.
  - $\hat{\beta}_0$  is the predicted intercept term.
  - $\hat{\beta}_1$  is the predicted coefficient term on the variable  $x$ .
  - $\hat{\varepsilon}$  is the predicted error term, known as the *residual*.
  - $\hat{y}$  is the predicted value of  $y$ . It does not include  $\hat{\varepsilon}$ .

# Least Squares

- The most common method for estimating a best-fitting regression line, is the *Ordinary Least Squares (OLS)* method.
- The *Least Squares* part refers to minimising the sum of squared residuals across all observations.

- i.e. minimise  $\sum_{i=1}^n (y_i - \hat{y}_i)^2$

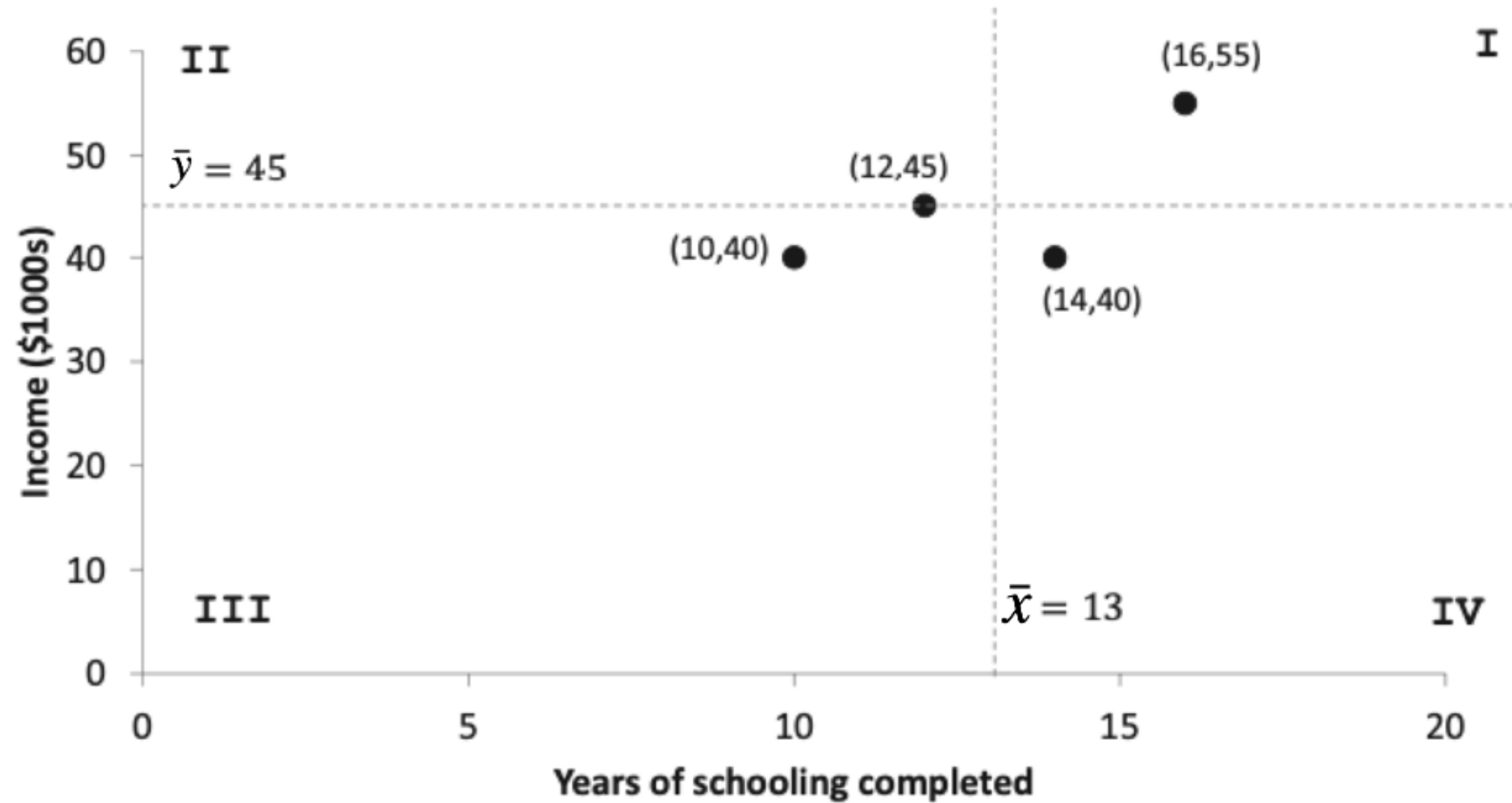
- Alternatively,  $\sum_{i=1}^n (y_i - (\hat{\beta}_0 + \hat{\beta}_1 x_i))^2$



# Example

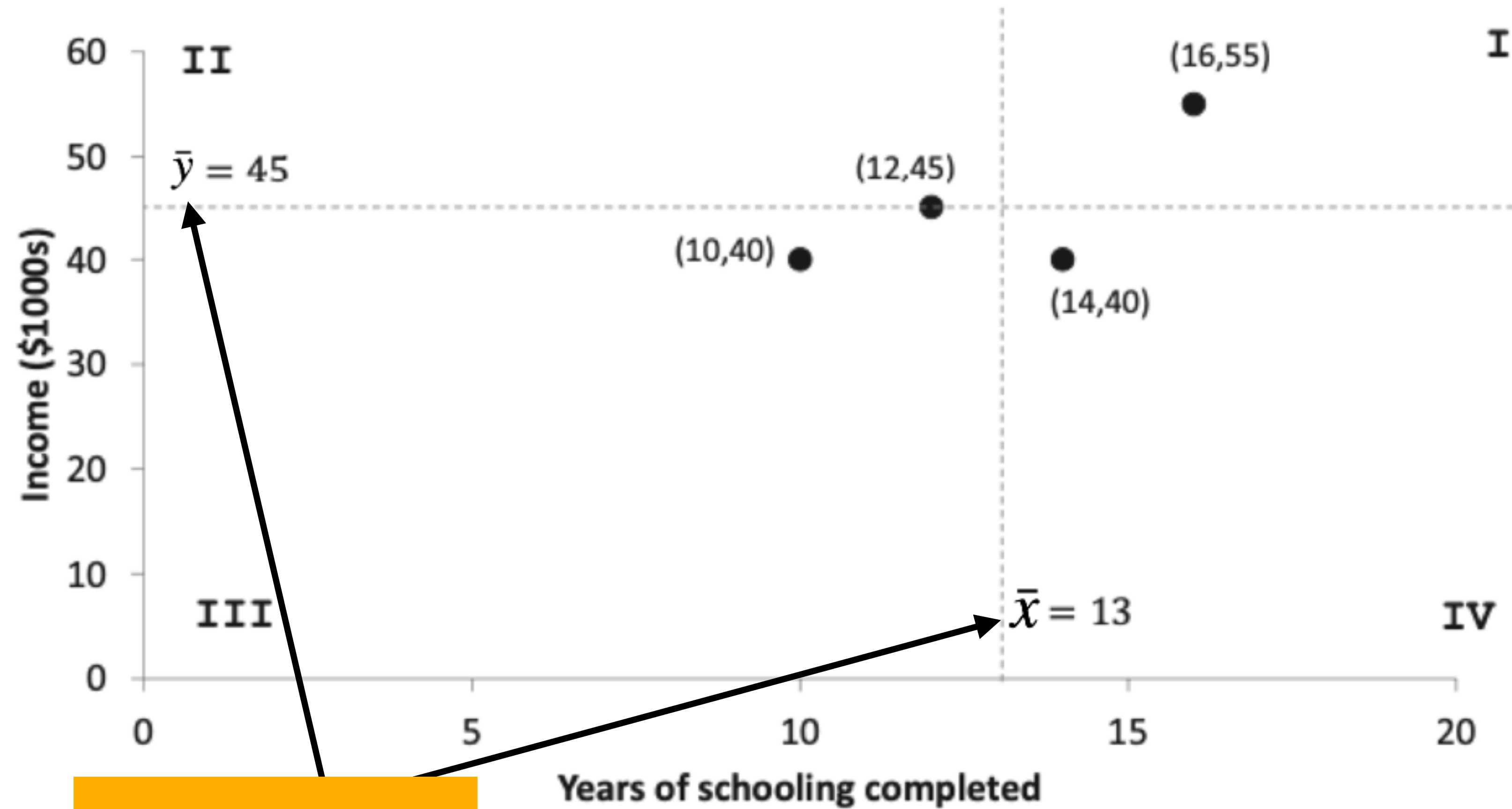
Person	Years of Schooling (x)	Income (\$1000s) (y)	Deviation from mean x	Deviation from mean y	Numerator for slope $(x_i - \bar{x}) \times (y_i - \bar{y})$	Denominator for slope $(x_i - \bar{x})^2$
1	10	40	-3	-5	15	9
2	12	45	-1	0	0	1
3	14	40	1	-5	-5	1
4	16	55	3	10	30	9
	$\bar{x} = 13$	$\bar{y} = 45$			40	20

# Example





# Example



Mean values.

# Example

- With the OLS method, we determine the estimated slope,  $\hat{\beta}_1$ , by:

$$\hat{\beta}_1 = \frac{\sum_{i=1}^n (x_i - \bar{x})(y_i - \bar{y})}{\sum_{i=1}^n (x_i - \bar{x})^2}$$

Person	Years of Schooling (x)	Income (\$1000s) (y)	Deviation from mean x	Deviation from mean y	Numerator for slope $(x_i - \bar{x}) \times (y_i - \bar{y})$	Denominator for slope $(x_i - \bar{x})^2$
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$$\hat{\beta}_1 = \frac{\sum_{i=1}^n (x_i - \bar{x})(y_i - \bar{y})}{\sum_{i=1}^n (x_i - \bar{x})^2}$$

$$\hat{\beta}_1 = \frac{40}{20} = 2$$

When  $x$  changes by 1 unit,  $y$  tends to be 2 units higher.

Person	Years of Schooling (x)	Income (\$1000s) (y)	Deviation from mean x	Deviation from mean y	Numerator for slope ( $x_i - \bar{x}$ ) $\times$ ( $y_i - \bar{y}$ )	Denominator for slope ( $x_i - \bar{x}$ ) <sup>2</sup>
1	10	40	-3	-5	15	9
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# Example

- Recall:  $\hat{y}_i = \hat{\beta}_0 + \hat{\beta}_1 x_i$
- We can say:  $\bar{y} = \hat{\beta}_0 + \hat{\beta}_1 \bar{x}$ 
  - I.e., the regression line goes through  $(\bar{x}, \bar{y})$ .
- Rearrange to:
  - $\hat{\beta}_0 = \bar{y} - \hat{\beta}_1 \bar{x}$

# Example

- $\hat{\beta}_0 = \bar{y} - \hat{\beta}_1 \bar{x}$   
 $= 45 - 2 \times 13 = 19$
- Substituting in  $\hat{\beta}_0$  and  $\hat{\beta}_1$  to  $\hat{y}_i = \hat{\beta}_0 + \hat{\beta}_1 x_i$ :
  - $\hat{y}_i = 19 + 2x_i$

Person	Years of Schooling (x)	Income (\$1000s) (y)	Deviation from mean x	Deviation from mean y	Numerator for slope ( $x_i - \bar{x}$ ) $\times$ ( $y_i - \bar{y}$ )	Denominator for slope ( $x_i - \bar{x}$ ) <sup>2</sup>
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# Total Sum of Squares (TSS)

- Also known as the *total variation*.

$$TSS = \sum_{i=1}^n (y_i - \bar{y})^2$$

- In the example to the right, TSS = 150.

Person	Years of Schooling (x)	Income (\$1000s) (y)	Deviation from mean x	Deviation from mean y	Numerator for slope ( $x_i - \bar{x}$ ) $\times$ ( $y_i - \bar{y}$ )	Denominator for slope ( $x_i - \bar{x}$ ) <sup>2</sup>
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# Total Sum of Squares (TSS)

- The Total Sum of Squares can be divided into two components:
  1.  $ExSS$  = Explained Sum of Squares = Total variation explained by the regression model.
  2.  $RSS$  = Residual Sum of Squares = Total variation unexplained by the regression model (or the sum of the squared residuals).
- $TSS = ExSS + RSS$
- $RSS = TSS - ExSS$

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  2.  $RSS$  = Residual Sum of Squares = Total variation unexplained by the regression model (or the sum of the squared residuals).
- $TSS = ExSS + RSS$
- $RSS = TSS - ExSS$

The regression model finds the set of coefficients that maximises  $ExSS$ , which in turn minimises  $RSS$ .

# Total Sum of Squares (TSS)

- $RSS = \sum_{i=1}^n (y_i - \hat{y}_i)^2$

- In our example:

Person	Years-of-schooling completed	Income (\$1000s)	Predicted income = 19 + 2x (\$1000s)	Residual
1	10	40	39	1
2	12	45	43	2
3	14	40	47	-7
4	16	55	51	4

$$RSS = \sum_{i=1}^n (y_i - \hat{y}_i)^2$$

$$= (40 - 39)^2 + (45 - 43)^2 + (40 - 47)^2 + (55 - 51)^2$$

$$= (1)^2 + (2)^2 + (-7)^2 + (4)^2 = 70$$



# Total Sum of Squares (TSS)

- We know:

- $TSS = 150$

- $RSS = 70$

Person	Years-of-schooling completed	Income (\$1000s)	Predicted income = 19 + 2x (\$1000s)	Residual
1	10	40	39	1
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- Therefore, as  $ExSS = TSS - RSS$ :

- $ExSS = 150 - 70 = 80$

- Also,  $\sum_{i=1}^n (\hat{y}_i - \bar{y})^2$

# $R^2$

- Another important statistic is  $R^2$ .
- Definition:  $R^2$  is the proportion of variation in the dependent variable ( $y$ ), that is explained by the explanatory variable ( $x$ ).

$$R^2 = \frac{ExSS}{TSS} = \frac{TSS - RSS}{TSS} = 1 - \frac{RSS}{TSS}$$

- For the education example:

$$R^2 = \frac{80}{150} = \frac{150 - 70}{150} = 1 - \frac{70}{150} = 0.533$$

# $R^2$

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- For the sample four people, 53.3% of the variation of income is explained by the variation in years-of-schooling. The remaining 46.7% is unexplained by the model.
- For Simple Linear Regression,  $R^2$  is equivalent to the square of the sample correlation (Product-Moment Correlation Coefficient),  $r_{x,y}$ :

$$R^2 = r_{x,y}^2 = \left( \frac{\sum_{i=1}^n (x_i - \bar{x})(y_i - \bar{y})}{\sqrt{\sum_{i=1}^n (x_i - \bar{x})^2} \sqrt{\sum_{i=1}^n (y_i - \bar{y})^2}} \right)^2$$

# $R^2$

- For the education example:

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- Interpretation of  $R^2$ :
  - Close to 1: Good fit of model.
  - Close to 0: Weak fit of model.



# Regression in R

```
adult <- read.csv("adult.data",header=F) # read the data
summary (adult$V13)
summary (adult$V5) # show summary of the two variables
cov(adult$V13,adult$V5) # show covariance of variables
cor(adult$V13,adult$V5) # show correlation of variables
cor(adult$V13,adult$V5)**2 # show PMCC squared / R2
fit <- lm(adult$V13 ~ adult$V5) # fit a linear model with V13 as Y
print (fit) # show the parameters of the model
summary(residuals(fit)) # summarize the distribution of residuals
summary(fit) # summarize the model.
# R shows the 'significance' of each parameter, based on a t-test
plot(adult$V5, adult$V13) # plot the data
abline(fit) # show the line of best fit on the data
```

# Regression in Gnuplot

- Scatter plot of hours worked vs. Years of education (as before):

set term png

set output "ageeducation.png"

set title "Hours versus education"

set xlabel "Years of education"

set ylabel "Hours worked"

set key under

- Add a line of best fit:

$$y(x)=a*x+b$$

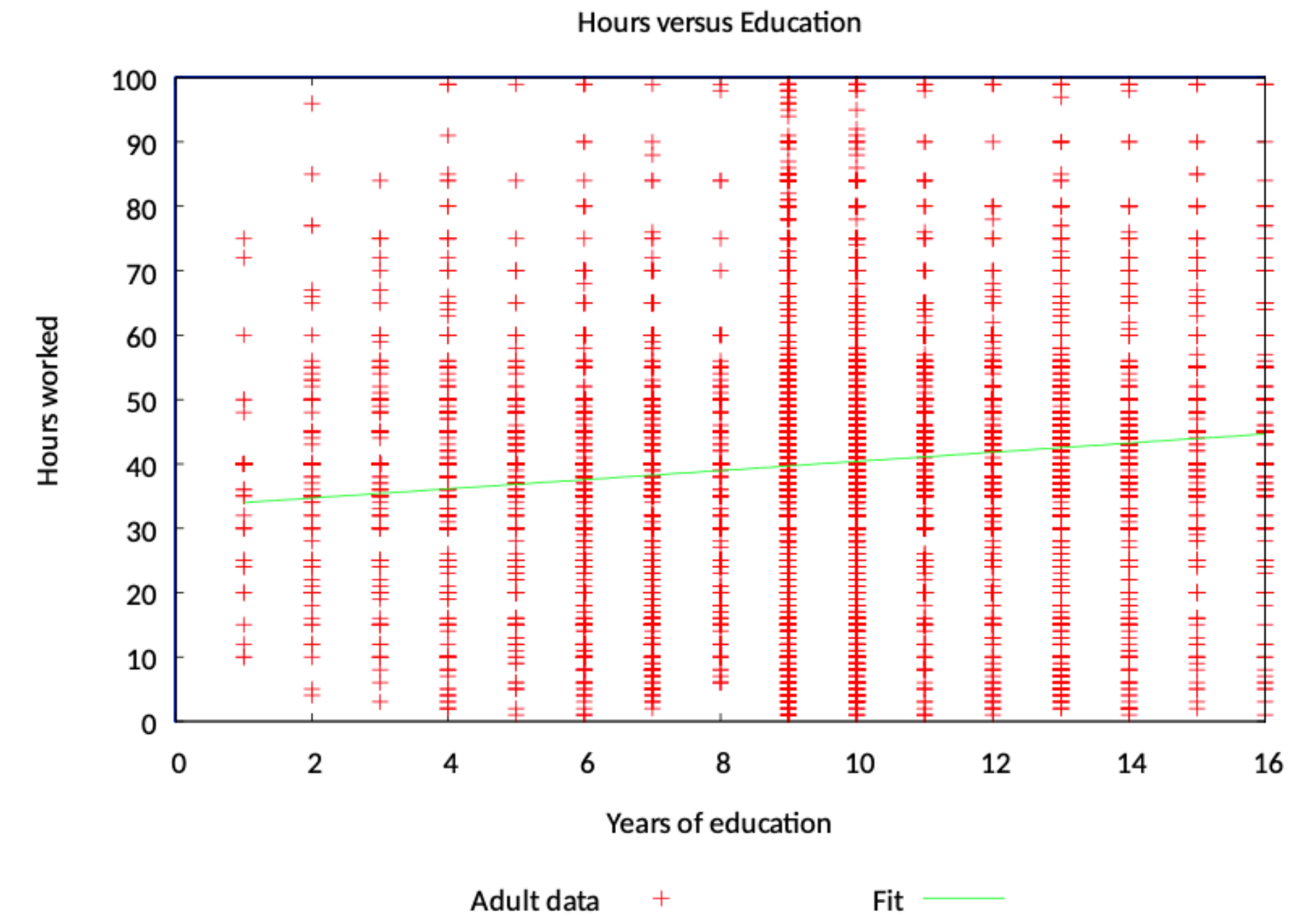
fit y(x) "adult/adult.data" using 5:13 via a,b

plot "adult/adult.data" u 5:13 w p t 'Adult', \ y(x) with lines title 'Fit'

# Regression in Gnuplot

- Output to standard output:

Final set of parameters		Asymptotic Standard Error	
<b>a</b>	= 0.710895	+/- 0.0263	(3.7%)
<b>b</b>	= 33.2711	+/- 0.2737	(0.8225%)



# Regression in Weka

- Open the data file, **remove** unwanted (non-numeric) attributes
- Under **classify** tab, choose “**functions/Simple Linear Regression**”
  - Select “use training set” for test options
  - Hit start!
- Partial output:

```
0.69 * education-num + 33.44
```

```
Time taken to build model: 0.03 seconds
```

```
=== Evaluation on training set ===
```

```
=== Summary ===
```

```
Correlation coefficient           0.1437
```

```
Mean absolute error              7.7668
```

```
Root mean squared error         12.2627
```



# Acknowledgements

- Graham Cormode [Warwick, CS910]
- Florin Ciucu [Warwick, CS430/CS910]
- Montgomery, D.C., Peck, E.A. and Vining, G.G., 2021. *Introduction to linear regression analysis*. John Wiley & Sons.
- Arkes, J., 2019. Regression analysis: A practical introduction. Routledge.
- Statistics 101: Logistic Regression, An Introduction. <https://www.youtube.com/watch?v=zAULhNrnuL4>. Brandon Foltz.

# Part B: Multiple Linear Regression, Non-Linear Regression & Logistic Regression

# Multiple Linear Regression

- Suppose we want to include more variables:
  - Model:  $y_i = ax_1 + bx_2 + cx_3 + \dots + z$
  - $y_i$ : dependent (response) variable
  - $x_i$ : explanatory variables
- We could follow same outline, write out squared error and minimise.
- Notation gets ugly, messy.
- Instead, can solve via matrix representation.

# Multiple Linear Regression

## Matrix Representation of Linear Regression

- Let the  $(d + 1)$  model parameters be  $(w_0, w_1, \dots, w_d) = \mathbf{w}$  (could instead use  $\beta$  here to be consistent with Simple Linear Regression if you wanted):

- Prediction for  $x$  will be  $f(x) = w_0 1 + \sum_{i=1}^d w_i x_i$ .

- Encode the  $n$  examples as a  $n \times (d + 1)$  matrix,  $X$ :

- First column is all 1s, for the constant term.

- Vector of  $n$  corresponding to  $y_i$  values,  $y$ .

$$\begin{pmatrix} 1 & x_{11} & x_{12} & x_{13} & \dots \\ 1 & x_{21} & x_{22} & x_{23} & \dots \\ 1 & x_{31} & x_{32} & x_{33} & \dots \\ \dots & \dots & \dots & \dots & \dots \end{pmatrix}$$

# Linear Algebra Refresher

- A  $r \times c$  matrix has  $r$  rows,  $c$  columns
  - $X_{i,j}$  is the entry in row  $i$  and column  $j$
- Transpose,  $X^T$  switches rows and columns:  $X_{i,j}^T = X_{j,i}$ 
  - $(X + Y)^T = X^T + Y^T$
  - $(XY)^T = Y^T X^T$



# Linear Algebra Refresher

- Multiplication: Multiply  $r \times n$  matrix  $X$  with  $n \times c$  matrix  $Y$  to get  $r \times c$  matrix  $Z$ 
  - $Z = XY$
  - $Z_{i,k} = \sum_{j=1}^n X_{i,j} Y_{j,k}$
- Identity Matrix  $I$  is  $n \times n$  matrix where  $IX = XI = X$ .

# Linear Algebra Refresher

- Addition: Add two  $r \times c$  matrices entry-wise,  $(X + Y)_{i,j} = X_{i,j} + Y_{i,j}$ .
- Inverse:  $X^{-1}$  is the matrix (if it exists) such that  $X^{-1}X = XX^{-1} = I$ .

# Sum of Squares Error

$$\mathbf{X} = \begin{bmatrix} 1 & x_1^{(1)} & \cdots & x_d^{(1)} \\ \vdots & & \vdots & \\ 1 & x_1^{(N)} & \cdots & x_d^{(N)} \end{bmatrix}, \quad \mathbf{y} = \begin{bmatrix} y_1 \\ \vdots \\ y_N \end{bmatrix}, \quad \mathbf{w} = \begin{bmatrix} w_0 \\ \vdots \\ w_d \end{bmatrix}$$

- Column vector of predictions on data is  $X\mathbf{w}$ .

- Residuals are the column  $(y - X\mathbf{w})$

- Residual Sum of Squares is now:

$$RSS(\mathbf{w}) = (y - X\mathbf{w})^T(y - X\mathbf{w}) = (y^T - \mathbf{w}^T X^T)(y - X\mathbf{w})$$

- $= y^T y - y^T X\mathbf{w} - \mathbf{w}^T X^T y + \mathbf{w}^T X^T X\mathbf{w}$

- The inner product of the residuals with themselves.

# Sum of Squares Error

- Taking partial derivative with respect to all values of  $\mathbf{w}$  yields the solution:
  - $\mathbf{w} = (X^T X)^{-1} X^T y$
  - Assuming that  $(X^T X)^{-1}$  exists.
  - I.e.,  $X$  cannot have linearly dependent columns.

# Prediction Using the Model

- Given a new data point  $x$ , define  $x' = [1, x_1, \dots, x_d]$ 
  - Prediction is  $x'\mathbf{w} = x'(X^T X)^{-1} X^T y$
- As before, quality of fit is given by the
  - Computed as fraction of the sum of squares explained by the regression
$$R^2 = 1 - \frac{RSS}{TSS}$$
- Same interpretation of  $R^2$  as in Simple Linear Regression:
  - Close to 1: Good fit of model.
  - Close to 0: Weak fit of model.



# Multiple Linear Regression in R

```
adult <- read.csv("adult.data",header=F) # read the data
fit <- lm(adult$V13 ~ adult$V5 + adult$V1)
#fit a linear model with V13 as Y, V1 and V5 as X
fit #show the parameters of the model
# Model:  $y = 31.2 + 0.06(\text{age}) + 0.70(\text{years of education})$ 
summary(fit)
#  $R^2 = 0.0260$ 
pairs(adult$V13~ adult$V1 + adult$V5)
# plots of pairs of vars
```

# Multiple Linear Regression in Weka

- Open the data file, **remove** unwanted (non-numeric) attributes
- Under *classify* tab, choose **“functions/LinearRegression”**
  - Select “use training set” for test options
  - Hit start!
- Partial output:

hours-per-week =

0.0545 \* age +  
0.6293 \* education-num +  
0.0001 \* capital-gain +  
0.0013 \* capital-loss +  
31.7487

Time taken to build model: 0.29 seconds

=== Evaluation on training set ===

Time taken to test model on training data: 0.16 seconds

=== Summary ===

Correlation coefficient	0.1747
Mean absolute error	7.7774
Root mean squared error	12.2008

# Dealing with Categorical Attributes

- Regression is **fundamentally numeric**:
  - But we can numerically encode categorical (explanatory) variables
- Simple case: binary attribute (e.g. Sex = Male or Female)
  - Create a variable that is **0 if male, 1 if female**
  - Include this new variable in the regression
- General categorical attributes (e.g. Country): “Dummy coding”
  - Create a binary variable for **each possibility**
  - E.g. England (T/F), Mexico (T/F), France (T/F)...
  - Include all these variables in the regression
  - Effectively, adds a different constant for each category

# Adult.data

- Build a regression model for hours worked:
  - Put in as many variables as possible.
  - R automatically handles categoric variables:
  - ```
fit3 <- lm(adult$V13 ~ adult$V1 + adult$V2 + adult$V4 + adult$V5 +  
adult$V6 + adult$V7 + adult$V8 + adult$V9 + adult$V10 + adult$V14 +  
adult$V15)
```

```
summary(fit3)
```
- Weka can automatically convert categoric values to numeric.

# Adult.data

- Multiple Linear Regression often gives greater  $R^2$  results!
- But we have built a complex model (dozens of variables/parameters)
- At risk of “kitchen sink regression”: throw in everything possible
  - May find false correlations, lead to erroneous conclusions.
  - Some variables significant: employment type (work class), education.
  - Others not: age, native-country, race.



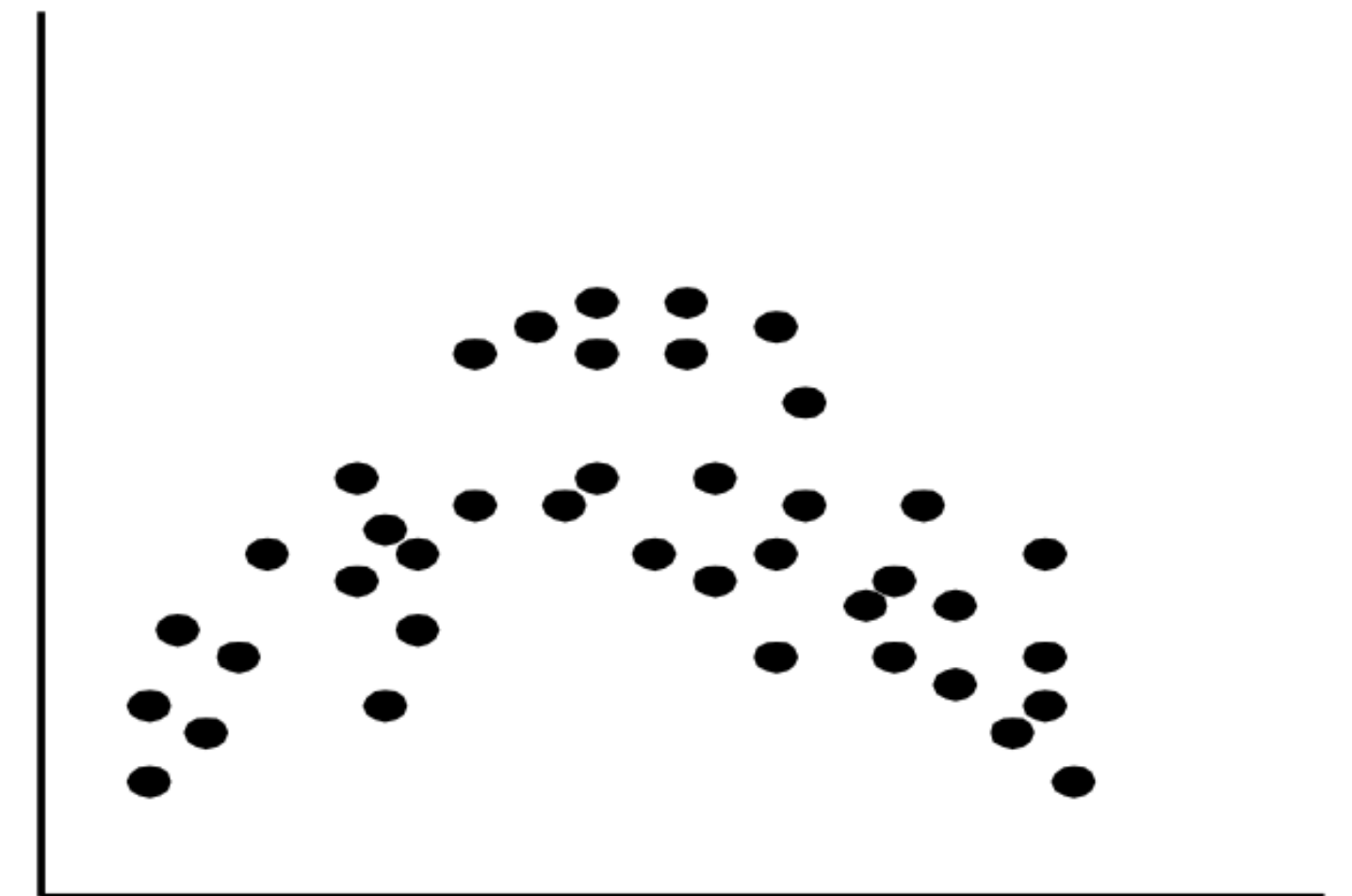
# Adult.data

## Education

- Two measures of education level in the data:
  - Years of education (numeric), Education level (categorical)
- How do they relate?
  - `fit4 <- lm(adult$V5 ~ adult$V4)`
  - $R^2 = 1$ !
  - `plot(adult$V5 ~ adult$V4)`
- Years of education entirely determined by education level:
  - Conjecture: years of education computed from education level!

# Fitting Non-Linear Models

- Not all relationships are linear
  - Some are quadratic, cubic, ...
  - exponential, logarithmic, ...
- Do we need to find new methods for each different model?
- Idea: try transforming the data so that we seek a linear model
  - Suppose we have a quadratic model:  $y = ax^2 + bx + c$
  - Introduce a new variable  $z = (x^2)$
  - Model is now  $y = az + bx + c$ : linear!
  - Use multiple linear regression to learn the parameters of this model



# Non-Linear Models

```
adult <- read.csv("adult.data",header=F) # read the data
```

```
fit <- lm(adult$V13 ~ adult$V5 + I(adult$V5^2) + I(adult$V5^3) + adult$V1 +  
I(adult$V1^2) + I(adult$V1^3))
```

```
#fit a linear model with V13 as Y, V1 and V5 as X
```

```
fit #show the parameters of the model
```

```
(Intercept)  adult$V5 I(adult$V5^2) I(adult$V5^3) adult$V1 I(adult$V1^2) I(adult$V1^3)  
-1.820e+01  1.706e+00 -2.389e-01  1.078e-02  3.426e+00 -6.190e-02  3.191e-04
```

```
summary(fit)
```

```
#  $R^2 = 0.148$ 
```

# Exponential Models

- Suppose that we want to learn a model of the form  $y = \alpha e^{\lambda x}$ 
  - For some unknown parameters  $\alpha, \lambda$
- Here, we can take the natural log of both sides:
  - $(\ln(y)) = (\ln(\alpha)) + \lambda x$ : **Simple Linear Regression**

$$\ln(xy) = \ln(x) + \ln(y)$$

# Categoric Outputs

- What about regression to predict **categoric attributes**?
  - Regression so far predicts a number.
  - Will focus on binary outputs.
- Can encode **True=1, False=0**, and try to use regression:
  - Predicts **0.03**: probably False
  - Predicts **0.82**: probably True
- Is it a sensible approach?:
  - Prediction of **13.3**: really true???
  - Prediction of **-5.7**: really false???



# Logistic Regression

- Logistic Regression is used to model the probability of some class or event occurring.
- Example: The probability that you will be accepted to study for an MSc at Warwick based on your grades (let's represent the grades as a number between 0 and 1000).
- Let *Accepted* be 1 if the applicant is accepted to study, and 0 otherwise.

| Grade | Accepted? |
|-------|-----------|
| 561   | 1         |
| 490   | 0         |
| 781   | 1         |
| 189   | 0         |
| 221   | 0         |
| 981   | 1         |
| 700   | 0         |
| 562   | 0         |
| 761   | 1         |
| 365   | 0         |

# Logistic Regression

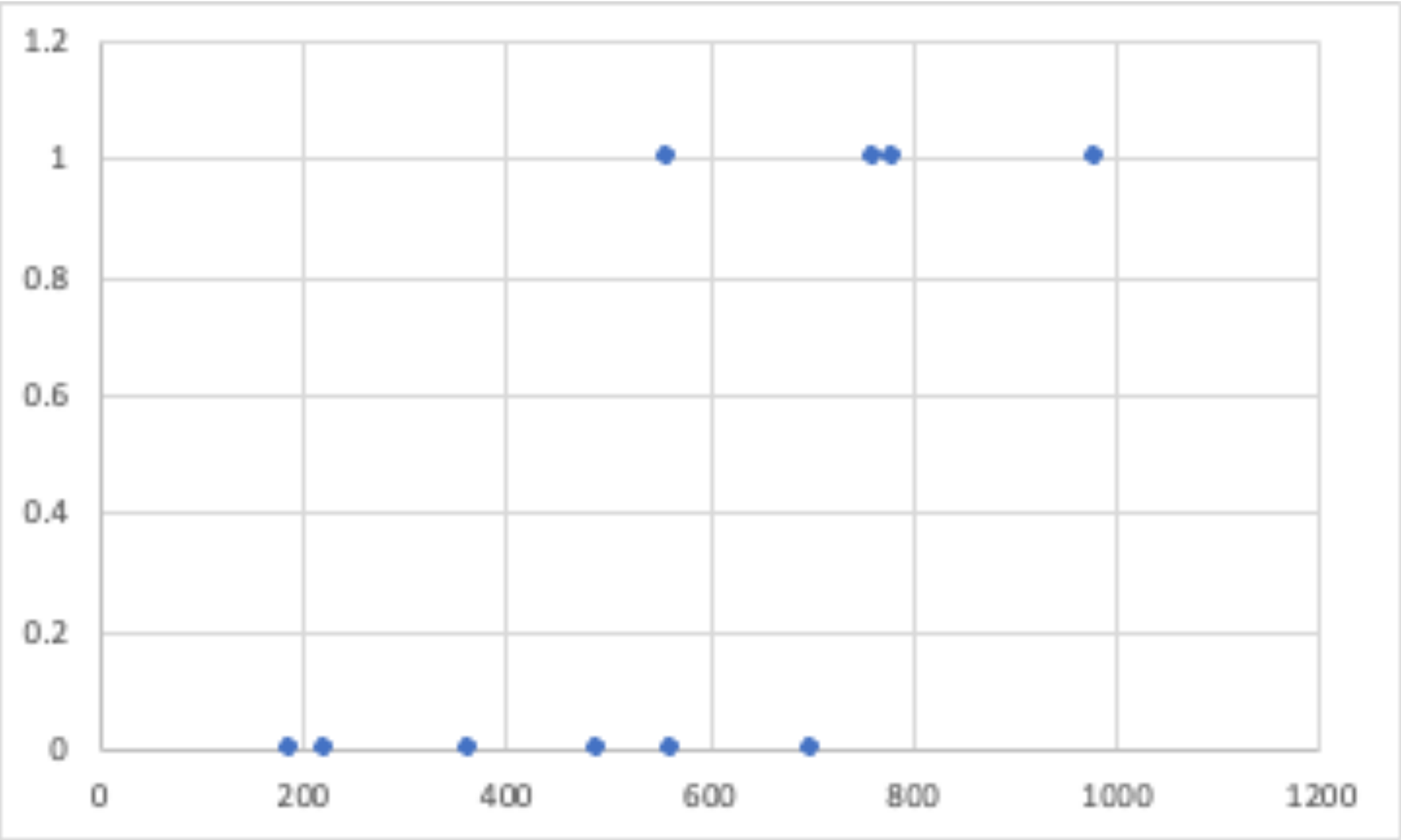
- Let's try to calculate the probability of an applicant with a score of 655 being accepted.

| Grade | Accepted? |
|-------|-----------|
| 561   | 1         |
| 490   | 0         |
| 781   | 1         |
| 189   | 0         |
| 221   | 0         |
| 981   | 1         |
| 700   | 0         |
| 562   | 0         |
| 761   | 1         |
| 365   | 0         |

# Logistic Regression

## Why Not Other Forms of Regression?

- Where would we draw our line of best fit?

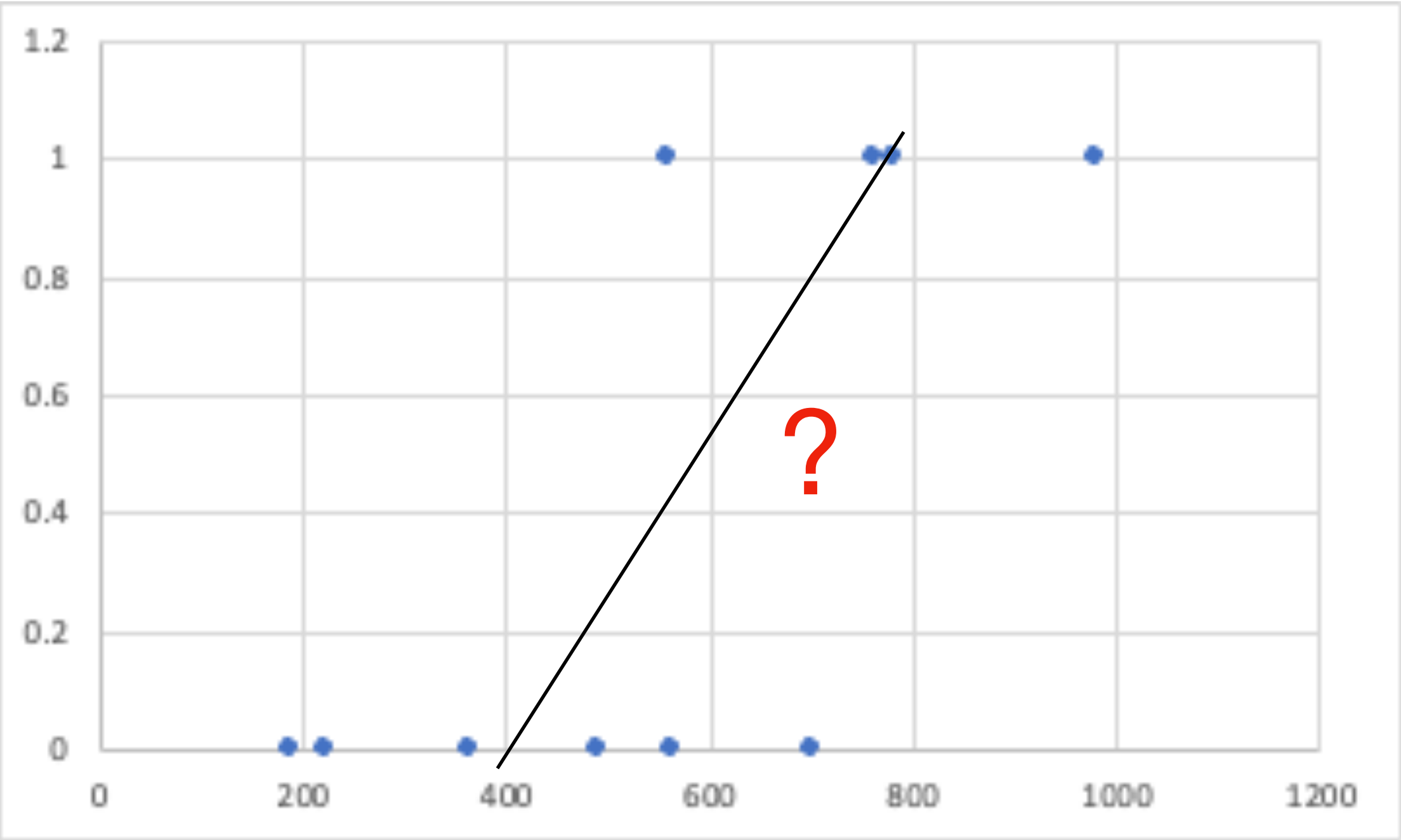


| Grade | Accepted? |
|-------|-----------|
| 561   | 1         |
| 490   | 0         |
| 781   | 1         |
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# Logistic Regression

## Why Not Other Forms of Regression?

- Where would we draw our line of best fit?



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# Logistic Regression

## Probability

- What is the probability of some event  $A$  occurring?

$$P(A) = \frac{\text{Number of outcomes of } A}{\text{Number of all possible outcomes}}$$

- Some examples:

- Toss a coin:  $P(\text{Heads}) = \frac{1}{2}$

- Roll an even number on a die:  $P(\text{Even number}) = \frac{3}{6} = \frac{1}{2}$

- Roll a number less than 6 on a die:  $P(\text{Roll} < 6) = \frac{5}{6}$

# Logistic Regression

## Odds

- What are the odds of some event occurring?

- $odds = \frac{p}{1 - p}$

where  $p$  is the probability of the event occurring.

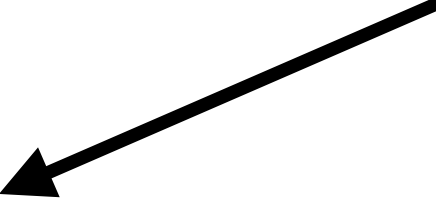
- Therefore, the odds of an event occurring, is the probability of the event occurring, divided by the probability of the event not occurring.

- Examples:

- Flipping a fair coin and getting heads:

- $P(heads) = p = \frac{1}{2} = 0.5$

- $Odds(heads) = \frac{0.5}{1 - 0.5} = \frac{0.5}{0.5} = 1$



**If odds are 1, then there is an equal number of outcomes where heads occur and where heads does not occur.**



# Logistic Regression

## Odds

- Examples (continued):

- Flipping a rigged coin and getting heads:

- $P(heads) = p = \frac{1}{4} = 0.25$

- $Odds(heads) = \frac{0.25}{1 - 0.25} = \frac{0.25}{0.75} = 0.3333$

3 times the number of outcomes where heads does not occur, compared to where heads does occur.

- Rolling a dice and getting a 6:

- $P(6) = p = \frac{1}{6} = 0.16666666$

- $Odds(6) = \frac{0.16666}{1 - 0.16666} = \frac{0.16666}{0.83333} = 0.2$

5 (i.e.,  $\frac{1}{0.2}$ ) times the number of outcomes where 6 does not occur, compared to where 6 does occur.

# Logistic Regression

## Odds

- Recall,  $odds = \frac{p}{1 - p}$ .
- Therefore:
  - As  $p \rightarrow 1$ ,  $odds \rightarrow \infty$ .
  - As  $p \rightarrow 0$ ,  $odds \rightarrow 0$ .

# Logistic Regression

## Odds Ratio

- The *Odds Ratio* is simply the ratio of two odds!
- For two events, ( $e_1$  and  $e_2$ ):

$$\begin{aligned} \text{Odds Ratio} &= \frac{\text{odds}(e_1)}{\text{odds}(e_2)} \\ &= \frac{\frac{p(e_1)}{1 - p(e_1)}}{\frac{p(e_2)}{1 - p(e_2)}} \end{aligned}$$

# Logistic Regression

## Odds Ratio

- Consider the following example:

- Flipping a fair coin and getting heads:

- $P(\text{heads}) = \frac{1}{2} = 0.5$

- $Odds(\text{heads}) = \frac{0.5}{1 - 0.5} = \frac{0.5}{0.5} = 1$

- Flipping a rigged coin and getting heads:

- $P(\text{heads}) = \frac{1}{4} = 0.25$

- $Odds(\text{heads}) = \frac{0.25}{1 - 0.25} = \frac{0.25}{0.75} = 0.3333$

$$\begin{aligned} Odds\ Ratio &= \frac{odds(e_1)}{odds(e_2)} \\ &= \frac{\frac{p(e_1)}{1 - p(e_1)}}{\frac{p(e_2)}{1 - p(e_2)}} \end{aligned}$$

- Let's say  $e_1$  is getting heads on the fair coin, and  $e_2$  is getting heads on the rigged coin.

$$Odds\ Ratio = \frac{odds(e_1)}{odds(e_2)}$$

- $$= \frac{1}{0.3333} = 3$$

- The odds of getting heads on the fair coin is three times greater than on the rigged coin.

# Logistic Regression

## Logit

- We are trying to calculate the probability  $p$  of some event happening.
  - Let's call the estimated  $p$ ,  $\hat{p}$ .
- We need to find a way to map our data to a probability distribution. We can do this using the natural log of the odds:

$$\ln(odds) = \ln\left(\frac{p}{1-p}\right) = \text{logit}(p)$$

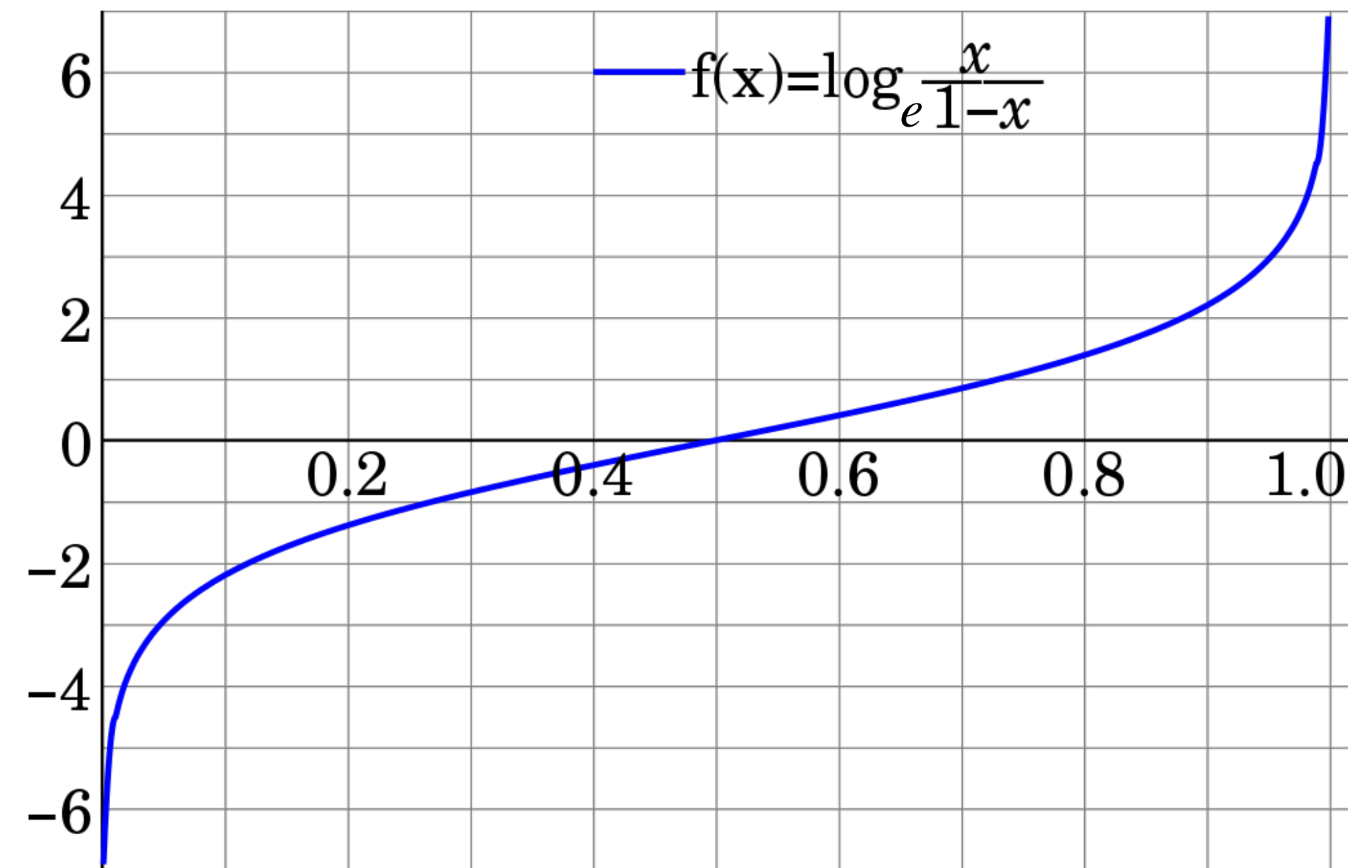
Remember,  
 $\ln(x) = \log_e x$

$$\text{Alternatively, } \ln(p) - \ln(1-p) = \text{logit}(p)$$

# Logistic Regression

## Logit

- $\text{logit}(p) = \ln\left(\frac{p}{1-p}\right)$ 
  - As  $p \rightarrow 1$ ,  $\text{logit}(p) \rightarrow \infty$ .
  - As  $p \rightarrow 0$ ,  $\text{logit}(p) \rightarrow -\infty$ .
  - When  $p = 0.5$ ,  $\text{logit}(p) = 0$ .
- We need our  $y$ -axis to be within the range 0 to 1 for probability...





# Logistic Regression

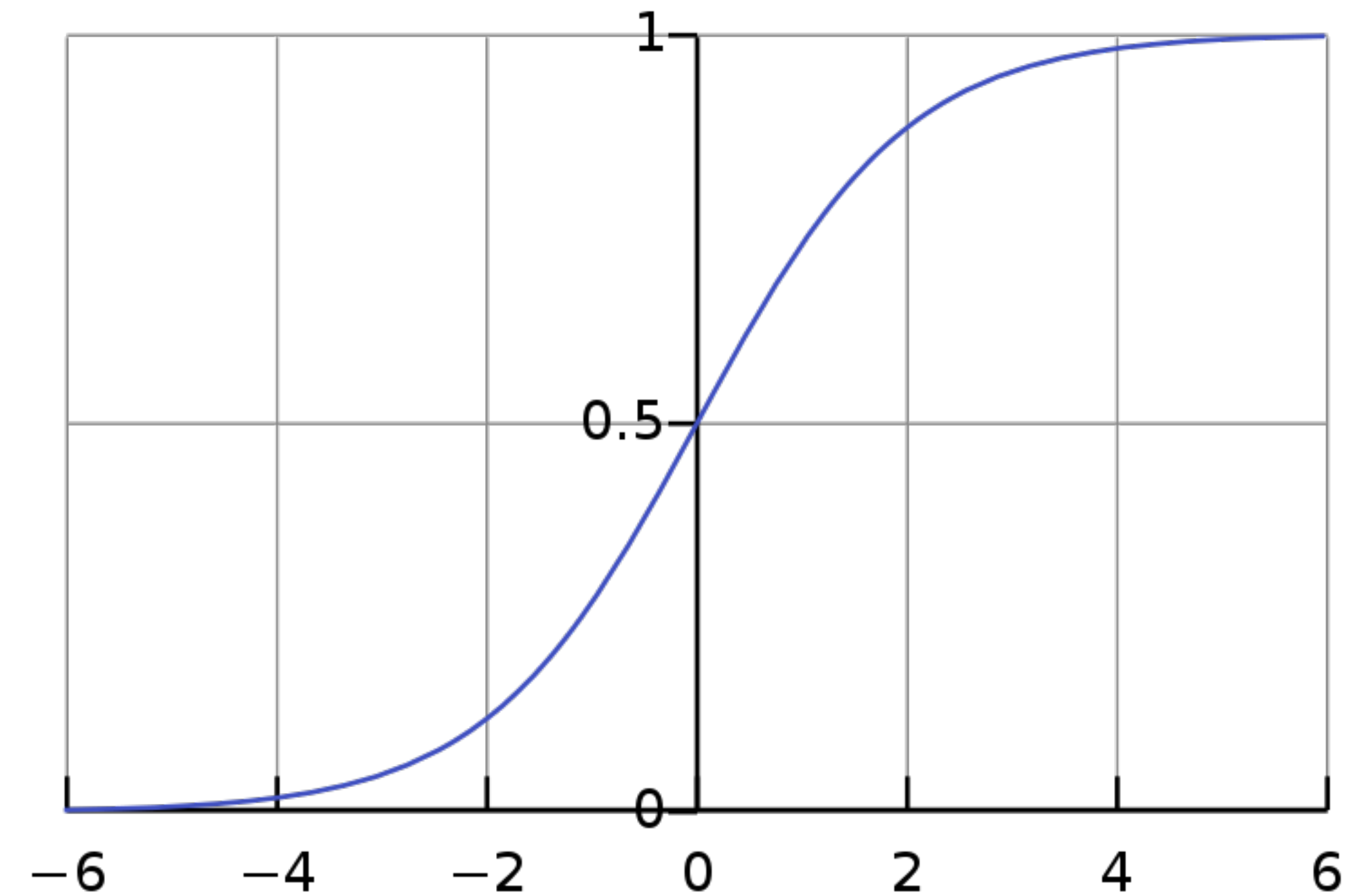
## The Inverse Logit

- $\text{logit}(p) = \ln\left(\frac{p}{1-p}\right)$
- $\text{logit}^{-1}(\alpha) = \left(\frac{1}{1+e^{-\alpha}}\right) = \left(\frac{e^{\alpha}}{1+e^{\alpha}}\right)$
- $\alpha$  is our linear combination of explanatory variables and their coefficients (i.e.  $\beta_0 + \beta_1 x_1 \dots$ )

# Logistic Regression

## The Inverse Logit

- Sigmoid function (“S” curve).
- Outcome of 0 and outcome of 1 is undefined.
  - As  $\alpha \rightarrow \infty$ ,  $\text{logit}^{-1}(\alpha) \rightarrow 1$ .
  - As  $\alpha \rightarrow -\infty$ ,  $\text{logit}^{-1}(\alpha) \rightarrow 0$ .
- Range from 0 to 1... good for probability!



# Logistic Regression

- The logit of  $p$  (or the natural log of the odds) is equivalent to a linear combination of the explanatory (independent) variables.

$$\text{logit}(p) = \ln\left(\frac{p}{1-p}\right) = \beta_0 + \beta_1 x_1$$

$$\frac{p}{1-p} = e^{\beta_0 + \beta_1 x_1}$$

- Simplify to get the estimated probability,  $\hat{p}$ :

$$\hat{p} = \frac{e^{\beta_0 + \beta_1 x_1}}{1 + e^{\beta_0 + \beta_1 x_1}}$$

# Logistic Regression

$$\hat{p} = \frac{e^{\beta_0 + \beta_1 x_1}}{1 + e^{\beta_0 + \beta_1 x_1}}$$

- Using our entry data again (shown to the right).
- Weka reports:
  - $\beta_0 = -8.1479, \beta_1 = 0.0126$
- Substitute into equation for row 3:
  - $\hat{p} = \frac{e^{-8.1479 + (0.0126 \times 781)}}{1 + e^{-8.1479 + (0.0126 \times 781)}} = 0.845...$
  - = 84.5% chance of accepted

| Grade | Accepted? |
|-------|-----------|
| 561   | 1         |
| 490   | 0         |
| 781   | 1         |
| 189   | 0         |
| 221   | 0         |
| 981   | 1         |
| 700   | 0         |
| 562   | 0         |
| 761   | 1         |
| 365   | 0         |

# Logistic Regression

$$\hat{p} = \frac{e^{\beta_0 + \beta_1 x_1}}{1 + e^{\beta_0 + \beta_1 x_1}}$$

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- = 84.5% chance of accepted

| Grade | Accepted? |
|-------|-----------|
| 561   | 1         |
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|       |           |
|       |           |
|       |           |
|       |           |
|       |           |
|       |           |
|       |           |
| 365   | 0         |

**Interpretation: Each grade increase of just 1 multiplies odds by  $e^{0.0126} = 1.013$ .**

# Logistic Regression

$$\hat{p} = \frac{e^{\beta_0 + \beta_1 x_1}}{1 + e^{\beta_0 + \beta_1 x_1}}$$

- Using our entry data again (shown to the right).
- Weka reports:
  - $\beta_0 = -8.1479$ ,  $\beta_1 = 0.0126$
- Odds of being accepted for row 3:
  - $Odds = \frac{0.845...}{1 - 0.845...} = 5.434...$
  - Therefore, the odds of being accepted with a grade of 781 is 5.434...

| Grade | Accepted? |
|-------|-----------|
| 561   | 1         |
| 490   | 0         |
| 781   | 1         |
| 189   | 0         |
| 221   | 0         |
| 981   | 1         |
| 700   | 0         |
| 562   | 0         |
| 761   | 1         |
| 365   | 0         |



# Logistic Regression

$$\hat{p} = \frac{e^{\beta_0 + \beta_1 x_1}}{1 + e^{\beta_0 + \beta_1 x_1}}$$

- $Odds = \frac{0.845...}{1 - 0.845...} = 5.434...$
- How about if we try to push our grade 1 higher (i.e. 782)? How does this change the odds?
- Step 1: Calculate the probability for 782:
  - $\hat{p} = 0.846...$
- Step 2: Calculate odds for 782:
  - $Odds = \frac{0.846...}{1 - 0.846...} = 5.503...$

| Grade | Accepted? |
|-------|-----------|
| 561   | 1         |
| 490   | 0         |
| 781   | 1         |
| 189   | 0         |
| 221   | 0         |
| 981   | 1         |
| 700   | 0         |
| 562   | 0         |
| 761   | 1         |
| 365   | 0         |

# Logistic Regression

$$\hat{p} = \frac{e^{\beta_0 + \beta_1 x_1}}{1 + e^{\beta_0 + \beta_1 x_1}}$$

- We can now calculate the odds ratio, which we can interpret as the increase in odds when we gain one additional grade point:

$$\begin{aligned} \text{Odds Ratio} &= \frac{\text{odds}(782)}{\text{odds}(781)} \\ &= \frac{5.503...}{5.434...} \\ &= 1.0127 \end{aligned}$$

- You can also see this value on your Weka output!

| Grade | Accepted? |
|-------|-----------|
| 561   | 1         |
| 490   | 0         |
| 781   | 1         |
| 189   | 0         |
| 221   | 0         |
| 981   | 1         |
| 700   | 0         |
| 562   | 0         |
| 761   | 1         |
| 365   | 0         |

# Logistic Regression in Weka

1. Select '**adult.arff**', remove unwanted attributes
2. Select the **classify** tab
3. Choose the classifier: '**classifiers/functions/Logistic**'
4. For test options, pick '**use training set**'
5. Pick the target attribute
6. Hit '**start**'
7. The result shows the model and some measures of quality

```
Time taken to build model: 6.35 seconds
=== Evaluation on training set ===
=== Summary ===
Correctly Classified Instances      40612      83.1497 %
Incorrectly Classified Instances    8230      16.8503 %
```

# Acknowledgements

- Graham Cormode [Warwick, CS910]
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- Montgomery, D.C., Peck, E.A. and Vining, G.G., 2021. *Introduction to linear regression analysis*. John Wiley & Sons.
- Arkes, J., 2019. Regression analysis: A practical introduction. Routledge.
- Statistics 101: Logistic Regression, An Introduction. <https://www.youtube.com/watch?v=zAULhNrnuL4>. Brandon Foltz.