arise:

2019 Data Science Internship

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Tools for Machine Learning and Data Mining

Linear and Logistic Regression

(Adapted from various sources)

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LEARNING OUTCOMES

- Understand the role of regression in data science
- Understand the basics of Linear Regression
- Measure the performance of a regression model
- Understand the basic of logistic regression

Regression

A form of statistical modeling that attempts to evaluate the relationship between one variable (termed the dependent variable) and one or more other variables (termed the independent variables). It is a form of global analysis as it only produces a single equation for the relationship.

A model where one continuous variable using one or more variables.

Linear Regression

Regression used to fit a linear model to data where the dependent variable is continuous:

$$Y = \beta_0 + \beta_1 X_1 + \beta_2 X_2 + \ldots + \beta_n X_n + \varepsilon$$

Given a set of points (Xi,Yi), we wish to find a linear function (or line in 2 dimensions) that “goes through” these points.

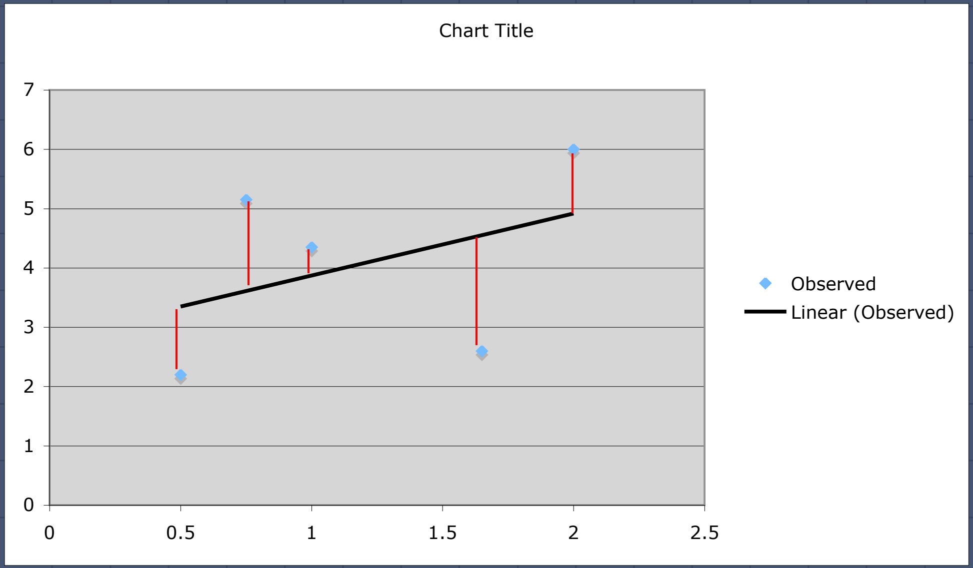
In general, the points are not exactly aligned:

- Find line that best fits the points

Residue

Error or residue:

- Observed value - Predicted value



Sum-squared Error (SSE)

$$SSE = \sum_{y} (y_{observed} - y_{predicted})^2$$

$$TSS = \sum_{y} (y_{observed} - \bar{y}_{observed})^2$$

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

PRACTICE

SN	Age	Height (CM)	CaloriesConsumedPerDay	weightIn5years (kg)
	55	169	1200	79
	25	170	2200	88
	67	166	1800	75
	89	173	2400	90
	33	155	1800	70
	21	158	800	61
	43	160	1100	73

weightIn5years (kg) [Predicted]
83
80
71
98
72
65
77

Given the following figures, calculate the
1) SSE, 2) TSS and 3) R-Squared for a model built with the the observed variables.

What is Best Fit?

The smaller the SSE, the better the fit

Hence,

- Linear regression attempts to minimize SSE (or similarly to maximize R2)

Assume 2 dimensions

$$Y = \beta_0 + \beta_1 X$$

Analytical Solution

$$\beta_0 = \frac{\sum y - \beta_1 \sum x}{n}$$

$$\beta_1 = \frac{n \sum xy - \sum x \sum y}{n \sum x^2 - \left(\sum x\right)^2}$$

Example (I)

x	y	x^2	xy
1.20	4.00	1.44	4.80
2.30	5.60	5.29	12.88
3.10	7.90	9.61	24.49
3.40	8.00	11.56	27.20
4.00	10.10	16.00	40.40
4.60	10.40	21.16	47.84
5.50	12.00	30.25	66.00
24.10	**58.00**	**95.31**	**223.61**

Target: $y=2x+1.5$

$$\beta_1 = \frac{n\sum xy - \sum x \sum y}{n\sum x^2 - \left(\sum x\right)^2}$$

$$= \frac{7 \times 223.61 - 24.10 \times 58.00}{7 \times 95.31 - 24.10^2}$$

$$= \frac{1565.27 - 1397.80}{667.17 - 580.81}$$

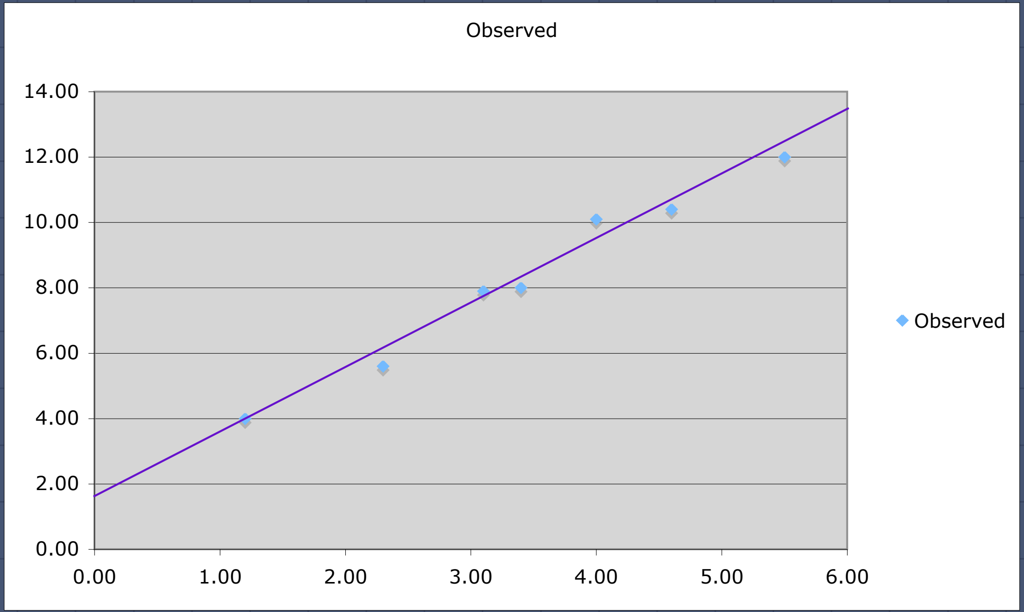
$$= \frac{167.47}{86.36} = \underline{\underline{1.94}}$$

$$\beta_0 = \frac{\sum y - \beta_1 \sum x}{n}$$

$$= \frac{58.00 - 1.94 \times 24.10}{7}$$

$$= \frac{11.27}{7} = \underline{\underline{1.61}}$$

Example (II)


Observed
14.00
12.00
10.00
8.00
6.00
4.00
2.00
0.00
0.00
1.00
2.00
3.00
4.00
5.00
6.00
Observed

Example (III)

x	y (obs)	y (pred)	SSE	TSS
1.20	4.00	3.94	0.004	18.367
2.30	5.60	6.07	0.221	7.213
3.10	7.90	7.62	0.078	0.149
3.40	8.00	8.21	0.044	0.082
4.00	10.10	9.37	0.533	3.292
4.60	10.40	10.53	0.017	4.470
5.50	12.00	12.28	0.078	13.796
			0.975	**47.369**

$$R^2 = 1 - \frac{SSE}{TSS} = 1 - \frac{0.975}{47.369} = 0.98$$

Logistic Regression

Regression used to fit a curve to data in which the dependent variable is binary, or dichotomous

Typical application: Medicine

- We might want to predict response to treatment, where we might code survivors as 1 and those who don’t survive as 0

Example

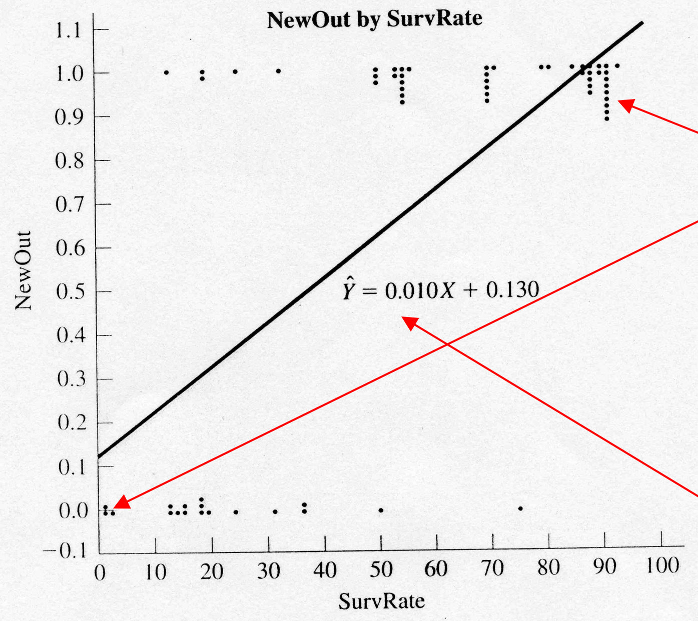


FIGURE 15·7 *Outcome as a function of SurvRate*

Observations:
For each value of SurvRate, the number of dots is the number of patients with that value of NewOut

Regression:
Standard linear regression

Problem: extending the regression line a few units left or right along the X axis produces predicted probabilities that fall outside of [0,1]

A Better Solution

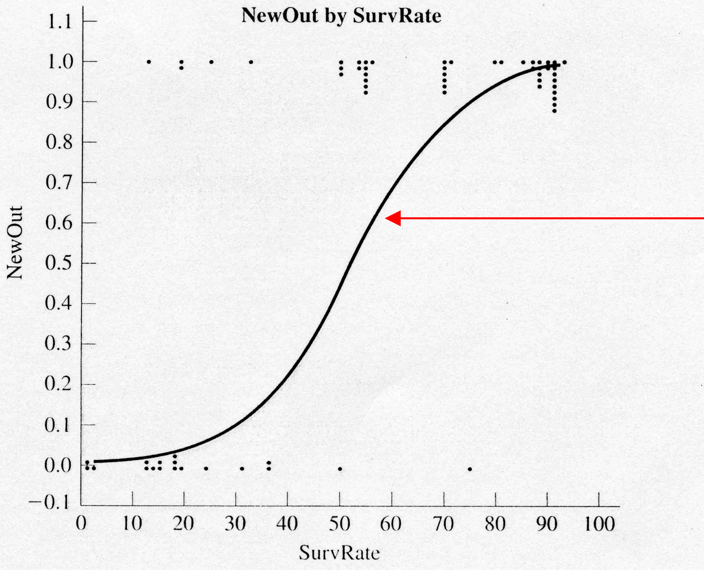


FIGURE 15.8 *More appropriate regression line for predicting outcome*

<u>Regression Curve</u>:
Sigmoid function!

(bounded by asymptotes *y*=0 and *y*=1)

Odds

Given some event with probability *p*, the odds of that event are given by:

$$\text{odds} = p \,/\, (1 - p)$$

Consider the following data

		Delinquent		
		Yes	**No**	**Total**
Testosterone	**Normal**	402	3614	4016
	High	101	345	446
		503	3959	4462

The odds of being delinquent if you are in the Normal group are:

pdelinquent/(1–pdelinquent) = (402/4016) / (1 - (402/4016)) = 0.1001 / 0.8889 = 0.111

Odds Ratio

The odds of being not delinquent in the Normal group is the reciprocal of this:

- 0.8999/0.1001 = 8.99

Now, for the High testosterone group

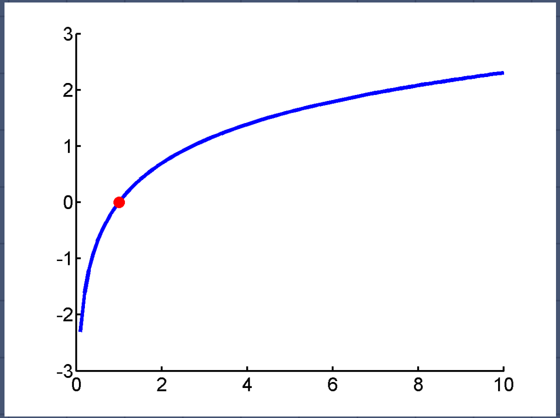
- odds(delinquent) = 101/345 = 0.293
- odds(not delinquent) = 345/101 = 3.416

When we go from Normal to High, the odds of being delinquent nearly triple:

- Odds ratio: 0.293/0.111 = 2.64
- 2.64 times more likely to be delinquent with high testosterone levels

Logit Transform

The logit is the natural log of the odds



logit(p) = ln(odds) = ln (p/(1-p))

Logistic Regression

In logistic regression, we seek a model:

$$\mathrm{logit}(p) = \beta_0 + \beta_1 X$$

That is, the log odds (logit) is assumed to be linearly related to the independent variable X

So, now we can focus on solving an ordinary (linear) regression!

Recovering Probabilities

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

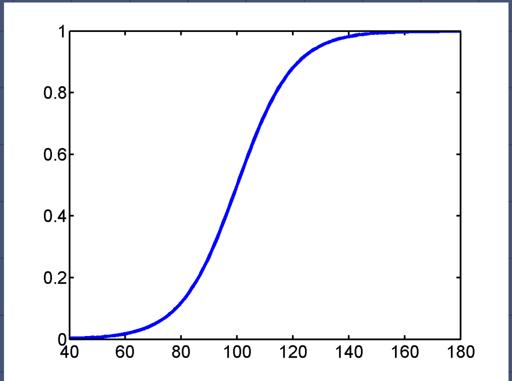
$$\Leftrightarrow \frac{p}{1-p} = e^{\beta_0 + \beta_1 X}$$

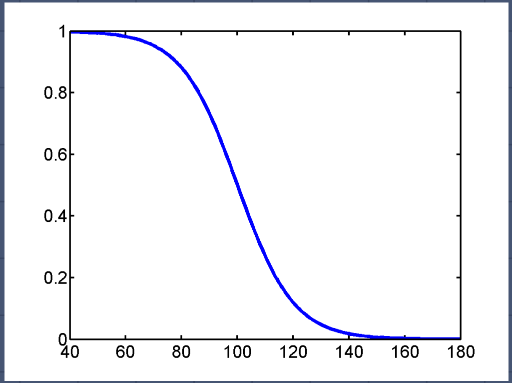
$$\Leftrightarrow p = \frac{e^{\beta_0 + \beta_1 X}}{1 + e^{\beta_0 + \beta_1 X}} = \frac{1}{1 + e^{-(\beta_0 + \beta_1 X)}}$$

which gives *p* as a sigmoid function!

Logistic Response Function

When the response variable is binary, the shape of the response function is often sigmoidal:





Sample Calculations

Suppose a cancer study yields:

- log odds = −2.6837 + 0.0812 SurvRate

Consider a patient with SurvRate = 40

- log odds = −2.6837 + 0.0812(40) = 0.5643
- odds = $e^{0.5643}$ = 1.758
- patient is 1.758 times more likely to be improved than not

Consider another patient with SurvRate = 41

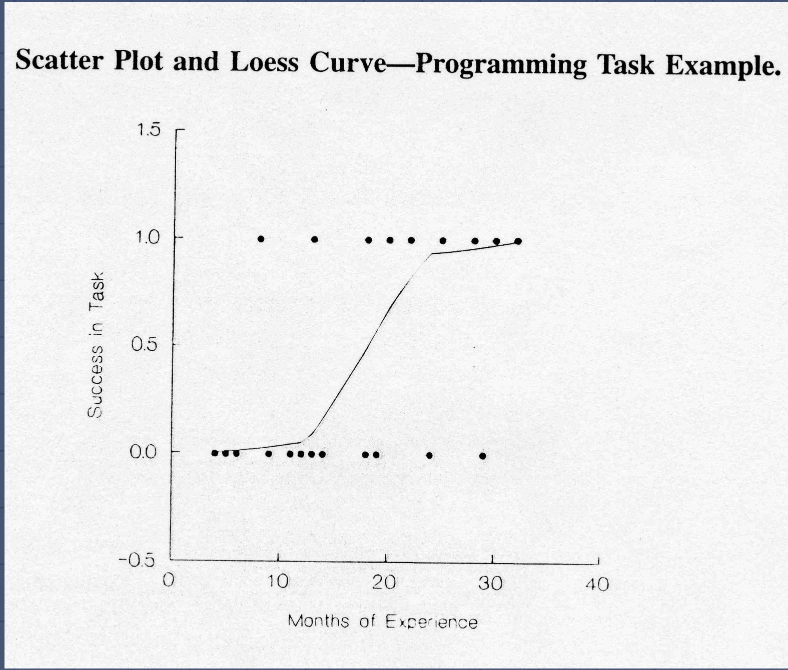
- log odds = −2.6837 + 0.0812(41) = 0.6455
- odds = $e^{0.6455}$ = 1.907
- patient's odds are 1.907/1.758 = 1.0846 times (or 8.5%) better than those of the previous patient

Using probabilities

- p40 = 0.6374 and p41 = 0.6560
- Improvements appear different with odds and with *p*

Example 1 (I)

- A systems analyst studied the effect of computer programming experience on ability to complete a task within a specified time
- Twenty-five persons selected for the study, with varying amounts of computer experience (in months)
- Results are coded in binary fashion: $Y = 1$ if task completed successfully; $Y = 0$, otherwise



Loess: form of local regression

Example 1 (II)

Results from a standard package give:

- β0 = −3.0597 and β1 = 0.1615

Estimated logistic regression function:

$$p = \frac{1}{1 + e^{3.0597 - 0.1615X}}$$

For example, the fitted value for X = 14 is:

$$p = \frac{1}{1 + e^{3.0597 - 0.1615(14)}} = 0.31$$

(Estimated probability that a person with 14 months experience will successfully complete the task)

Example 1 (III)

We know that the probability of success increases sharply with experience

- Odds ratio: exp(β1) = e0.1615 = 1.175
- Odds increase by 17.5% with each additional month of experience

A unit increase of one month is quite small, and we might want to know the change in odds for a longer difference in time

- For c units of X: exp(cβ1)

Example 1 (IV)

Suppose we want to compare individuals with relatively little experience to those with extensive experience, say 10 months versus 25 months (c = 15)

- Odds ratio: e15x0.1615 = 11.3
- Odds of completing the task increase 11-fold!

Example 2 (I)

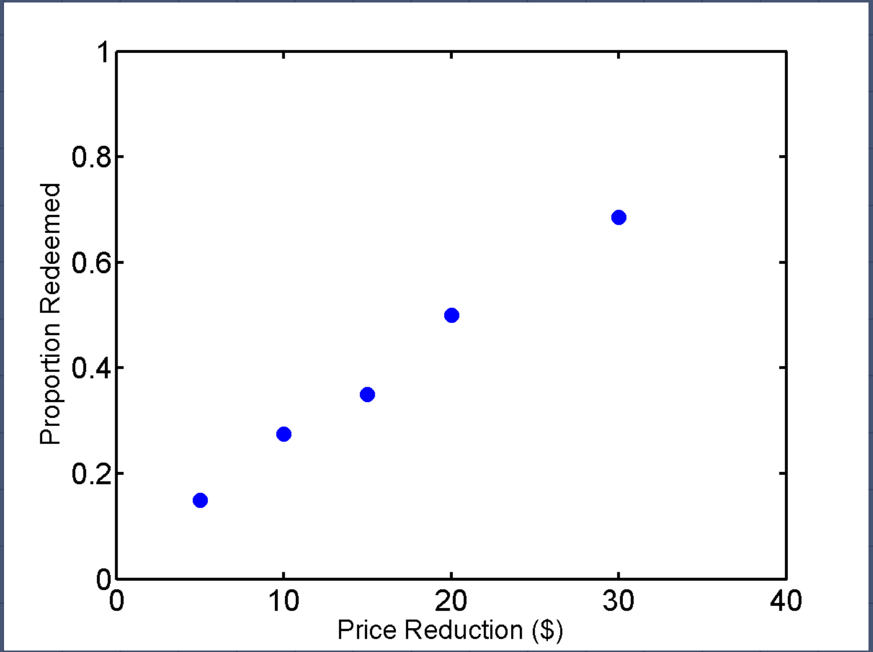
In a study of the effectiveness of coupons offering a price reduction, 1,000 homes were selected and coupons mailed

Coupon price reductions: 5, 10, 15, 20, and 30 dollars

200 homes assigned at random to each coupon value

X: amount of price reduction

Y: binary variable indicating whether or not coupon was redeemed



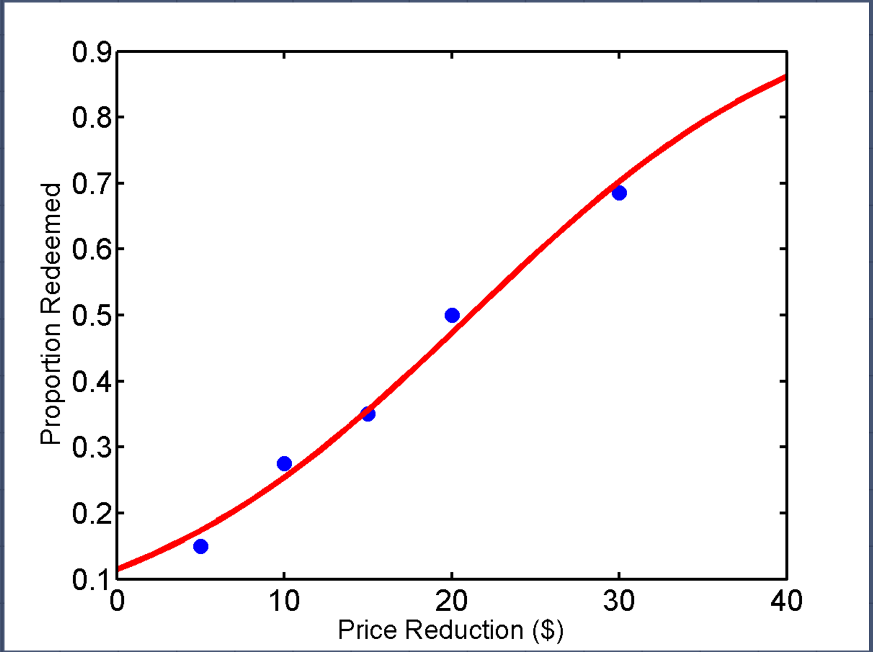
Example 2 (II)

Fitted response function

- $\beta_0 = -2.04$ and $\beta_1 = 0.097$

Odds ratio: $\exp(\beta_1) = e^{0.097} = 1.102$

Odds of a coupon being redeemed are estimated to increase by 10.2% with each $1 increase in the coupon value (i.e., $1 in price reduction)



Putting it to Work

For each value of X, you may not have probability but rather a number of <x,y> pairs from which you can extract frequencies and hence probabilities

- Raw data: <12,0>, <12,1>, <14,0>, <12,1>, <14,1>, <14,1>, <12,0>, <12,0>
- Probability data (p=1, 3rd entry is number of occurrences in raw data): <12, 0.4, 5>, <14, 0.66, 3>
- Odds ratio data…

Coronary Heart Disease (I)

Age Group	Coronary Heart Disease		Total	
	No	Yes		
1	9	1	10	(20-29)
2	13	2	15	(30-34)
3	9	3	12	(35-39)
4	10	5	15	(40-44)
5	7	6	13	(45-49)
6	3	5	8	(50-54)
7	4	13	17	(55-59)
8	2	8	10	(60-69)
Total	57	43	100	

Coronary Heart Disease (II)

Age Group	p(CHD)=1	odds	log odds	#occ
1	0.1000	0.1111	-2.1972	10
2	0.1333	0.1538	-1.8718	15
3	0.2500	0.3333	-1.0986	12
4	0.3333	0.5000	-0.6931	15
5	0.4615	0.8571	-0.1542	13
6	0.6250	1.6667	0.5108	8
7	0.7647	3.2500	1.1787	17
8	0.8000	4.0000	1.3863	10

Coronary Heart Disease (III)

X (AG)	Y (log odds)	X^2	XY	#occ
1	-2.1972	1.0000	-2.1972	10
2	-1.8718	4.0000	-3.7436	15
3	-1.0986	9.0000	-3.2958	12
4	-0.6931	16.0000	-2.7726	15
5	-0.1542	25.0000	-0.7708	13
6	0.5108	36.0000	3.0650	8
7	1.1787	49.0000	8.2506	17
8	1.3863	64.0000	11.0904	10
448	**-37.6471**	**2504.0000**	**106.3981**	**100**

Note: the sums reflect the number of occurrences (Sum(X) = X1.#occ(X1)+…+X8.#occ(X8), etc.)

Coronary Heart Disease (IV)

Results from regression:

- $\beta 0 = -2.856$ and $\beta 1 = 0.5535$

Age Group	p(CHD)=1	est. p
1	0.1000	0.0909
2	0.1333	0.1482
3	0.2500	0.2323
4	0.3333	0.3448
5	0.4615	0.4778
6	0.6250	0.6142
7	0.7647	0.7346
8	0.8000	0.8280

SSE	**0.0028**
TSS	**0.5265**
R2	**0.9946**

Summary

Regression is a powerful data mining technique

- It provides prediction
- It offers insight on the relative power of each variable

We have focused on the case of a single independent variable

- What about the general case?