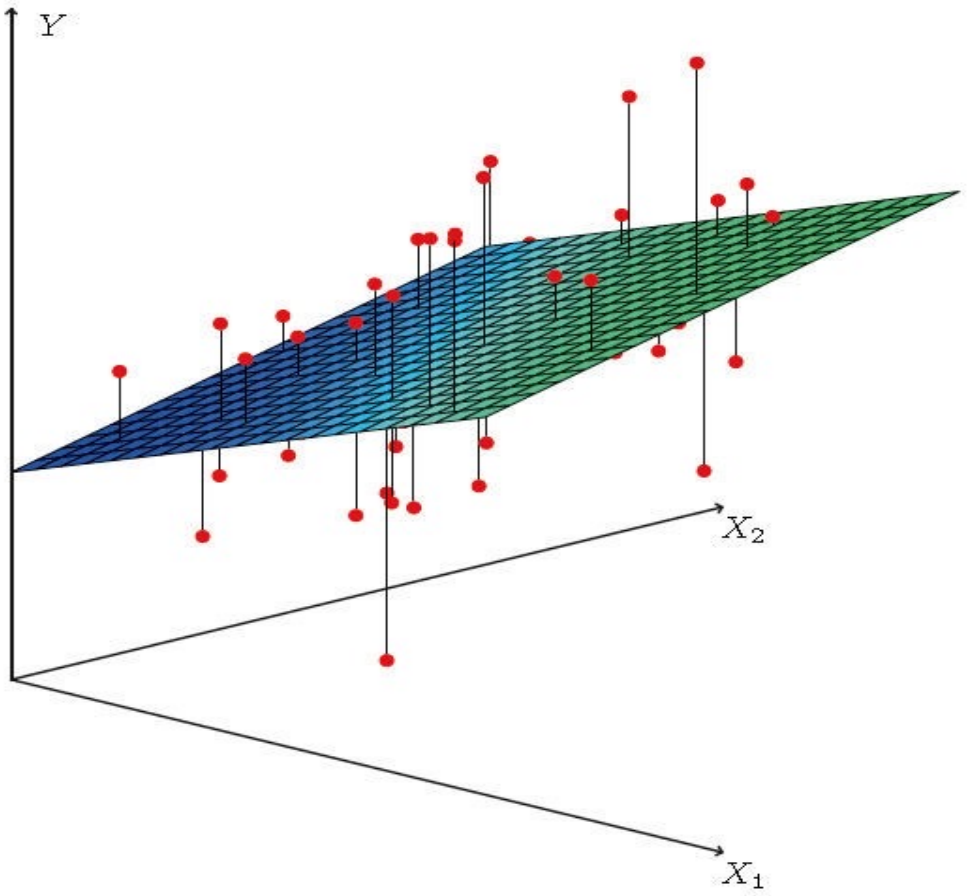
DSCI 552, Machine Learning for Data Science

University of Southern California

M. R. Rajati, PhD

Lesson 2
Linear Regression

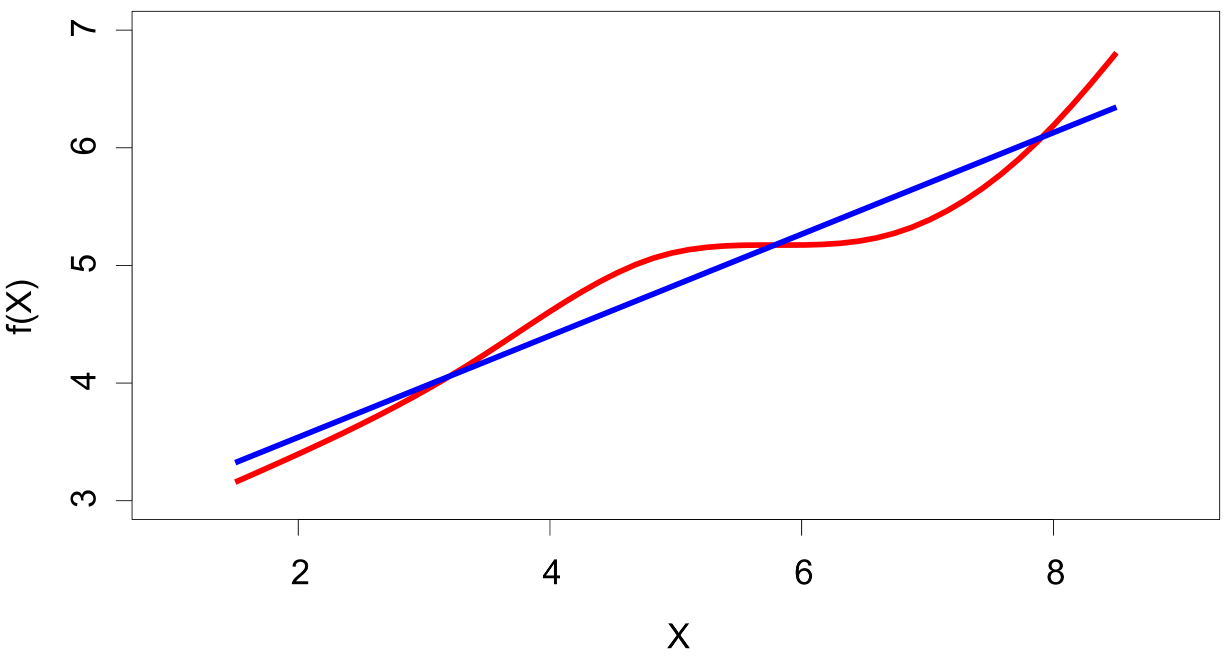


Linear Regression

- Linear regression is a simple approach to supervised learning. It assumes that the dependence of Y on $X_1, X_2, \ldots X_p$ is linear.

Linear regression

- Although it may seem overly simplistic, linear regression is extremely useful both conceptually and practically.



Linear regression for the advertising data

Consider the advertising data shown on the next slide. Questions we might ask:

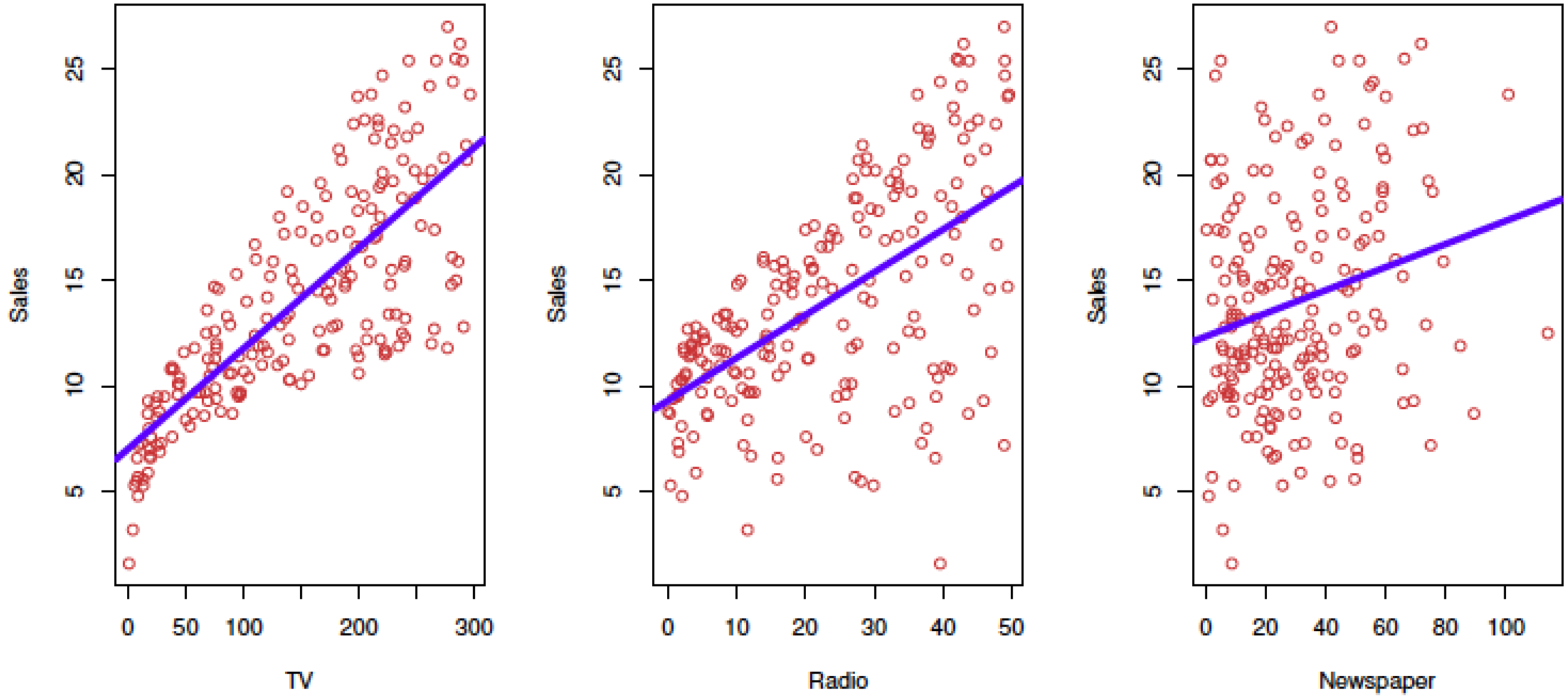
- Is there a relationship between advertising budget and sales?
- How strong is the relationship between advertising budget and sales?

Linear regression for the advertising data

Consider the advertising data shown on the next slide. Questions we might ask:

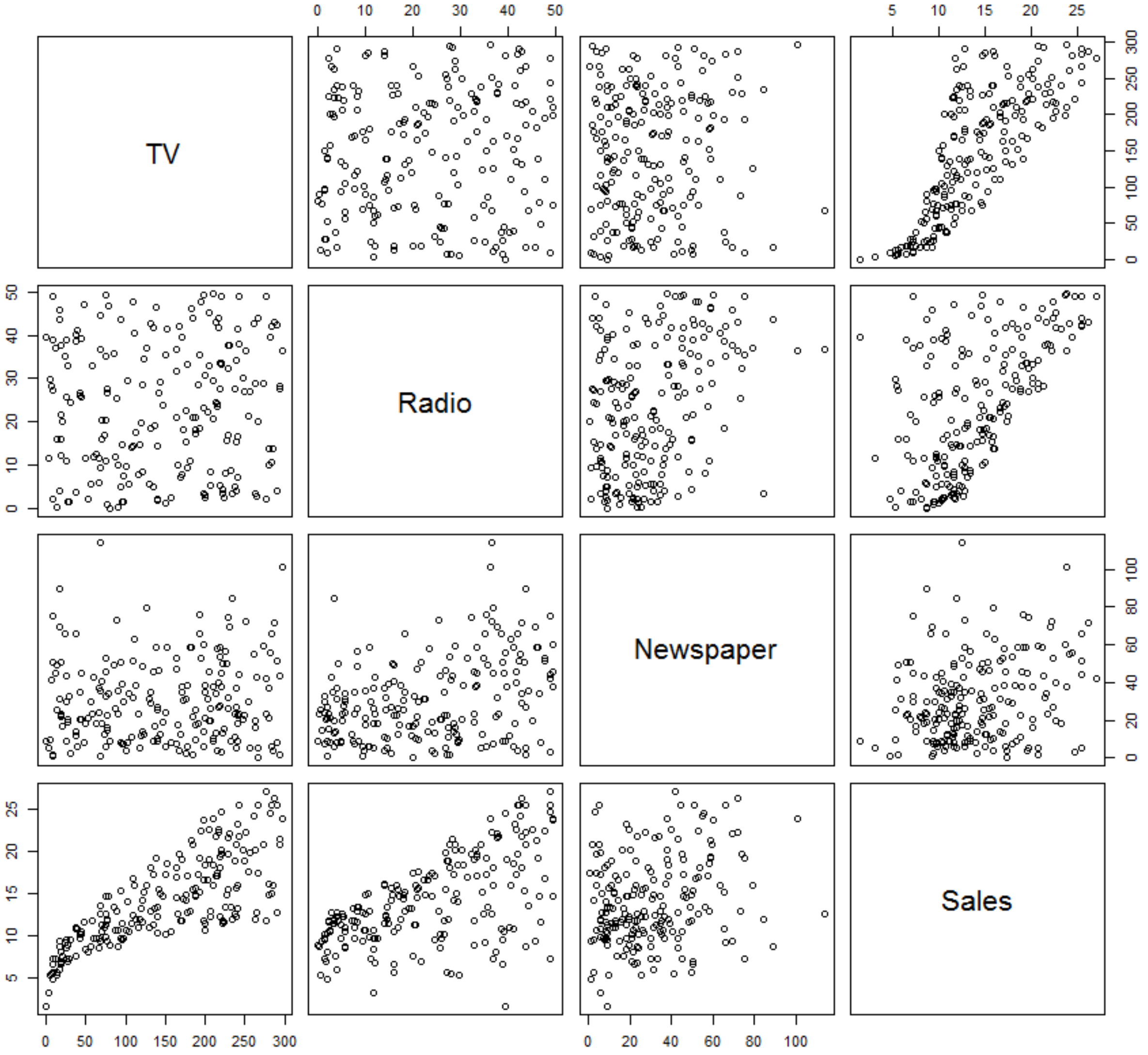
- Which media contribute to sales?
- How accurately can we predict future sales?
- Is the relationship linear?
- Is there synergy among the advertising media?

Advertising data



Case 1: Advertisement Data

```
Advertising=read.csv("http://www-bcf.usc.edu/~gareth/ISL/Advertising.csv", header=TRUE);
newdata=Advertising[,-1]
fix(newdata)
View(newdata)
names(newdata)
pairs(newdata)
```



Simple linear regression using a single predictor *X*.

- *We assume a model*

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

where β_0 and β_1 are two unknown constants that represent the *intercept* and *slope*, also known as *coefficients* or *parameters*, and ε is the error term.

Simple linear regression using a single predictor X.

- Given some estimates $\hat{\beta}_0$ and $\hat{\beta}_1$ for the model coefficients, we predict future sales using

$$\hat{y} = \hat{\beta}_0 + \hat{\beta}_1 x,$$

where $\hat{y}$ indicates a prediction of Y on the basis of $X = x$. The *hat* symbol denotes an estimated value.

Estimation of the parameters by least squares

- Let $\hat{y}_i = \hat{\beta}_0 + \hat{\beta}_1 x_i$ be the prediction for Y based on the ith value of X. Then $e_i = y_i - \hat{y}_i$ represents the i^{th} *residual*

Estimation of the parameters by least squares

- Let $\hat{y}_i = \hat{\beta}_0 + \hat{\beta}_1 x_i$ be the prediction for Y based on the ith value of X. Then $e_i = y_i - \hat{y}_i$ represents the ith residual
- We define the *residual sum of squares* (RSS) as $\mathrm{RSS} = e_1^2 + e_2^2 + \cdots + e_n^2$

or equivalently as

$$\mathrm{RSS} = (y_1 - \hat{\beta}_0 - \hat{\beta}_1 x_1)^2 + (y_2 - \hat{\beta}_0 - \hat{\beta}_1 x_2)^2 + \ldots + (y_n - \hat{\beta}_0 - \hat{\beta}_1 x_n)^2.$$

Normality of ε

- Note that in the following, the statistical results including confidence intervals, hypothesis testing assume that ε is normally distributed with mean zero and standard deviation σ.

Estimation of the parameters by least squares

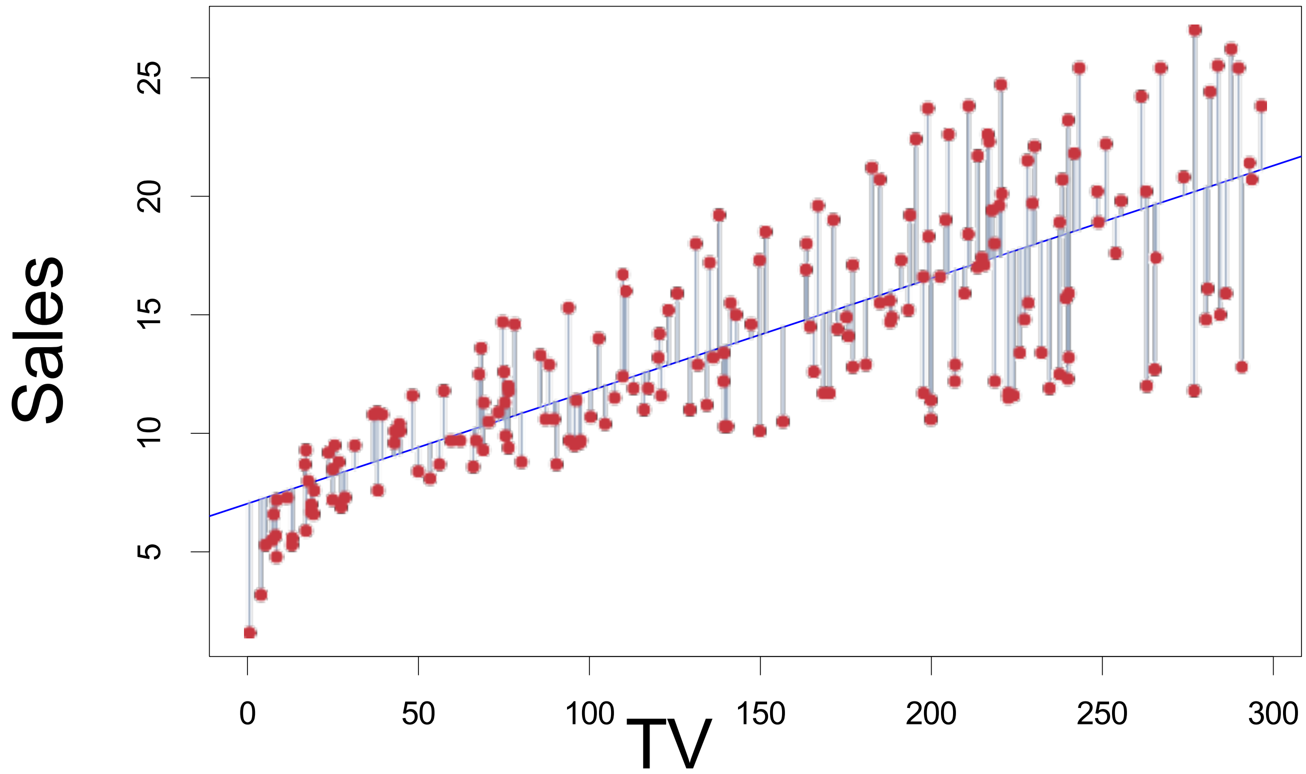
The least squares approach chooses $\hat{\beta}_0$and $\hat{\beta}_1$to minimize the RSS. The minimizing values can be shown to be

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

$$\hat{\beta}_0 = \bar{y} - \hat{\beta}_1 \bar{x},$$

where $\bar{y} \equiv \frac{1}{n}\sum_{i=1}^{n} y_i$ and $\bar{x} \equiv \frac{1}{n}\sum_{i=1}^{n} x_i$ are the sample means.

Example: advertising data



The least squares fit for the regression of `sales` onto `TV`. In this case a linear fit captures the essence of the relationship, although it is somewhat deficient in the left of the plot.

Assessing the Accuracy of the Coefficient Estimates

- The standard error of an estimator reflects how it varies under repeated sampling. We have

$$\mathrm{SE}(\hat{\beta}_1)^2 = \frac{\sigma^2}{\sum_{i=1}^{n}(x_i - \bar{x})^2}, \quad \mathrm{SE}(\hat{\beta}_0)^2 = \sigma^2 \left[\frac{1}{n} + \frac{\bar{x}^2}{\sum_{i=1}^{n}(x_i - \bar{x})^2}\right]$$

where $\sigma^2 = \mathrm{Var}(\varepsilon)$

Assessing the Accuracy of the Coefficient Estimates

- These standard errors can be used to compute confidence intervals. A 95% confidence interval is defined as a range of values such that 95% of times, the range will contain the true unknown value of the parameter. It has the form $\hat{\beta}_1 \pm 2 \cdot \mathrm{SE}(\hat{\beta}_1)$.

Confidence intervals — continued

That is, there is approximately a 95% chance that the interval

$$\left[\hat{\beta}_1 - 2 \cdot \mathrm{SE}(\hat{\beta}_1),\ \hat{\beta}_1 + 2 \cdot \mathrm{SE}(\hat{\beta}_1)\right]$$

will contain the true value of β_1 (under a scenario where we got repeated samples like the present sample)

Confidence intervals — continued

In fact, an interval that will contain the true unknown value of the parameter β_1 in 1-α percent of times is

$$\left[\hat{\beta}_1 - 2 \cdot \mathrm{SE}(\hat{\beta}_1),\ \hat{\beta}_1 + 2 \cdot \mathrm{SE}(\hat{\beta}_1)\right]$$

Approximate CI for 1-α=0.95 (by the textbook)

$$[\hat{\beta}_1 - t_{n-2,\alpha/2}.\,\mathrm{SE}(\hat{\beta}_1), \hat{\beta}_1 + t_{n-2,\alpha/2}.\,\mathrm{S\hat{E}}(\beta_1)]$$

More accurate CI

Student’s t distribution

Student's t-distribution (or simply the t-distribution) is any member of a family of continuous probability distributions that arises when estimating the mean of a normally distributed population in situations where the sample size is small and the population standard deviation is unknown.

Student’s t distribution

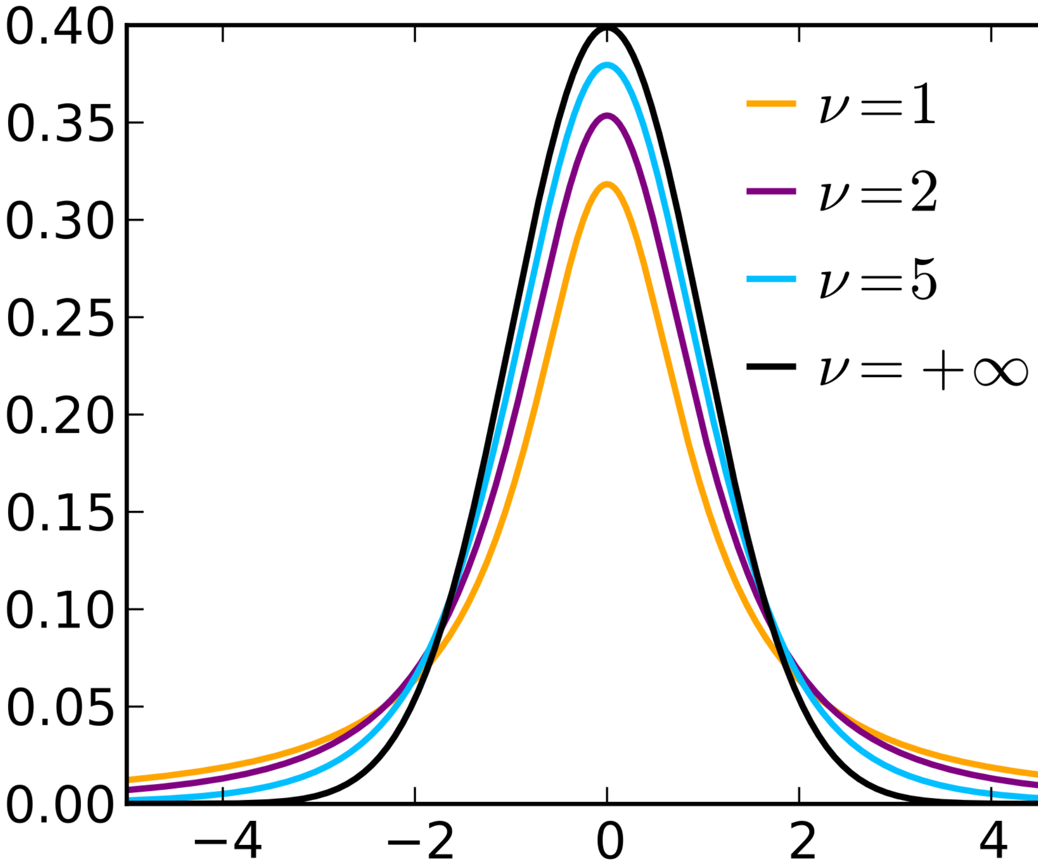
It was developed by William Sealy Gosset under the pseudonym Student.

The family is parameterized by a parameter ν, which is called the degrees of freedom.

The distribution is bell-shaped and has a zero mean, but its tails are heavier than the standard normal distribution.

Student’s t distribution

t



Student's t distribution

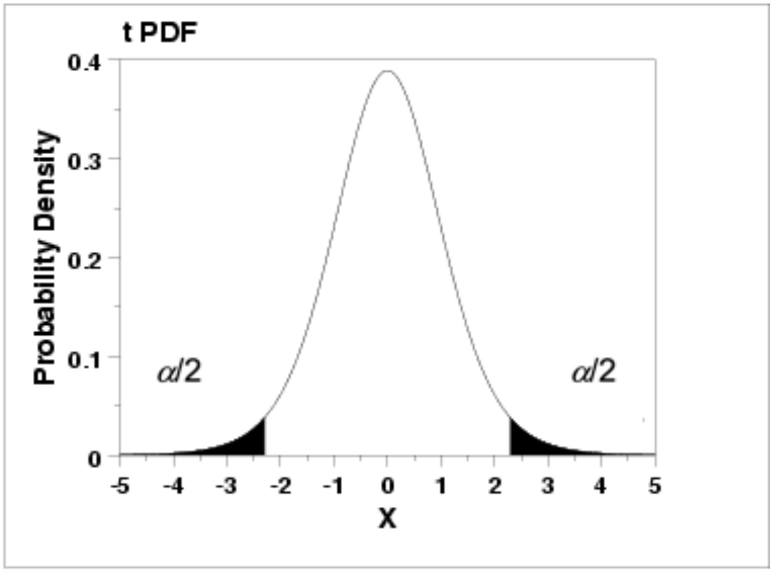
When $\nu \to \infty$, $t_\nu \to Z$, where Z is a standard normal distribution, i.e., a normal distribution with mean zero and standard deviation 1.

Student’s t distribution-cut off points

By $t_{n-2,\alpha/2}$, we mean:

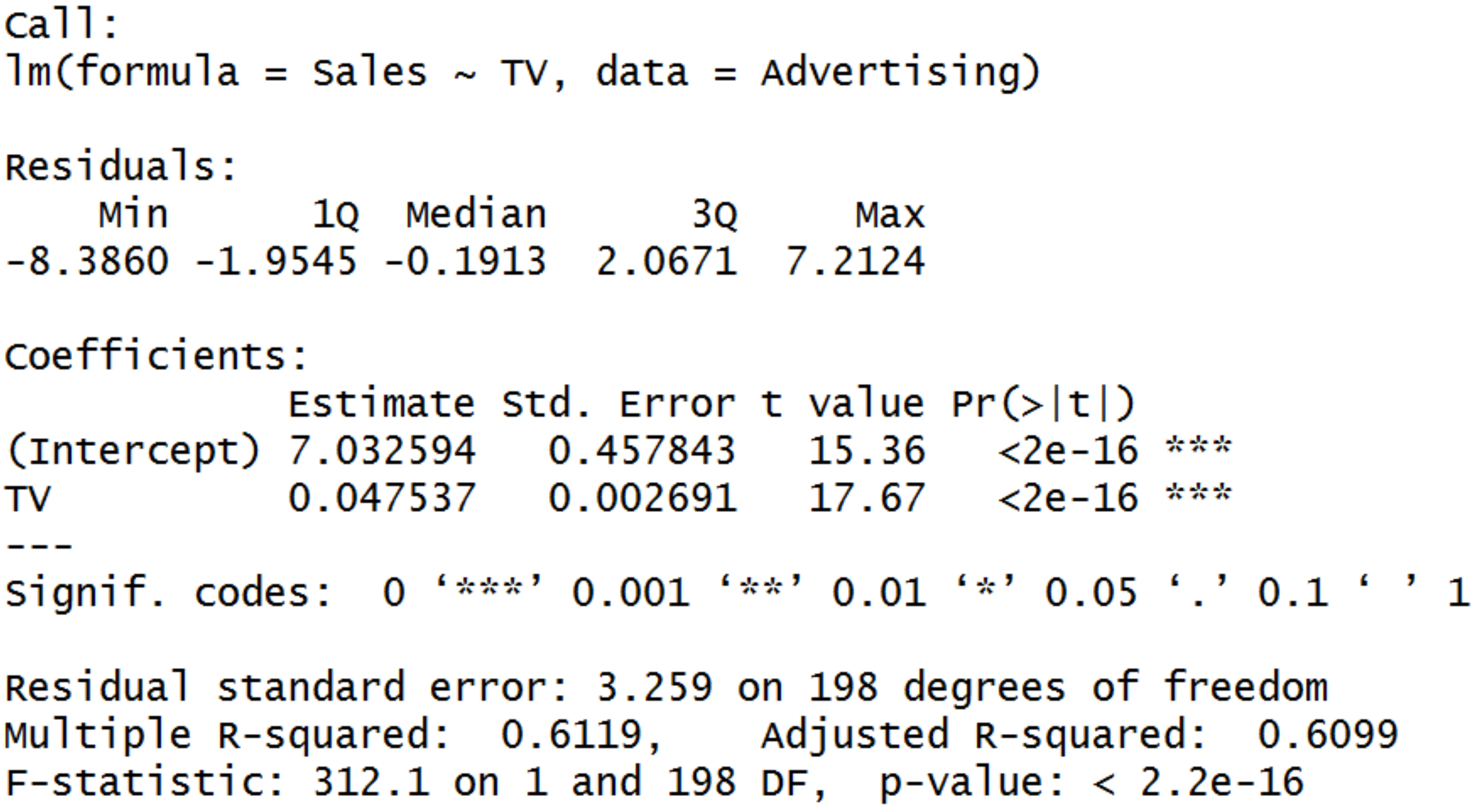
$\Pr(t_{n-2} > t_{n-2,\alpha/2}) = \alpha/2$

In other words, the area under the pdf of the *t* distribution with *n*-2 degrees of freedom is $\alpha/2$ to the right of $t_{n-2,\alpha/2}$.



Advertisement Data for simple linear regression

lm.fit=lm(Sales~TV,data=Advertising) ## to get Table 3.1
summary(lm.fit)
names(lm.fit)
coef(lm.fit)
confint(lm.fit)



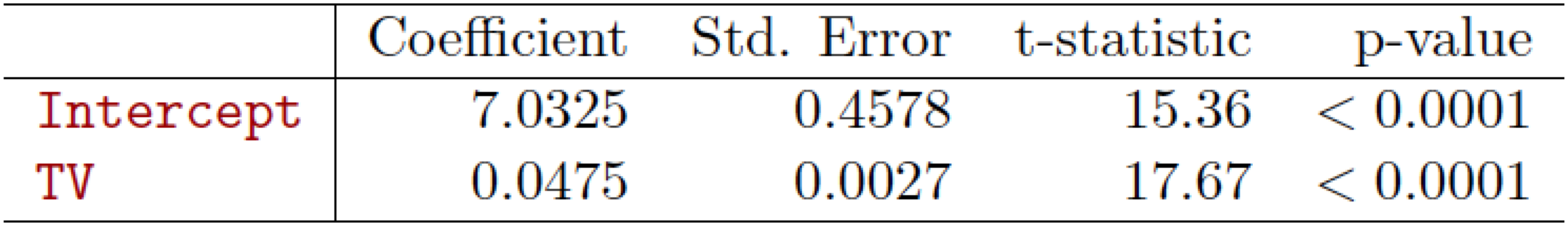
```
Call:
lm(formula = Sales ~ TV, data = Advertising)

Residuals:
    Min      1Q  Median      3Q     Max 
-8.3860 -1.9545 -0.1913  2.0671  7.2124 

Coefficients:
            Estimate Std. Error t value Pr(>|t|)    
(Intercept) 7.032594   0.457843   15.36   <2e-16 ***
TV          0.047537   0.002691   17.67   <2e-16 ***
---
Signif. codes:  0 ‘***’ 0.001 ‘**’ 0.01 ‘*’ 0.05 ‘.’ 0.1 ‘ ’ 1

Residual standard error: 3.259 on 198 degrees of freedom
Multiple R-squared:  0.6119,    Adjusted R-squared:  0.6099 
F-statistic: 312.1 on 1 and 198 DF,  p-value: < 2.2e-16
```

Results for the advertising data



	Coefficient	Std. Error	t-statistic	p-value
Intercept	7.0325	0.4578	15.36	< 0.0001
TV	0.0475	0.0027	17.67	< 0.0001

Confidence intervals — continued

For the advertising data, the 95% confidence interval for β_1 is approximately [0.042, 0.053]

$$\left[\hat{\beta}_1 - 2 \cdot \mathrm{SE}(\hat{\beta}_1),\ \hat{\beta}_1 + 2 \cdot \mathrm{SE}(\hat{\beta}_1)\right]$$

Approximate CI for 1-α=0.95 (by the textbook)

$$[\hat{\beta}_1 - t_{n-2,\alpha/2}.\,\mathrm{SE}(\hat{\beta}_1), \hat{\beta}_1 + t_{n-2,\alpha/2}.\,\mathrm{S\hat{E}}(\beta_1)]$$

More accurate CI

Hypothesis testing

- Standard errors can also be used to perform *hypothesis tests* on the coefficients. The most common hypothesis test involves testing the *null hypothesis* of

  H_0 :There is no relationship between X and Y

  versus the *alternative hypothesis*

  H_A :There is some relationship between X and Y .

Hypothesis testing

- Mathematically, this corresponds to testing

$$H_0 : \beta_1 = 0$$

versus

$$H_A : \beta_1 \neq 0,$$

since if $\beta_1 = 0$ then the model reduces to $Y = \beta_0 + \varepsilon$, and X is not associated with Y.

Hypothesis testing — continued

- To test the null hypothesis, we compute a *t-statistic*, given by

$$t = \frac{\hat{\beta}_1 - 0}{\mathrm{SE}(\hat{\beta}_1)}$$

- This will have a *t*-distribution with $n - 2$ degrees of freedom, assuming $\beta_1 = 0$.

Hypothesis testing — continued

- If the null hypothesis is true, the probability of observing $t > t_{n-2,\alpha/2}$or $t < t_{n-2,\alpha/2}$ would be *α*. *α* is the probability of rejecting a true null hypothesis, i.e. a *Type-I error*, and should be set ahead of time (metaphorically, by your boss). Why? Usually, *α* is selected to be 5%.

Rejection Region Approach

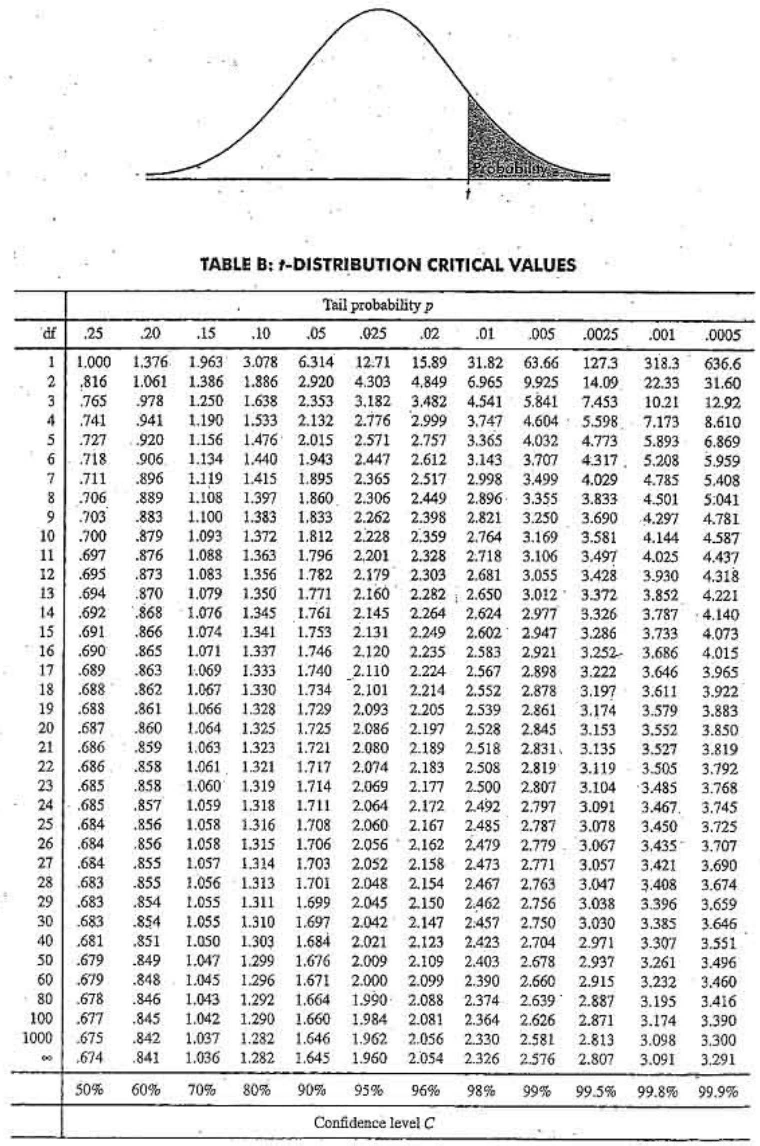


TABLE B: t-DISTRIBUTION CRITICAL VALUES

	Tail probability p											
df	.25	.20	.15	.10	.05	.025	.02	.01	.005	.0025	.001	.0005
1	1.000	1.376	1.963	3.078	6.314	12.71	15.89	31.82	63.66	127.3	318.3	636.6
2	.816	1.061	1.386	1.886	2.920	4.303	4.849	6.965	9.925	14.09	22.33	31.60
3	.765	.978	1.250	1.638	2.353	3.182	3.482	4.541	5.841	7.453	10.21	12.92
4	.741	.941	1.190	1.533	2.132	2.776	2.999	3.747	4.604	5.598	7.173	8.610
5	.727	.920	1.156	1.476	2.015	2.571	2.757	3.365	4.032	4.773	5.893	6.869
6	.718	.906	1.134	1.440	1.943	2.447	2.612	3.143	3.707	4.317	5.208	5.959
7	.711	.896	1.119	1.415	1.895	2.365	2.517	2.998	3.499	4.029	4.785	5.408
8	.706	.889	1.108	1.397	1.860	2.306	2.449	2.896	3.355	3.833	4.501	5.041
9	.703	.883	1.100	1.383	1.833	2.262	2.398	2.821	3.250	3.690	4.297	4.781
10	.700	.879	1.093	1.372	1.812	2.228	2.359	2.764	3.169	3.581	4.144	4.587
11	.697	.876	1.088	1.363	1.796	2.201	2.328	2.718	3.106	3.497	4.025	4.437
12	.695	.873	1.083	1.356	1.782	2.179	2.303	2.681	3.055	3.428	3.930	4.318
13	.694	.870	1.079	1.350	1.771	2.160	2.282	2.650	3.012	3.372	3.852	4.221
14	.692	.868	1.076	1.345	1.761	2.145	2.264	2.624	2.977	3.326	3.787	4.140
15	.691	.866	1.074	1.341	1.753	2.131	2.249	2.602	2.947	3.286	3.733	4.073
16	.690	.865	1.071	1.337	1.746	2.120	2.235	2.583	2.921	3.252	3.686	4.015
17	.689	.863	1.069	1.333	1.740	2.110	2.224	2.567	2.898	3.222	3.646	3.965
18	.688	.862	1.067	1.330	1.734	2.101	2.214	2.552	2.878	3.197	3.611	3.922
19	.688	.861	1.066	1.328	1.729	2.093	2.205	2.539	2.861	3.174	3.579	3.883
20	.687	.860	1.064	1.325	1.725	2.086	2.197	2.528	2.845	3.153	3.552	3.850
21	.686	.859	1.063	1.323	1.721	2.080	2.189	2.518	2.831	3.135	3.527	3.819
22	.686	.858	1.061	1.321	1.717	2.074	2.183	2.508	2.819	3.119	3.505	3.792
23	.685	.858	1.060	1.319	1.714	2.069	2.177	2.500	2.807	3.104	3.485	3.768
24	.685	.857	1.059	1.318	1.711	2.064	2.172	2.492	2.797	3.091	3.467	3.745
25	.684	.856	1.058	1.316	1.708	2.060	2.167	2.485	2.787	3.078	3.450	3.725
26	.684	.856	1.058	1.315	1.706	2.056	2.162	2.479	2.779	3.067	3.435	3.707
27	.684	.855	1.057	1.314	1.703	2.052	2.158	2.473	2.771	3.057	3.421	3.690
28	.683	.855	1.056	1.313	1.701	2.048	2.154	2.467	2.763	3.047	3.408	3.674
29	.683	.854	1.055	1.311	1.699	2.045	2.150	2.462	2.756	3.038	3.396	3.659
30	.683	.854	1.055	1.310	1.697	2.042	2.147	2.457	2.750	3.030	3.385	3.646
40	.681	.851	1.050	1.303	1.684	2.021	2.123	2.423	2.704	2.971	3.307	3.551
50	.679	.849	1.047	1.299	1.676	2.009	2.109	2.403	2.678	2.937	3.261	3.496
60	.679	.848	1.045	1.296	1.671	2.000	2.099	2.390	2.660	2.915	3.232	3.460
80	.678	.846	1.043	1.292	1.664	1.990	2.088	2.374	2.639	2.887	3.195	3.416
100	.677	.845	1.042	1.290	1.660	1.984	2.081	2.364	2.626	2.871	3.174	3.390
1000	.675	.842	1.037	1.282	1.646	1.962	2.056	2.330	2.581	2.813	3.098	3.300
∞	.674	.841	1.036	1.282	1.645	1.960	2.054	2.326	2.576	2.807	3.091	3.291
	50%	60%	70%	80%	90%	95%	96%	98%	99%	99.5%	99.8%	99.9%
	Confidence level C											

Rejection Region Approach

Rejection Region Approach

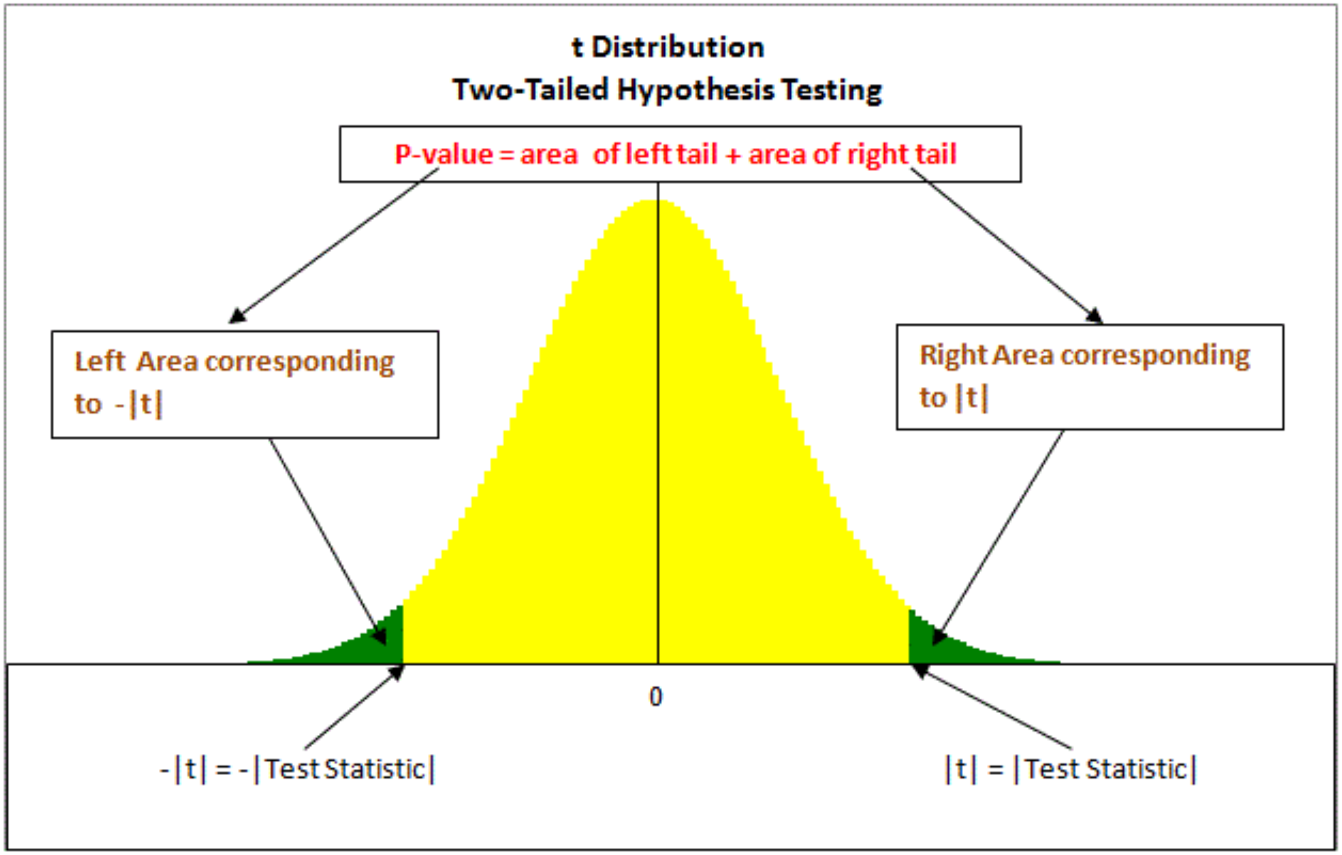
Hypothesis testing — continued

- Using statistical software, it is easy to compute the probability of observing any value equal to |*t*| or larger. We call this probability the *p-value*.

$$t = \frac{\hat{\beta}_1 - 0}{\mathrm{SE}(\hat{\beta}_1)}$$

Hypothesis testing — continued

- We call this probability the *p-value*.



Hypothesis testing — continued

- If the p-value is very small, it means that the probability of seeing a *t* statistic extremer than what was observed assuming that $\beta_1 = 0$ is very small. So we reject the null.

Advertisement Data for simple linear regression

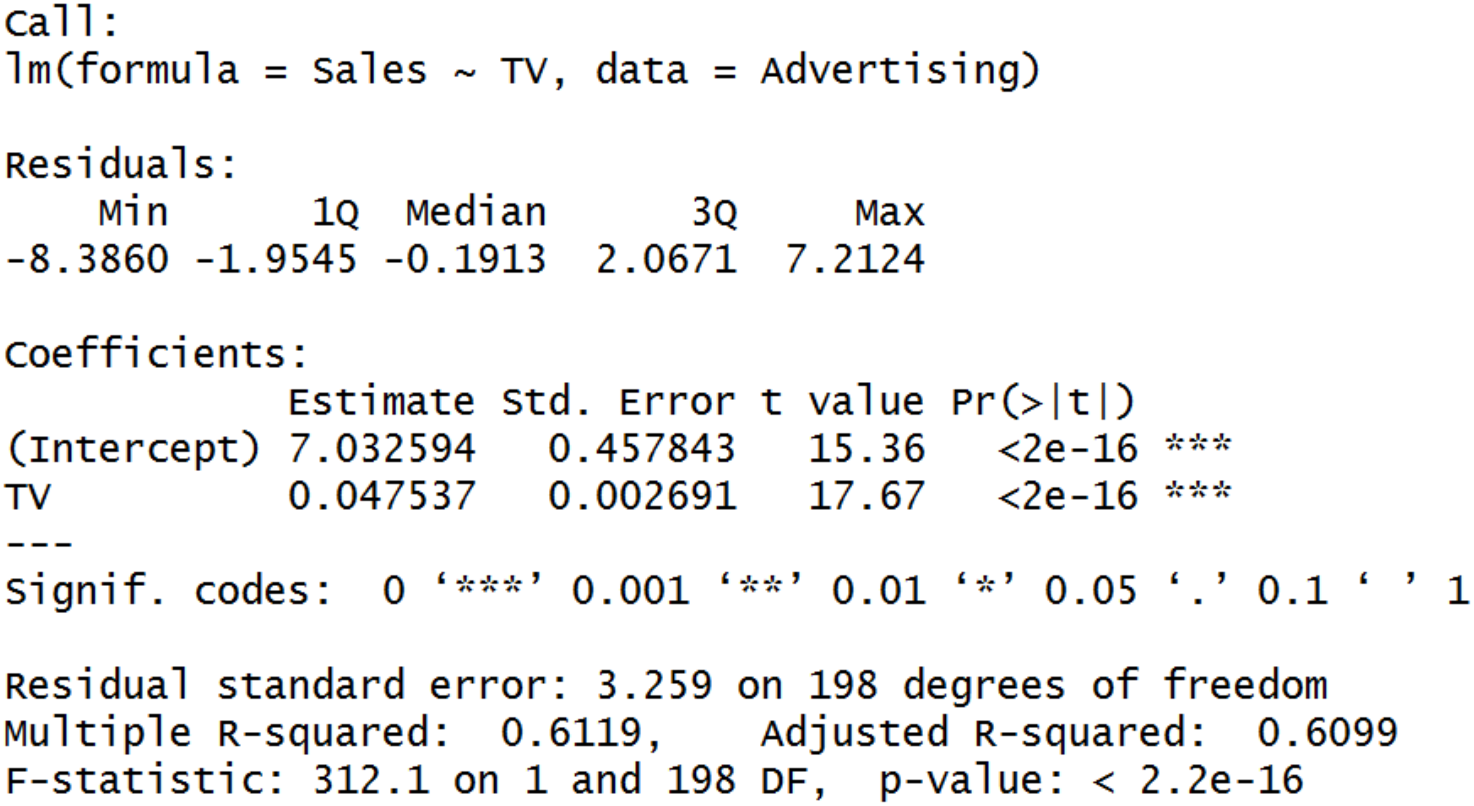
lm.fit=lm(Sales~TV,data=Advertising) ## to get Table 3.1

summary(lm.fit)

names(lm.fit)

coef(lm.fit)

confint(lm.fit)



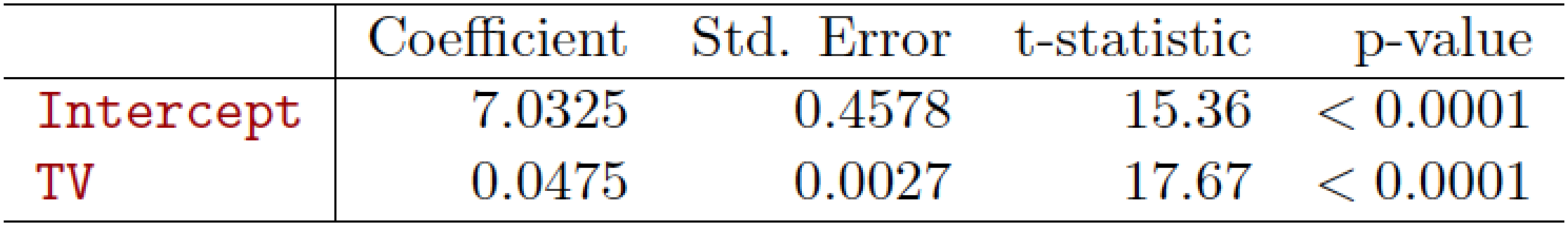
```
Call:
lm(formula = Sales ~ TV, data = Advertising)

Residuals:
    Min      1Q  Median      3Q     Max 
-8.3860 -1.9545 -0.1913  2.0671  7.2124 

Coefficients:
            Estimate Std. Error t value Pr(>|t|)    
(Intercept) 7.032594   0.457843   15.36   <2e-16 ***
TV          0.047537   0.002691   17.67   <2e-16 ***
---
Signif. codes:  0 ‘***’ 0.001 ‘**’ 0.01 ‘*’ 0.05 ‘.’ 0.1 ‘ ’ 1

Residual standard error: 3.259 on 198 degrees of freedom
Multiple R-squared:  0.6119,    Adjusted R-squared:  0.6099 
F-statistic: 312.1 on 1 and 198 DF,  p-value: < 2.2e-16
```

Results for the advertising data



	Coefficient	Std. Error	t-statistic	p-value
`Intercept`	7.0325	0.4578	15.36	< 0.0001
`TV`	0.0475	0.0027	17.67	< 0.0001

Inferences about the Slope: t Test Example

$$t = \frac{\hat{\beta}_1 - 0}{\mathrm{SE}(\hat{\beta}_1)}$$

Test Statistic: **t = 17.76**

From Software output:

$\hat{\beta}_1$ $SE(\hat{\beta}_1)$ t

	Coefficients	***Standard Error***	***t Stat***	***P-value***
Intercept	**7.0325**	**0.4578**	**15.36**	**<0.0001**
TV	**.0475**	**0.0027**	**17.67**	**<0.0001**

H_0: $\beta_1 = 0$

H_1: $\beta_1 \neq 0$

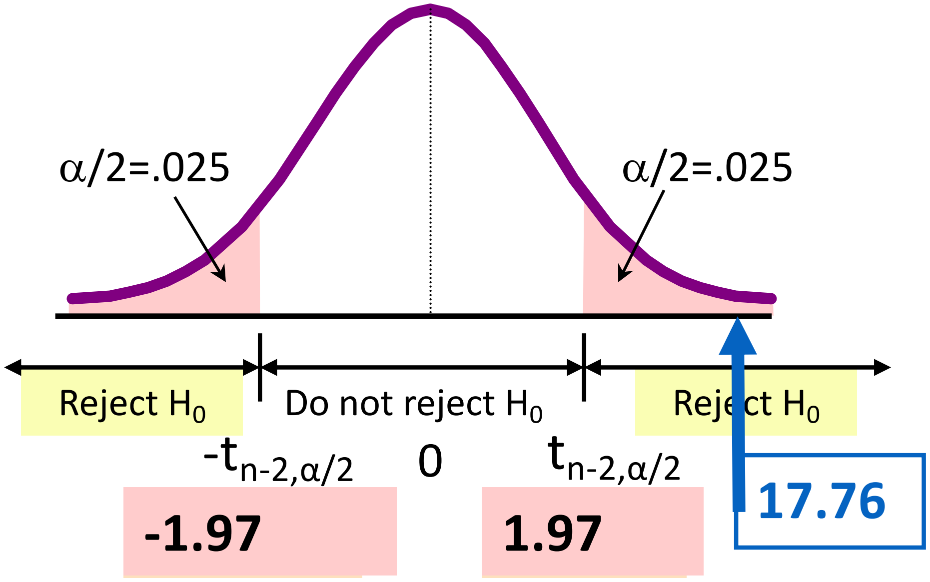
Inferences about the Slope: t Test Example

$H_0: \beta_1 = 0$
$H_1: \beta_1 \neq 0$

d.f. = n-2 = 198

$t_{198,.025} = 1.97$

Test Statistic: **$t = 17.76$**

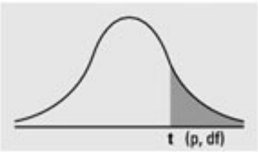


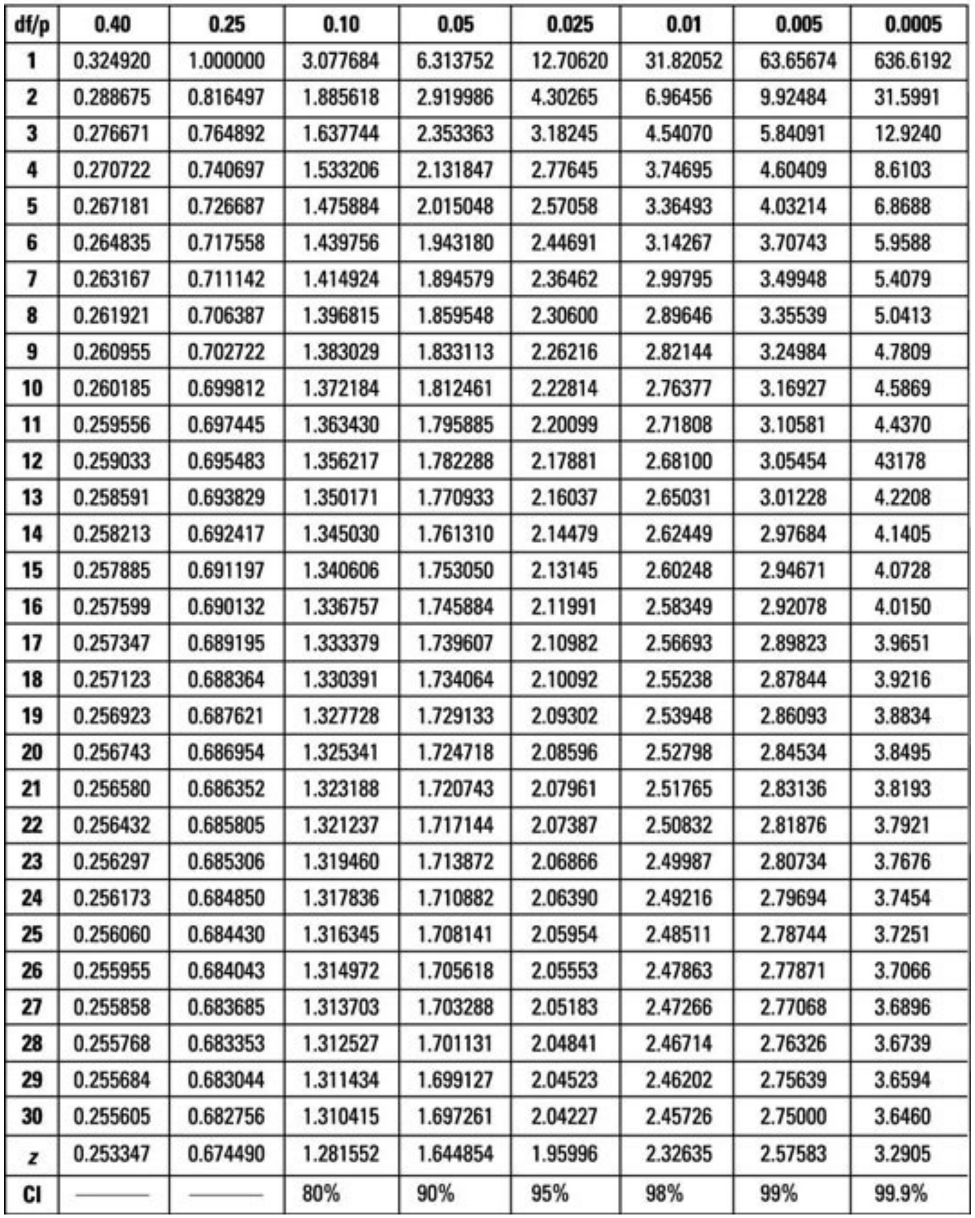
Decision:
Reject H_0

Conclusion:

There is sufficient evidence that TV affects sales

Numbers in each row of the table are values on a *t*-distribution with (*df*) degrees of freedom for selected right-tail (greater-than) probabilities (*p*).





df/p	0.40	0.25	0.10	0.05	0.025	0.01	0.005	0.0005
1	0.324920	1.000000	3.077684	6.313752	12.70620	31.82052	63.65674	636.6192
2	0.288675	0.816497	1.885618	2.919986	4.30265	6.96456	9.92484	31.5991
3	0.276671	0.764892	1.637744	2.353363	3.18245	4.54070	5.84091	12.9240
4	0.270722	0.740697	1.533206	2.131847	2.77645	3.74695	4.60409	8.6103
5	0.267181	0.726687	1.475884	2.015048	2.57058	3.36493	4.03214	6.8688
6	0.264835	0.717558	1.439756	1.943180	2.44691	3.14267	3.70743	5.9588
7	0.263167	0.711142	1.414924	1.894579	2.36462	2.99795	3.49948	5.4079
8	0.261921	0.706387	1.396815	1.859548	2.30600	2.89646	3.35539	5.0413
9	0.260955	0.702722	1.383029	1.833113	2.26216	2.82144	3.24984	4.7809
10	0.260185	0.699812	1.372184	1.812461	2.22814	2.76377	3.16927	4.5869
11	0.259556	0.697445	1.363430	1.795885	2.20099	2.71808	3.10581	4.4370
12	0.259033	0.695483	1.356217	1.782288	2.17881	2.68100	3.05454	43178
13	0.258591	0.693829	1.350171	1.770933	2.16037	2.65031	3.01228	4.2208
14	0.258213	0.692417	1.345030	1.761310	2.14479	2.62449	2.97684	4.1405
15	0.257885	0.691197	1.340606	1.753050	2.13145	2.60248	2.94671	4.0728
16	0.257599	0.690132	1.336757	1.745884	2.11991	2.58349	2.92078	4.0150
17	0.257347	0.689195	1.333379	1.739607	2.10982	2.56693	2.89823	3.9651
18	0.257123	0.688364	1.330391	1.734064	2.10092	2.55238	2.87844	3.9216
19	0.256923	0.687621	1.327728	1.729133	2.09302	2.53948	2.86093	3.8834
20	0.256743	0.686954	1.325341	1.724718	2.08596	2.52798	2.84534	3.8495
21	0.256580	0.686352	1.323188	1.720743	2.07961	2.51765	2.83136	3.8193
22	0.256432	0.685805	1.321237	1.717144	2.07387	2.50832	2.81876	3.7921
23	0.256297	0.685306	1.319460	1.713872	2.06866	2.49987	2.80734	3.7676
24	0.256173	0.684850	1.317836	1.710882	2.06390	2.49216	2.79694	3.7454
25	0.256060	0.684430	1.316345	1.708141	2.05954	2.48511	2.78744	3.7251
26	0.255955	0.684043	1.314972	1.705618	2.05553	2.47863	2.77871	3.7066
27	0.255858	0.683685	1.313703	1.703288	2.05183	2.47266	2.77068	3.6896
28	0.255768	0.683353	1.312527	1.701131	2.04841	2.46714	2.76326	3.6739
29	0.255684	0.683044	1.311434	1.699127	2.04523	2.46202	2.75639	3.6594
30	0.255605	0.682756	1.310415	1.697261	2.04227	2.45726	2.75000	3.6460
z	0.253347	0.674490	1.281552	1.644854	1.95996	2.32635	2.57583	3.2905
CI	———	———	80%	90%	95%	98%	99%	99.9%

Assessing the Overall Accuracy of the Model

- We compute the *Residual Standard Error*

$$\mathrm{RSE} = \sqrt{\frac{1}{n-2}\mathrm{RSS}} = \sqrt{\frac{1}{n-2}\sum_{i=1}^{n}(y_i - \hat{y}_i)^2},$$

where the *residual sum-of-squares* is $RSS = \sum_{i=1}^{n}(y_i - \hat{y}_i)^2$

Assessing the Overall Accuracy of the Model

- The *Residual Standard Error* is used to estimate the variance of the noise ε, i.e. to measure how much on average the response deviated from the regression line.

$$\mathrm{RSE} = \sqrt{\frac{1}{n-2}\mathrm{RSS}} = \sqrt{\frac{1}{n-2}\sum_{i=1}^{n}(y_i - \hat{y}_i)^2},$$

Explanatory Power of a Linear Regression Equation

Total variation is made up of two parts:

$$\text{TSS} = \text{Regression SS} + \text{RSS}$$

Total Sum of Squares

Regression Sum of Squares

Error (residual) Sum of Squares

$$= \sum (y_i - \bar{y})^2$$

$$= \sum (\hat{y}_i - \bar{y})^2$$

$$= \sum (y_i - \hat{y}_i)^2$$

where:

$\bar{y}$ = Average value of the dependent variable

y_i = Observed values of the dependent variable

$\hat{y}_i$ = Predicted value of y for the given x_i value

Explanatory Power of a Linear Regression Equation

TSS = total sum of squares

Measures the variation of the y_i values around their mean, $\bar{y}$

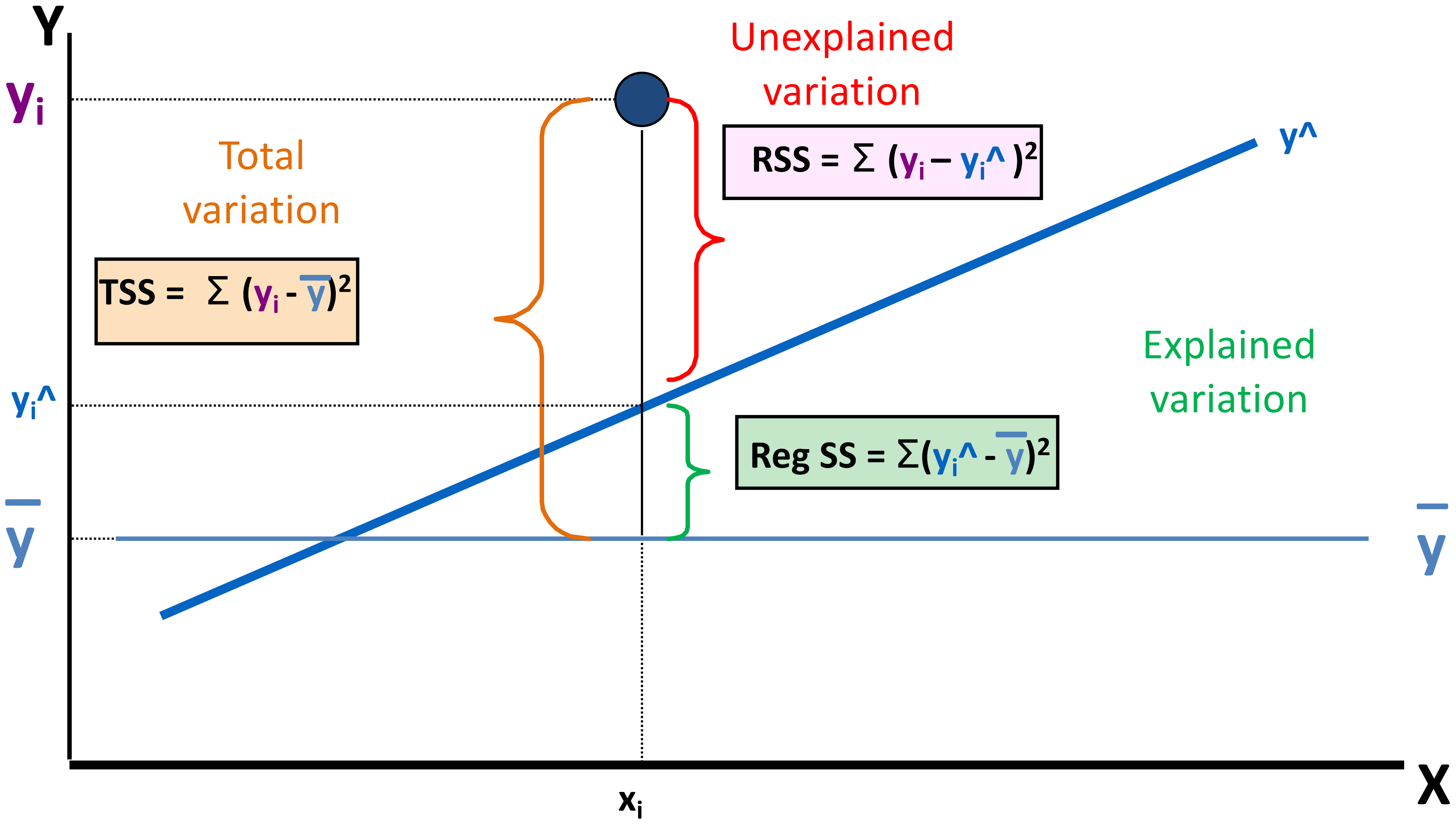
Regression SS = regression sum of squares

Explained variation attributable to the linear relationship between *X* and *Y*

RSS = Residual (error) sum of squares

Variation attributable to factors other than the linear relationship between *X* and *Y*

Explanatory Power of a Linear Regression Equation



Unexplained variation

RSS = $\Sigma\ (y_i - y_i\text{^})^2$

Total variation

TSS = $\Sigma\ (y_i - \bar{y})^2$

Explained variation

Reg SS = $\Sigma(y_i\text{^} - \bar{y})^2$

Assessing the Overall Accuracy of the Model

- We are interested in the ratio of variation explained to total variation, i.e.
- $$\frac{RegSS}{TSS} = -$$

Assessing the Overall Accuracy of the Model

- *R-squared* or fraction of total variation explained is

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

where $\mathrm{TSS} = \sum_{i=1}^{n}(y_i - \bar{y})^2$ is the *total sum of squares*.

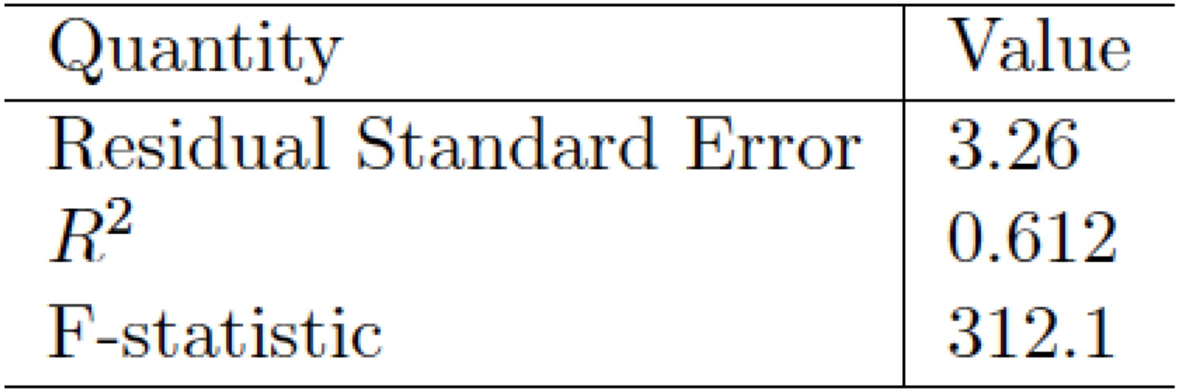
Assessing the Overall Accuracy of the Model

- It can be shown that in this simple linear regression setting that $R^2 = r^2$, where *r* is the correlation between *X* and *Y*:

$$r = \frac{\sum_{i=1}^{n}(x_i - \overline{x})(y_i - \overline{y})}{\sqrt{\sum_{i=1}^{n}(x_i - \overline{x})^2}\sqrt{\sum_{i=1}^{n}(y_i - \overline{y})^2}}.$$

$$= \frac{S_{XY}}{S_X S_Y}$$

Advertising data results



Quantity	Value
Residual Standard Error	3.26
R^2	0.612
F-statistic	312.1

Multiple Linear Regression

- Here our model is

$$Y = \beta_0 + \beta_1 X_1 + \beta_2 X_2 + \cdots + \beta_p X_p + \varepsilon,$$

- We interpret β_j as the average effect on Y of a one unit increase in X_j , holding all other predictors fixed. In the advertising example, the model becomes

$$\text{sales} = \beta_0 + \beta_1 \times \text{TV} + \beta_2 \times \text{radio} + \beta_3 \times \text{newspaper} + \varepsilon.$$

Interpreting regression coefficients

- The ideal scenario is when the predictors are uncorrelated — a *balanced design*:
  - Each coefficient can be estimated and tested separately.
  - Interpretations such as *“a unit change in X_j is associated with a β_j change in Y on average, while all the other variables stay fixed”*, are possible.

Interpreting regression coefficients

- Correlations amongst predictors cause problems:
  - The variance of all coefficients tends to increase, sometimes dramatically
  - Interpretations become hazardous — when X_j changes, everything else changes.

Interpreting regression coefficients

- ***Claims of causality*** **should be avoided for observational data.**

The woes of (interpreting) regression coefficients

"Data Analysis and Regression"
Mosteller and Tukey 1977

- a regression coefficient β_j estimates the expected change in Y per unit change in X_j, *with all other predictors held fixed*. But predictors usually change together!

The woes of (interpreting) regression coefficients

- Example: Y total amount of change in your pocket;
  X_1 = # of coins; X_2 = # of pennies, nickels and dimes.
  By itself, regression coefficient of Y on X_2 will be > 0. But how about with X_1 in model?

The woes of (interpreting) regression coefficients

- Y = number of tackles by a football player in a season; W and H are his weight and height.
- Fitted regression model is $\hat{Y} = b_0 + 0.50W - 0.10H$. How do we interpret $\hat{\beta}_2 < 0$?

Two quotes by famous Statisticians

“Essentially, all models are wrong, but some are useful”

George Box

Two quotes by famous Statisticians

“The only way to find out what will happen when a complex system is disturbed is to disturb the system, not merely to observe it passively”

Fred Mosteller and John Tukey, paraphrasing George Box

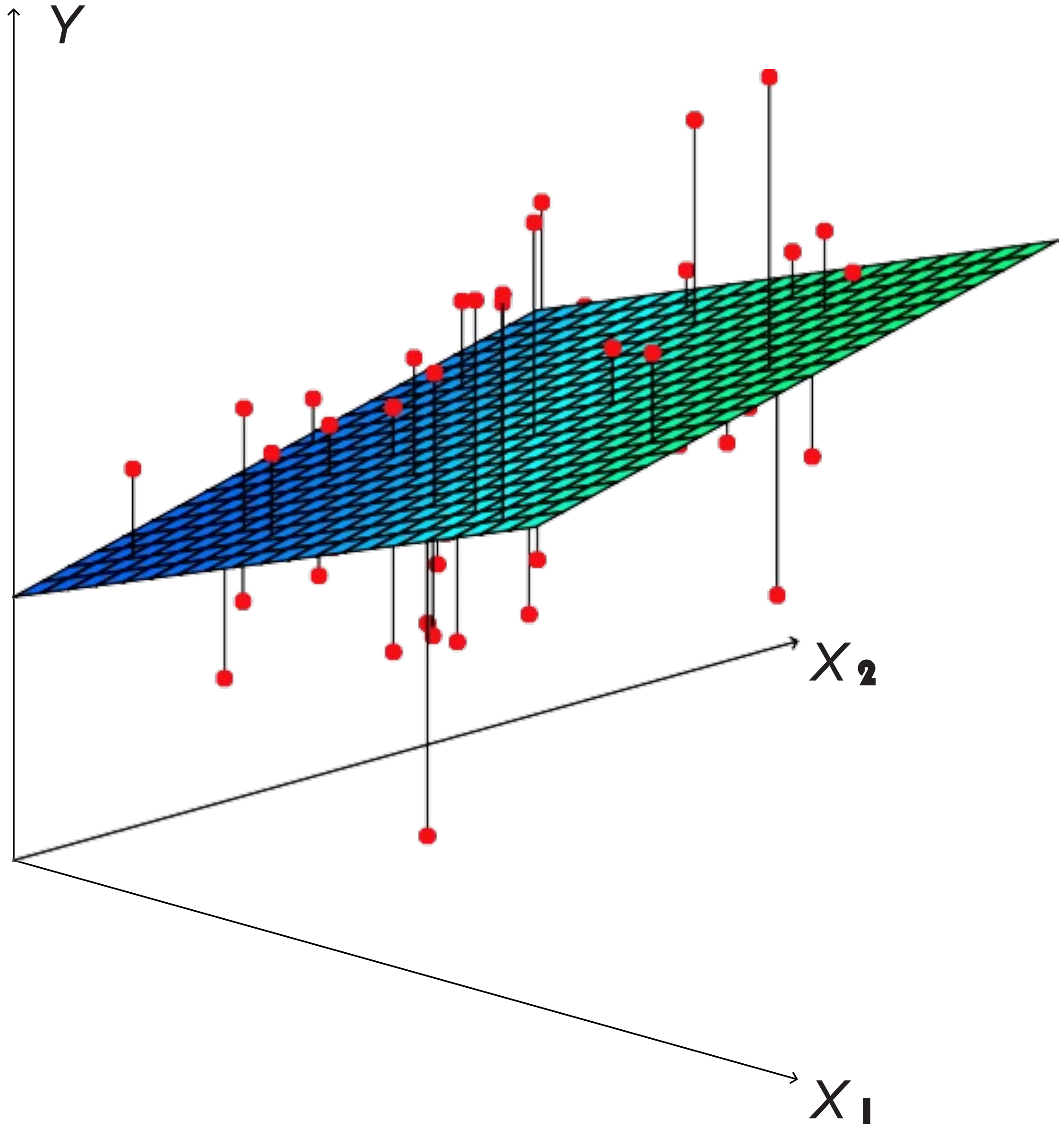
Estimation and Prediction for Multiple Regression

- Given estimates $\hat{\beta}_0, \hat{\beta}_1, . . . \hat{\beta}_p$, we can make predictions using the formula
- $\hat{y} = \hat{\beta}_0 + \hat{\beta}_1 x_1 + \hat{\beta}_2 x_2 + \cdots + \hat{\beta}_p x_p.$
- We estimate $\beta_0, \beta_1, . . . , \beta_p$ as the values that minimize the sum of squared residuals RSS

Estimation and Prediction for Multiple Regression

$$\begin{aligned} \text{RSS} &= \sum_{i=1}^{n}(y_i - \hat{y}_i)^2 \\ &= \sum_{i=1}^{n}(y_i - \hat{\beta}_0 - \hat{\beta}_1 x_{i1} - \hat{\beta}_2 x_{i2} - \cdots - \hat{\beta}_p x_{ip})^2 \end{aligned}$$

This is done using standard statistical software. The values $\hat{\beta}_0$, $\hat{\beta}_1, \ldots, \hat{\beta}_p$ that minimize RSS are the multiple least squares regression coefficient estimates.


Y
X 2
X 1

Confidence intervals for Multiple Regression

An interval that will contain the true unknown value of the parameter β_i in 1-α percent of times is

$$\left[\hat{\beta}_i - t_{n-p-1,\alpha/2}.\,\mathrm{SE}(\hat{\beta}_i), \hat{\beta}_i + t_{n-p-1,\alpha/2}.\,\mathrm{S\hat{E}}(\beta_i)\right]$$

Hypothesis testing

- Standard errors can also be used to perform *hypothesis tests* on the coefficients. The most common hypothesis test involves testing the *null hypothesis* of

H_0 :There is no relationship between X_i and Y

versus the *alternative hypothesis*

H_A :There is some relationship between X_i and Y .

Hypothesis testing

- Mathematically, this corresponds to testing

$$H_0 : \beta_i = 0$$

versus

$$H_A : \beta_i \neq 0,$$

since if $\beta_i = 0$ then X_i is not associated with Y.

Hypothesis testing

- In general, to test the following hypothesis

$$H_0 : \beta_i = \beta$$

versus

$$H_A : \beta_i \neq \beta,$$

we use a t-statistic:

Hypothesis testing — continued

- To test the null hypothesis, we compute a *t-statistic*, given by

$$t = \frac{\hat{\beta}_i - \beta}{\mathrm{SE}(\hat{\beta}_i)}$$

Usually zero

- This will have a *t*-distribution with $n - p - 1$ degrees of freedom, assuming $\beta_i = \beta$.

Hypothesis testing — continued

- Using statistical software, it is easy to compute the probability of observing any value equal to $|t|$ or larger. We call this probability the *p-value*.

$$t = \frac{\hat{\beta}_i - \beta}{\mathrm{SE}(\hat{\beta}_i)}$$

Usually zero

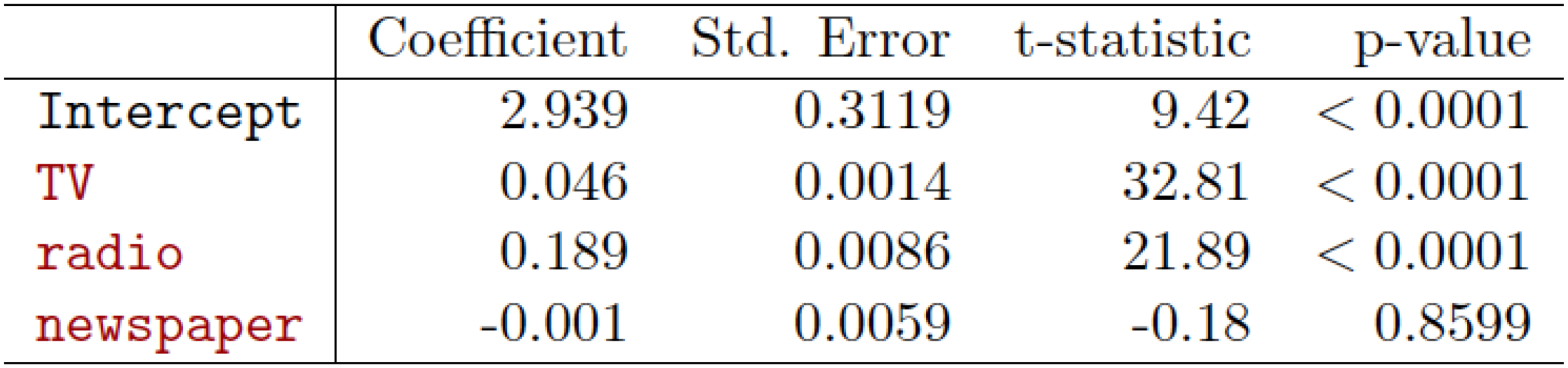
Hypothesis testing — continued

- If the p-value is very small, it means that the probability of seeing a *t* statistic extremer than what was observed (assuming that $\beta_i = \beta$) is very small. So we reject the null.

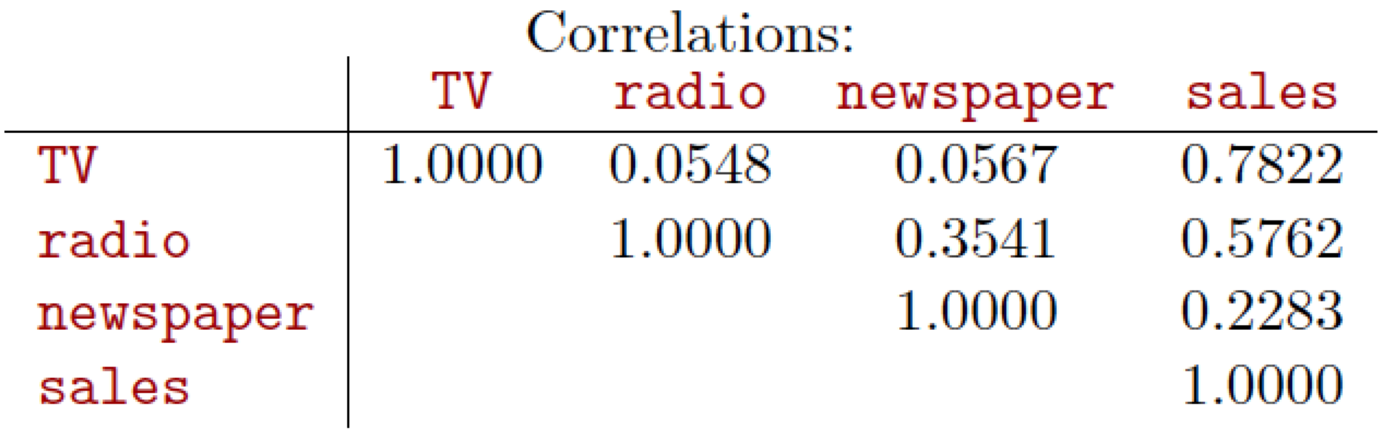
Rejection Region Approach

- Similar to simple regression

Results for advertising data



	Coefficient	Std. Error	t-statistic	p-value
Intercept	2.939	0.3119	9.42	< 0.0001
TV	0.046	0.0014	32.81	< 0.0001
radio	0.189	0.0086	21.89	< 0.0001
newspaper	-0.001	0.0059	-0.18	0.8599



Correlations:

	TV	radio	newspaper	sales
TV	1.0000	0.0548	0.0567	0.7822
radio		1.0000	0.3541	0.5762
newspaper			1.0000	0.2283
sales				1.0000

Some important questions

1. *Is at least one of the predictors $X_1, X_2, \ldots, X_p$ useful in predicting the response?*

2. *Do all the predictors help to explain Y, or is only a subset of the predictors useful?*

Some important questions

3. *How well does the model fit the data?*

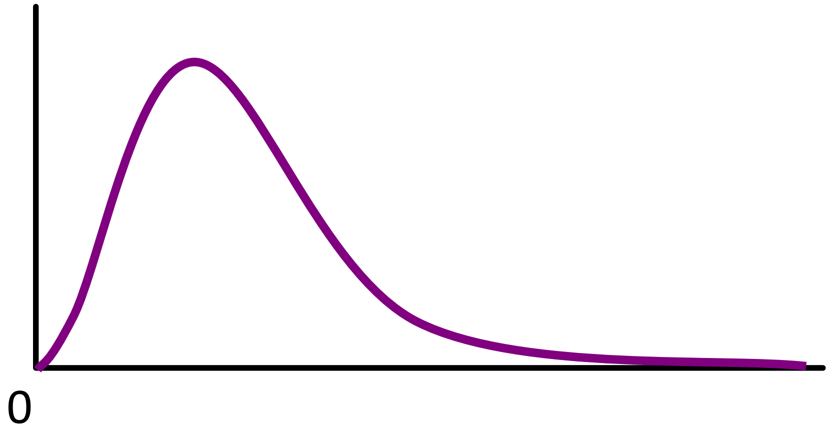
4. *Given a set of predictor values, what response value should we predict, and how accurate is our prediction?*

Is at least one predictor useful?

For the first question, we can use the F-statistic

$$F = \frac{(\mathrm{TSS} - \mathrm{RSS})/p}{\mathrm{RSS}/(n-p-1)} \sim F_{p,n-p-1}$$

Quantity	Value
Residual Standard Error	1.69
R^2	0.897
F-statistic	570



Tests on Regression Coefficients

Tests on All Coefficients

F-Test for Overall Significance of the Model

Shows if there is a linear relationship between all of the *X* variables considered together and *Y*

Use *F* test statistic

Hypotheses:

H_0: $\beta_1 = \beta_2 = \ldots = \beta_p = 0$ (no linear relationship)

H_1: at least one $\beta_i \neq 0$ (at least one independent variable affects *Y*)

F-Test for Overall Significance

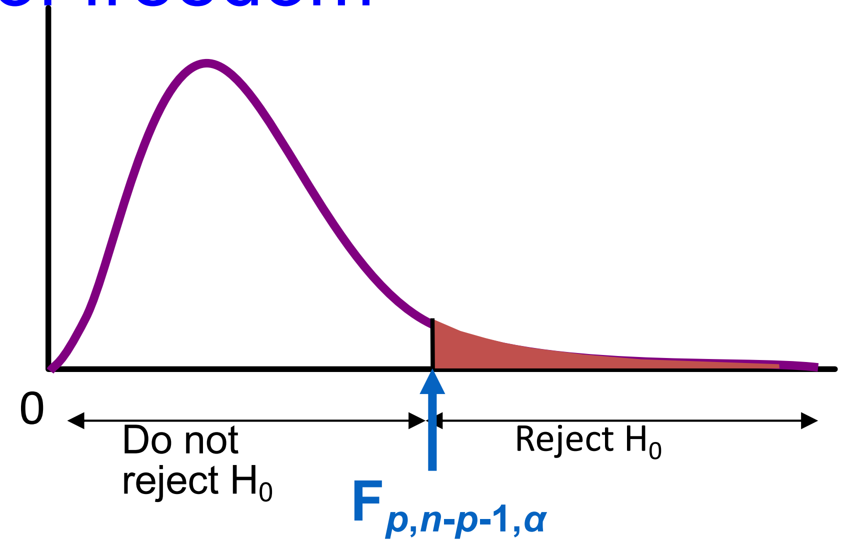
Test statistic:

$$F = \frac{(\mathrm{TSS} - \mathrm{RSS})/p}{\mathrm{RSS}/(n-p-1)} \sim F_{p,n-p-1}$$

where F has p (numerator) and $(n - p - 1)$ (denominator) degrees of freedom

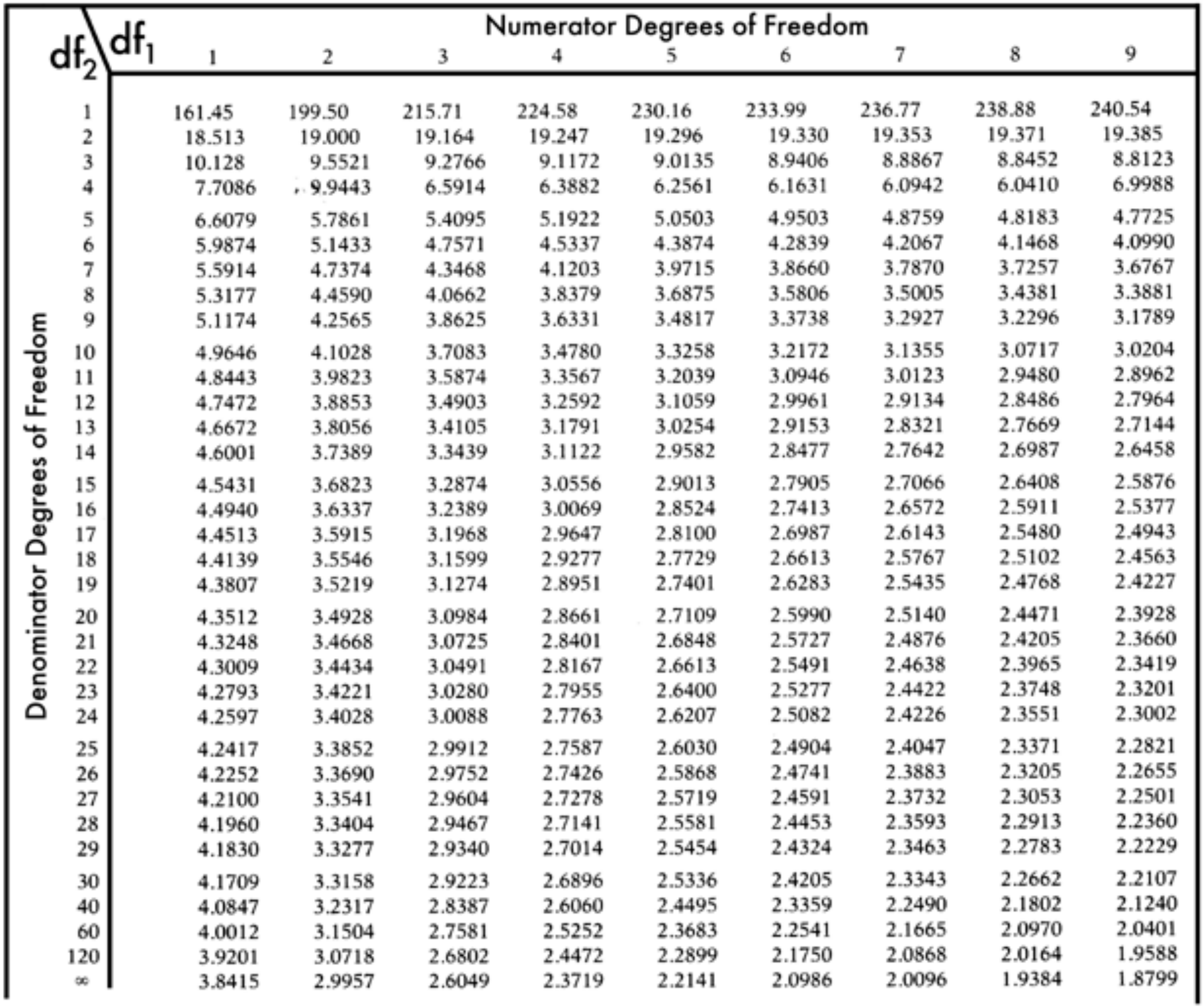
The decision rule is

Reject H_0 if $F > F_{p,n-p-1,\alpha}$



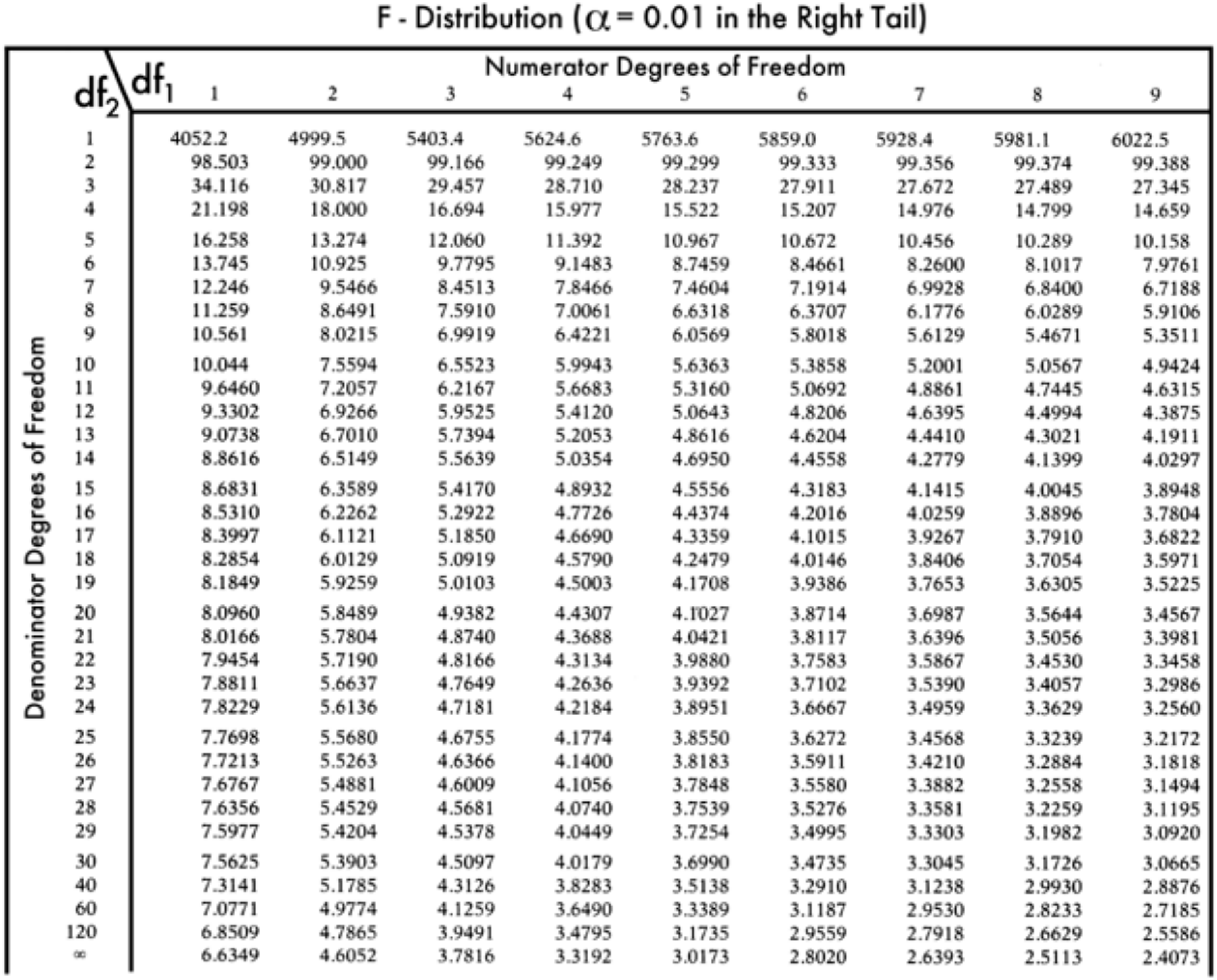
F-Test for Overall Significance

F - Distribution (α = 0.05 in the Right Tail)



Denominator Degrees of Freedom	Numerator Degrees of Freedom								
$df_2 \backslash df_1$	1	2	3	4	5	6	7	8	9
1	161.45	199.50	215.71	224.58	230.16	233.99	236.77	238.88	240.54
2	18.513	19.000	19.164	19.247	19.296	19.330	19.353	19.371	19.385
3	10.128	9.5521	9.2766	9.1172	9.0135	8.9406	8.8867	8.8452	8.8123
4	7.7086	9.9443	6.5914	6.3882	6.2561	6.1631	6.0942	6.0410	6.9988
5	6.6079	5.7861	5.4095	5.1922	5.0503	4.9503	4.8759	4.8183	4.7725
6	5.9874	5.1433	4.7571	4.5337	4.3874	4.2839	4.2067	4.1468	4.0990
7	5.5914	4.7374	4.3468	4.1203	3.9715	3.8660	3.7870	3.7257	3.6767
8	5.3177	4.4590	4.0662	3.8379	3.6875	3.5806	3.5005	3.4381	3.3881
9	5.1174	4.2565	3.8625	3.6331	3.4817	3.3738	3.2927	3.2296	3.1789
10	4.9646	4.1028	3.7083	3.4780	3.3258	3.2172	3.1355	3.0717	3.0204
11	4.8443	3.9823	3.5874	3.3567	3.2039	3.0946	3.0123	2.9480	2.8962
12	4.7472	3.8853	3.4903	3.2592	3.1059	2.9961	2.9134	2.8486	2.7964
13	4.6672	3.8056	3.4105	3.1791	3.0254	2.9153	2.8321	2.7669	2.7144
14	4.6001	3.7389	3.3439	3.1122	2.9582	2.8477	2.7642	2.6987	2.6458
15	4.5431	3.6823	3.2874	3.0556	2.9013	2.7905	2.7066	2.6408	2.5876
16	4.4940	3.6337	3.2389	3.0069	2.8524	2.7413	2.6572	2.5911	2.5377
17	4.4513	3.5915	3.1968	2.9647	2.8100	2.6987	2.6143	2.5480	2.4943
18	4.4139	3.5546	3.1599	2.9277	2.7729	2.6613	2.5767	2.5102	2.4563
19	4.3807	3.5219	3.1274	2.8951	2.7401	2.6283	2.5435	2.4768	2.4227
20	4.3512	3.4928	3.0984	2.8661	2.7109	2.5990	2.5140	2.4471	2.3928
21	4.3248	3.4668	3.0725	2.8401	2.6848	2.5727	2.4876	2.4205	2.3660
22	4.3009	3.4434	3.0491	2.8167	2.6613	2.5491	2.4638	2.3965	2.3419
23	4.2793	3.4221	3.0280	2.7955	2.6400	2.5277	2.4422	2.3748	2.3201
24	4.2597	3.4028	3.0088	2.7763	2.6207	2.5082	2.4226	2.3551	2.3002
25	4.2417	3.3852	2.9912	2.7587	2.6030	2.4904	2.4047	2.3371	2.2821
26	4.2252	3.3690	2.9752	2.7426	2.5868	2.4741	2.3883	2.3205	2.2655
27	4.2100	3.3541	2.9604	2.7278	2.5719	2.4591	2.3732	2.3053	2.2501
28	4.1960	3.3404	2.9467	2.7141	2.5581	2.4453	2.3593	2.2913	2.2360
29	4.1830	3.3277	2.9340	2.7014	2.5454	2.4324	2.3463	2.2783	2.2229
30	4.1709	3.3158	2.9223	2.6896	2.5336	2.4205	2.3343	2.2662	2.2107
40	4.0847	3.2317	2.8387	2.6060	2.4495	2.3359	2.2490	2.1802	2.1240
60	4.0012	3.1504	2.7581	2.5252	2.3683	2.2541	2.1665	2.0970	2.0401
120	3.9201	3.0718	2.6802	2.4472	2.2899	2.1750	2.0868	2.0164	1.9588
∞	3.8415	2.9957	2.6049	2.3719	2.2141	2.0986	2.0096	1.9384	1.8799

F-Test for Overall Significance



F - Distribution ($\alpha = 0.01$ in the Right Tail)

Denominator Degrees of Freedom

	Numerator Degrees of Freedom								
df_2 \ df_1	1	2	3	4	5	6	7	8	9
1	4052.2	4999.5	5403.4	5624.6	5763.6	5859.0	5928.4	5981.1	6022.5
2	98.503	99.000	99.166	99.249	99.299	99.333	99.356	99.374	99.388
3	34.116	30.817	29.457	28.710	28.237	27.911	27.672	27.489	27.345
4	21.198	18.000	16.694	15.977	15.522	15.207	14.976	14.799	14.659
5	16.258	13.274	12.060	11.392	10.967	10.672	10.456	10.289	10.158
6	13.745	10.925	9.7795	9.1483	8.7459	8.4661	8.2600	8.1017	7.9761
7	12.246	9.5466	8.4513	7.8466	7.4604	7.1914	6.9928	6.8400	6.7188
8	11.259	8.6491	7.5910	7.0061	6.6318	6.3707	6.1776	6.0289	5.9106
9	10.561	8.0215	6.9919	6.4221	6.0569	5.8018	5.6129	5.4671	5.3511
10	10.044	7.5594	6.5523	5.9943	5.6363	5.3858	5.2001	5.0567	4.9424
11	9.6460	7.2057	6.2167	5.6683	5.3160	5.0692	4.8861	4.7445	4.6315
12	9.3302	6.9266	5.9525	5.4120	5.0643	4.8206	4.6395	4.4994	4.3875
13	9.0738	6.7010	5.7394	5.2053	4.8616	4.6204	4.4410	4.3021	4.1911
14	8.8616	6.5149	5.5639	5.0354	4.6950	4.4558	4.2779	4.1399	4.0297
15	8.6831	6.3589	5.4170	4.8932	4.5556	4.3183	4.1415	4.0045	3.8948
16	8.5310	6.2262	5.2922	4.7726	4.4374	4.2016	4.0259	3.8896	3.7804
17	8.3997	6.1121	5.1850	4.6690	4.3359	4.1015	3.9267	3.7910	3.6822
18	8.2854	6.0129	5.0919	4.5790	4.2479	4.0146	3.8406	3.7054	3.5971
19	8.1849	5.9259	5.0103	4.5003	4.1708	3.9386	3.7653	3.6305	3.5225
20	8.0960	5.8489	4.9382	4.4307	4.1027	3.8714	3.6987	3.5644	3.4567
21	8.0166	5.7804	4.8740	4.3688	4.0421	3.8117	3.6396	3.5056	3.3981
22	7.9454	5.7190	4.8166	4.3134	3.9880	3.7583	3.5867	3.4530	3.3458
23	7.8811	5.6637	4.7649	4.2636	3.9392	3.7102	3.5390	3.4057	3.2986
24	7.8229	5.6136	4.7181	4.2184	3.8951	3.6667	3.4959	3.3629	3.2560
25	7.7698	5.5680	4.6755	4.1774	3.8550	3.6272	3.4568	3.3239	3.2172
26	7.7213	5.5263	4.6366	4.1400	3.8183	3.5911	3.4210	3.2884	3.1818
27	7.6767	5.4881	4.6009	4.1056	3.7848	3.5580	3.3882	3.2558	3.1494
28	7.6356	5.4529	4.5681	4.0740	3.7539	3.5276	3.3581	3.2259	3.1195
29	7.5977	5.4204	4.5378	4.0449	3.7254	3.4995	3.3303	3.1982	3.0920
30	7.5625	5.3903	4.5097	4.0179	3.6990	3.4735	3.3045	3.1726	3.0665
40	7.3141	5.1785	4.3126	3.8283	3.5138	3.2910	3.1238	2.9930	2.8876
60	7.0771	4.9774	4.1259	3.6490	3.3389	3.1187	2.9530	2.8233	2.7185
120	6.8509	4.7865	3.9491	3.4795	3.1735	2.9559	2.7918	2.6629	2.5586
∞	6.6349	4.6052	3.7816	3.3192	3.0173	2.8020	2.6393	2.5113	2.4073

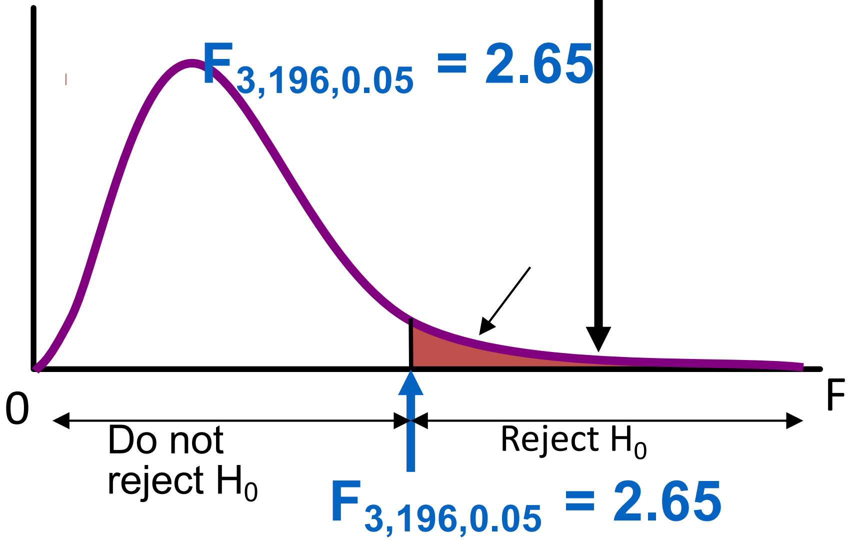
F-Test for Overall Significance

H_0: $\beta_1 = \beta_2 = \beta_3 = 0$
H_1: Not all three of β_1, β_2, β_3 are zero

$df_1 = 3$ $df_2 = 200\text{-}3\text{-}1$

Critical Value:

$F_{3,196,0.05} = 2.65$



Test Statistic: F=570

$$F = \frac{(\text{TSS} - \text{RSS})/p}{\text{RSS}/(n-p-1)} \sim F_{p,n-p-1}$$

Decision:

Since F test statistic is in the rejection region (p-value < .05), reject H_0

Conclusion:

There is evidence that at least one independent variable affects Y

Deciding on the important variables

- The most direct approach is called *all subsets* or *best subsets* regression: we compute the least squares fit for all possible subsets and then choose between them based on some criterion that balances training error with model size.

Deciding on the important variables

- However we often can't examine all possible models, since they are 2^p of them; for example when $p = 40$ there are over a trillion models!
- Instead we need an automated approach that searches through a subset of them. We discuss two commonly use approaches next.

Forward selection

- Begin with the *null model* — a model that contains an intercept but no predictors.
- Fit *p* simple linear regressions and add to the null model the variable that results in the lowest RSS.

Forward selection

- Add to that model the variable that results in the lowest RSS amongst all two-variable models.
- Continue until some stopping rule is satisfied, for example when all remaining variables have a p-value above some threshold.

Backward selection

- Start with all variables in the model.
- Remove the variable with the largest p-value — that is, the variable that is the least statistically significant.
- The new (p − 1)-variable model is fit, and the variable with the largest p-value is removed.

Backward selection

- Continue until a stopping rule is reached. For instance, we may stop when all remaining variables have a significant

  p-value defined by some significance threshold.

Model selection — continued

- Later we discuss more systematic criteria for choosing an "optimal" member in the path of models produced by forward or backward stepwise selection.

Model selection — continued

- These include *Mallow's* C_p, *Akaike information criterion (AIC)*, *Bayesian information criterion (BIC)*, *adjusted* R^2 and *Cross-validation (CV)*.

Other Considerations in the Regression Model

Qualitative Predictors

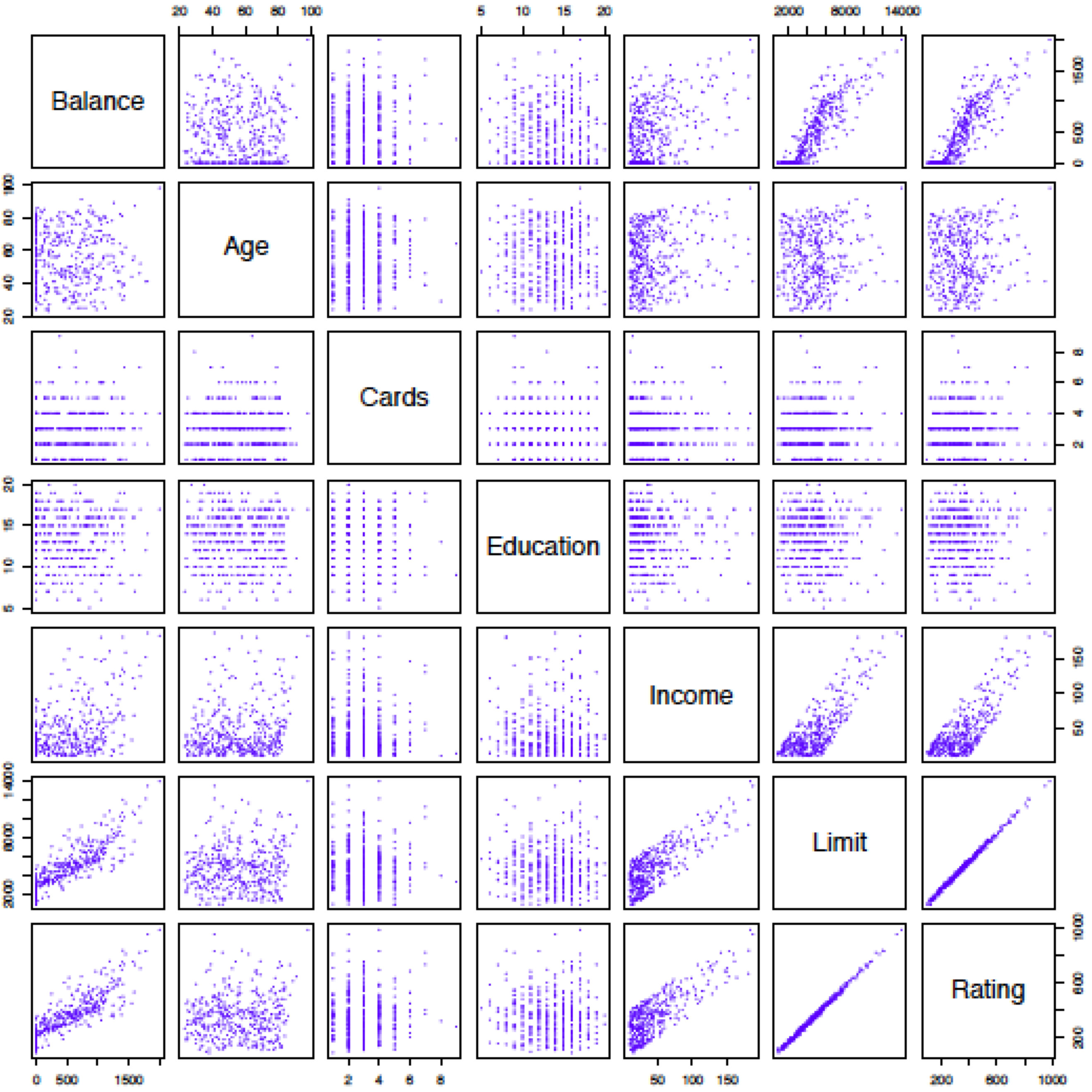
- Some predictors are not *quantitative* but are *qualitative*, taking a discrete set of values.
- These are also called *categorical* predictors or *factor variables*.

Other Considerations in the Regression Model

See for example the scatterplot matrix of the credit card data in the next slide.

In addition to the 7 quantitative variables shown, there are four qualitative variables: gender, student (student status), status (marital status), and ethnicity (Caucasian, African American (AA) or Asian).

Credit Card Data



Qualitative Predictors — cont'd

Example: investigate differences in credit card balance between males and females, ignoring the other variables. We create a new variable

$$x_i = \begin{cases} 1 & \text{if } i\text{th person is female} \\ 0 & \text{if } i\text{th person is male} \end{cases}$$

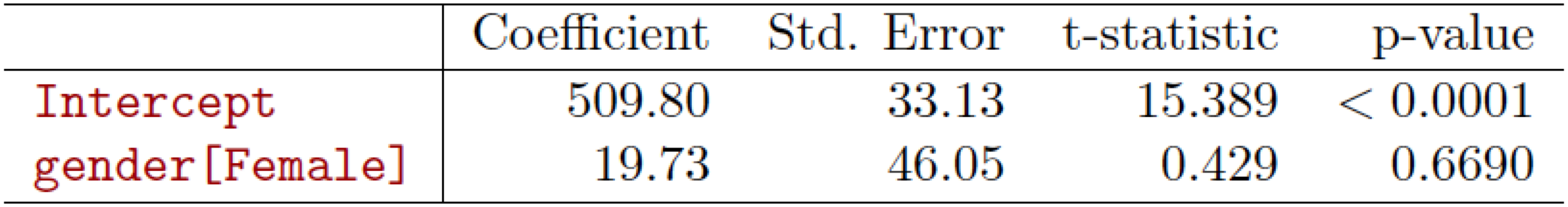
Resulting model:

$$y_i = \beta_0 + \beta_1 x_i + \epsilon_i = \begin{cases} \beta_0 + \beta_1 + \epsilon_i & \text{if } i\text{th person is female} \\ \beta_0 + \epsilon_i & \text{if } i\text{th person is male.} \end{cases}$$

Intrepretation?

Credit card data — continued

Results for gender model:



	Coefficient	Std. Error	t-statistic	p-value
`Intercept`	509.80	33.13	15.389	< 0.0001
`gender[Female]`	19.73	46.05	0.429	0.6690

Qualitative predictors with more than two levels

- With more than two levels, we create additional dummy variables. For example, for the ethnicity variable we create two dummy variables. The first could be

$$x_{i1} = \begin{cases} 1 & \text{if } i\text{th person is Asian} \\ 0 & \text{if } i\text{th person is not Asian,} \end{cases}$$

and the second could be

$$x_{i2} = \begin{cases} 1 & \text{if } i\text{th person is Caucasian} \\ 0 & \text{if } i\text{th person is not Caucasian.} \end{cases}$$

Qualitative predictors with more than two levels

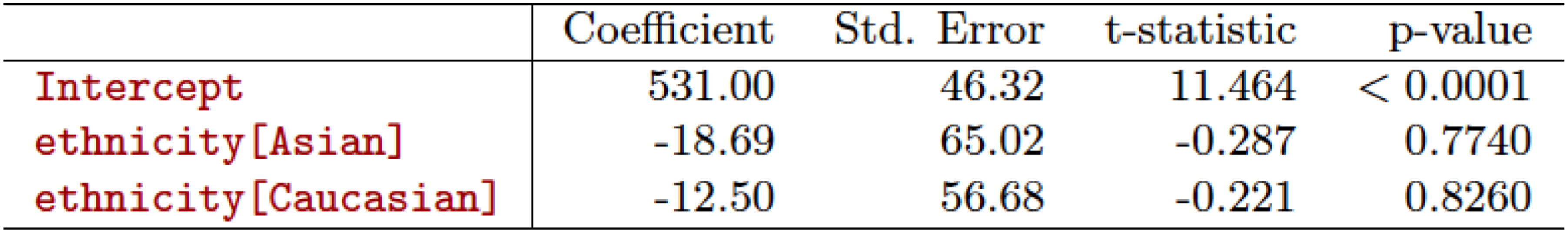
- Then both of these variables can be used in the regression equation, in order to obtain the model

$$y_i = \beta_0+\beta_1 x_{i1}+\beta_2 x_{i2}+\epsilon_i = \begin{cases} \beta_0 + \beta_1 + \epsilon_i & \text{if } i\text{th person is Asian} \\ \beta_0 + \beta_2 + \epsilon_i & \text{if } i\text{th person is Caucasian} \\ \beta_0 + \epsilon_i & \text{if } i\text{th person is AA.} \end{cases}$$

Qualitative predictors with more than two levels

- There will always be one fewer dummy variable than the number of levels. The level with no dummy variable — African American in this example — is known as the *baseline*.

Results for ethnicity



	Coefficient	Std. Error	t-statistic	p-value
Intercept	531.00	46.32	11.464	< 0.0001
ethnicity[Asian]	-18.69	65.02	-0.287	0.7740
ethnicity[Caucasian]	-12.50	56.68	-0.221	0.8260

Extensions of the Linear Model

Removing the additive assumption:
interactions and *nonlinearity*

Interactions:

- In our previous analysis of the Advertising data, we assumed that the effect on sales of increasing one advertising medium is independent of the amount spent on the other media.

Extensions of the Linear Model

- For example, the linear model

$$\widehat{\texttt{sales}} = \beta_0 + \beta_1 \times \texttt{TV} + \beta_2 \times \texttt{radio} + \beta_3 \times \texttt{newspaper}$$

states that the average effect on sales of a one-unit increase in TV is always β_1, regardless of the amount spent on radio.

Interactions — continued

- But suppose that spending money on radio advertising actually increases the effectiveness of TV advertising, so that the slope term for TV should increase as radio increases.

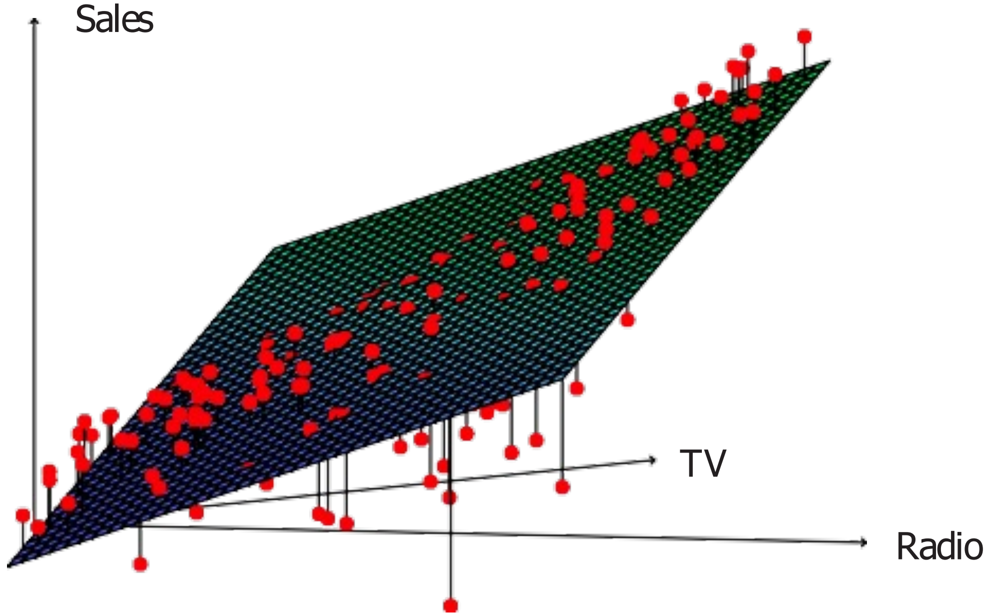
Interactions — continued

- In this situation, given a fixed budget of $100, 000, spending half on radio and half on TV may increase sales more than allocating the entire amount to either TV or to radio.

Interactions — continued

- In marketing, this is known as a *synergy* effect, and in statistics it is referred to as an *interaction* effect.

Interaction in the Advertising data?



When levels of either TV or radio are low, then the true sales are lower than predicted by the linear model.

But when advertising is split between the two media, then the model tends to underestimate sales.

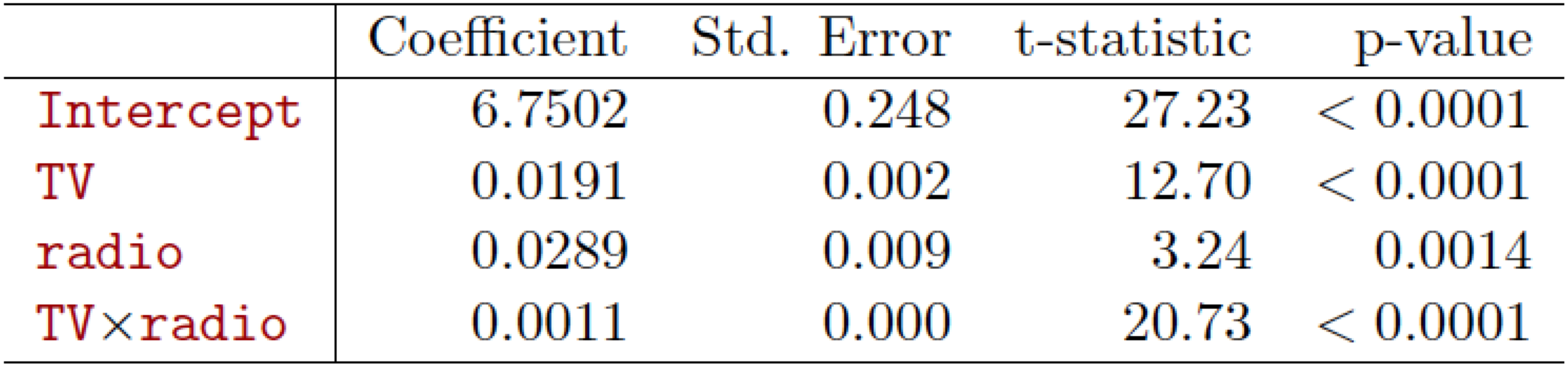
Modelling interactions — Advertising data

Model takes the form

$$\text{sales} = \beta_0 + \beta_1 \times \text{TV} + \beta_2 \times \text{radio} + \beta_3 \times (\text{radio} \times \text{TV}) + \varepsilon$$

$$= \beta_0 + (\beta_1 + \beta_3 \times \text{radio}) \times \text{TV} + \beta_2 \times \text{radio} + \varepsilon$$

Results:



	Coefficient	Std. Error	t-statistic	p-value
Intercept	6.7502	0.248	27.23	< 0.0001
TV	0.0191	0.002	12.70	< 0.0001
radio	0.0289	0.009	3.24	0.0014
TV×radio	0.0011	0.000	20.73	< 0.0001

Interpretation

- The results in this table suggest that interactions are important.
- The p-value for the interaction term TV×radio is extremely low, indicating that there is strong evidence for $H_A: \beta_3 \neq 0$.

Interpretation

- The R^2 for the interaction model is 96.8%, compared to only 89.7% for the model that predicts sales using TV and radio without an interaction term.

Interpretation — continued

- This means that (96.8 − 89.7)/(100 − 89.7) = 69% of the variability in sales that remains after fitting the additive model has been explained by the interaction term.

Interpretation — continued

- The coefficient estimates in the table suggest that an increase in TV advertising of $1, 000 is associated with increased sales of $(\hat{\beta}_1 + \hat{\beta}_3 \times \text{radio}) \times 1000 = 19 + 1.1 \times \text{radio}$ units.

Interpretation — continued

- An increase in radio advertising of $1, 000 will be associated with an increase in sales of $(\hat{\beta}_2 + \hat{\beta}_3 \times \text{TV}) \times 1000 = 29 + 1.1 \times \text{TV}$ units.

Hierarchy

- Sometimes it is the case that an interaction term has a very small p-value, but the associated main effects (in this case, TV and radio) do not.
- The *hierarchical principle*:

  If we include an interaction in a model, we should also include the main effects, even if the p-values associated with their coefficients are not significant.

Hierarchy — continued

- The rationale for this principle is that interactions are hard to interpret in a model without main effects — their meaning is changed.
- Specifically, the interaction terms also contain main effects, if the model has no main effect terms.

Interaction between Quantitative and Qualitative Variables

Consider the Credit data set, and suppose that we wish to predict balance using income (quantitative) and student (qualitative).

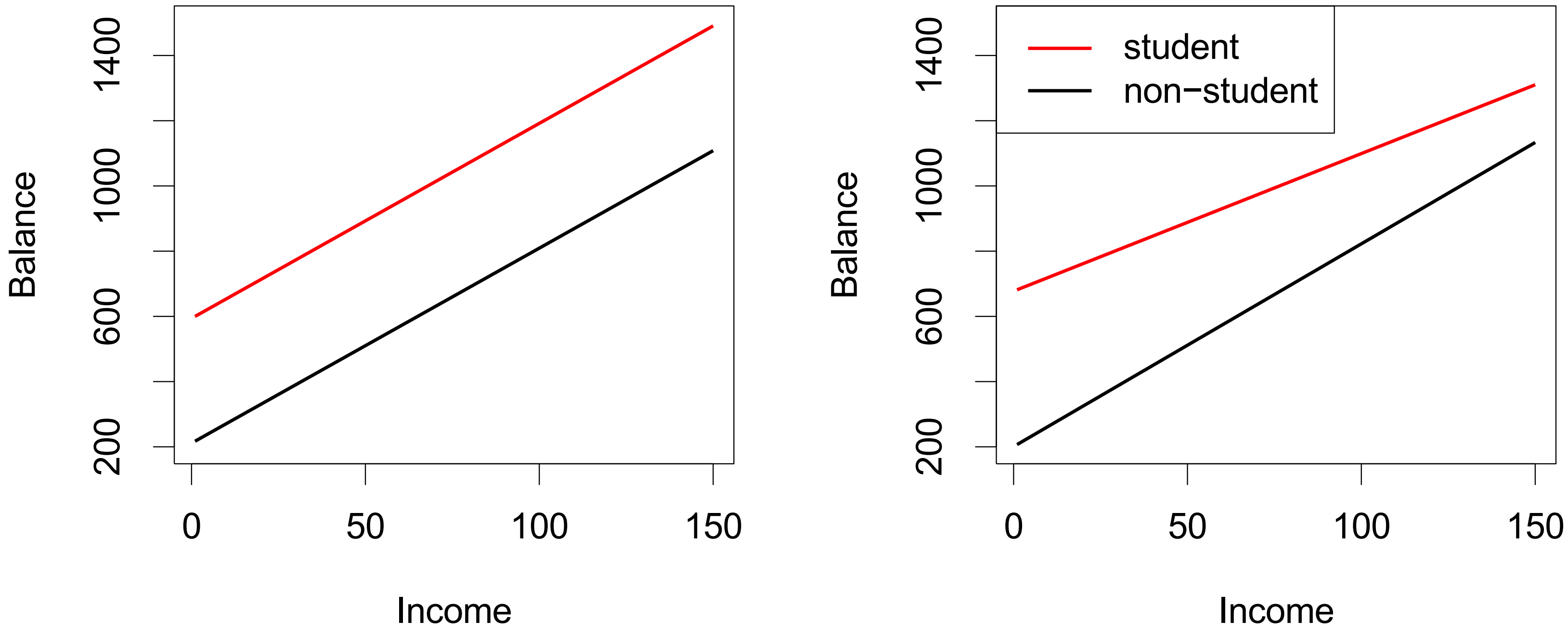
Without an interaction term, the model takes the form

$$\begin{aligned}
\texttt{balance}_i &\approx \beta_0 + \beta_1 \times \texttt{income}_i + \begin{cases} \beta_2 & \text{if } i\text{th person is a student} \\ 0 & \text{if } i\text{th person is not a student} \end{cases} \\
&= \beta_1 \times \texttt{income}_i + \begin{cases} \beta_0 + \beta_2 & \text{if } i\text{th person is a student} \\ \beta_0 & \text{if } i\text{th person is not a student.} \end{cases}
\end{aligned}$$

Interaction between Quantitative and Qualitative Variables

With interactions, it takes the form

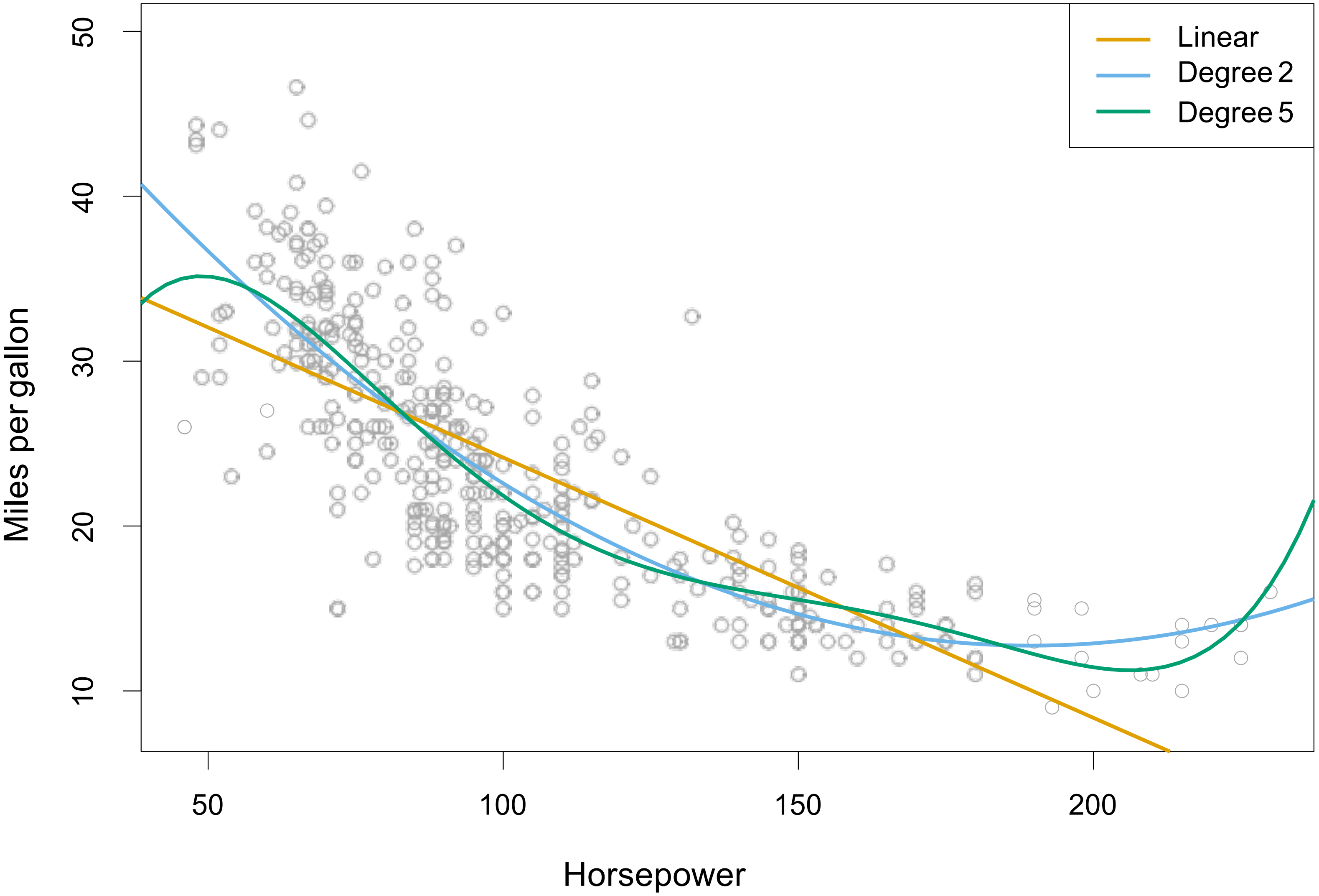
$$
\begin{aligned}
\texttt{balance}_i &\approx \beta_0 + \beta_1 \times \texttt{income}_i + \begin{cases} \beta_2 + \beta_3 \times \texttt{income}_i & \text{if student} \\ 0 & \text{if not student} \end{cases} \\
&= \begin{cases} (\beta_0 + \beta_2) + (\beta_1 + \beta_3) \times \texttt{income}_i & \text{if student} \\ \beta_0 + \beta_1 \times \texttt{income}_i & \text{if not student} \end{cases}
\end{aligned}
$$



Credit data; Left: no interaction between income and student. Right: with an interaction term between income and student.

Non-linear effects of predictors

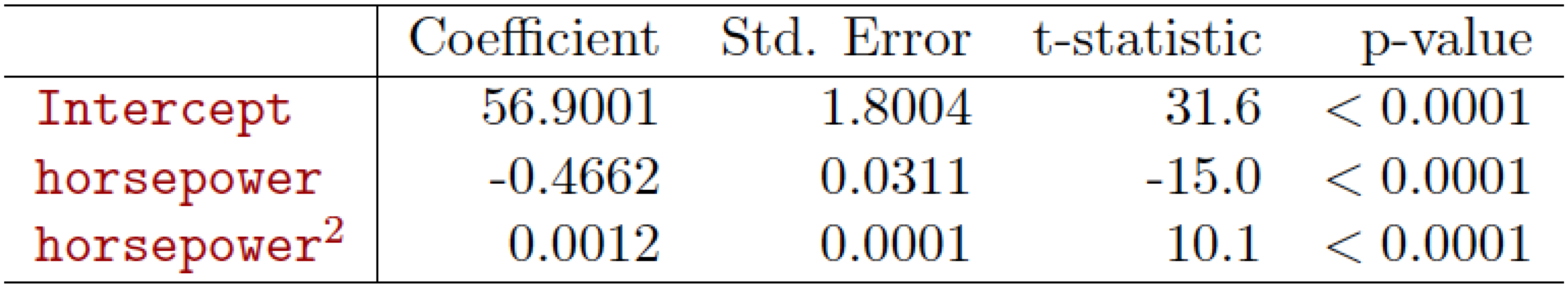
polynomial regression on Auto data



The figure suggests that

$$\text{mpg} = \beta_0 + \beta_1 \times \text{horsepower} + \beta_2 \times \text{horsepower}^2 + \varepsilon$$

may provide a better fit.



	Coefficient	Std. Error	t-statistic	p-value
`Intercept`	56.9001	1.8004	31.6	< 0.0001
`horsepower`	-0.4662	0.0311	-15.0	< 0.0001
$\texttt{horsepower}^2$	0.0012	0.0001	10.1	< 0.0001

What we did not cover

Outliers

Non-constant variance of error terms

High leverage points

Collinearity

See text Section 3.33

Generalizations of the Linear Model

In much of the rest of this course, we discuss methods that expand the scope of linear models and how they are fit

Generalizations of the Linear Model

- *Classification problems:* logistic regression, support vector machines
- *Non-linearity:* kernel smoothing, splines and generalized additive models; nearest neighbor methods.

Generalizations of the Linear Model

- *Interactions:* Tree-based methods, bagging, random forests and boosting (these also capture non-linearities)
- *Regularized fitting:* Ridge regression and lasso

Appendix: More on Qualitative/ Categorical Variables

Material from:

https://www.analyticsvidhya.com/blog/2015/11/easy-methods-deal-categorical-variables-predictive-modeling/

Qualitative/ Categorical Variables

- Challenges faced while dealing with categorical variables:
- A categorical variable has too many levels. This pulls down performance level of the model. For example, a cat. variable “zip code” would
  have numerous levels.

Qualitative/ Categorical Variables

- Challenges faced while dealing with categorical variables:
- A categorical variable has levels which rarely occur. Many of these levels have minimal chance of making a real impact on model fit. For example, a variable ‘disease’ might have some levels which would rarely occur.

Qualitative/ Categorical Variables

- Challenges faced while dealing with categorical variables:
  - There is one level which always occurs i.e. for most of the observations in data set there is only one level. Variables with such levels fail to make a positive impact on model performance due to very low variation.

Qualitative/ Categorical Variables

- Challenges faced while dealing with categorical variables:
- If the categorical variable is masked, it becomes a laborious task to decipher its meaning. Such situations are commonly found in data science competitions.

Qualitative/ Categorical Variables

- Challenges faced while dealing with categorical variables:
- You can’t fit categorical variables into a regression equation in their raw form. They must be treated.

Qualitative/ Categorical Variables

- Challenges faced while dealing with categorical variables:
- Most of the algorithms (or ML libraries) produce better result with numerical variable. In python, library “sklearn” requires features in numerical arrays.

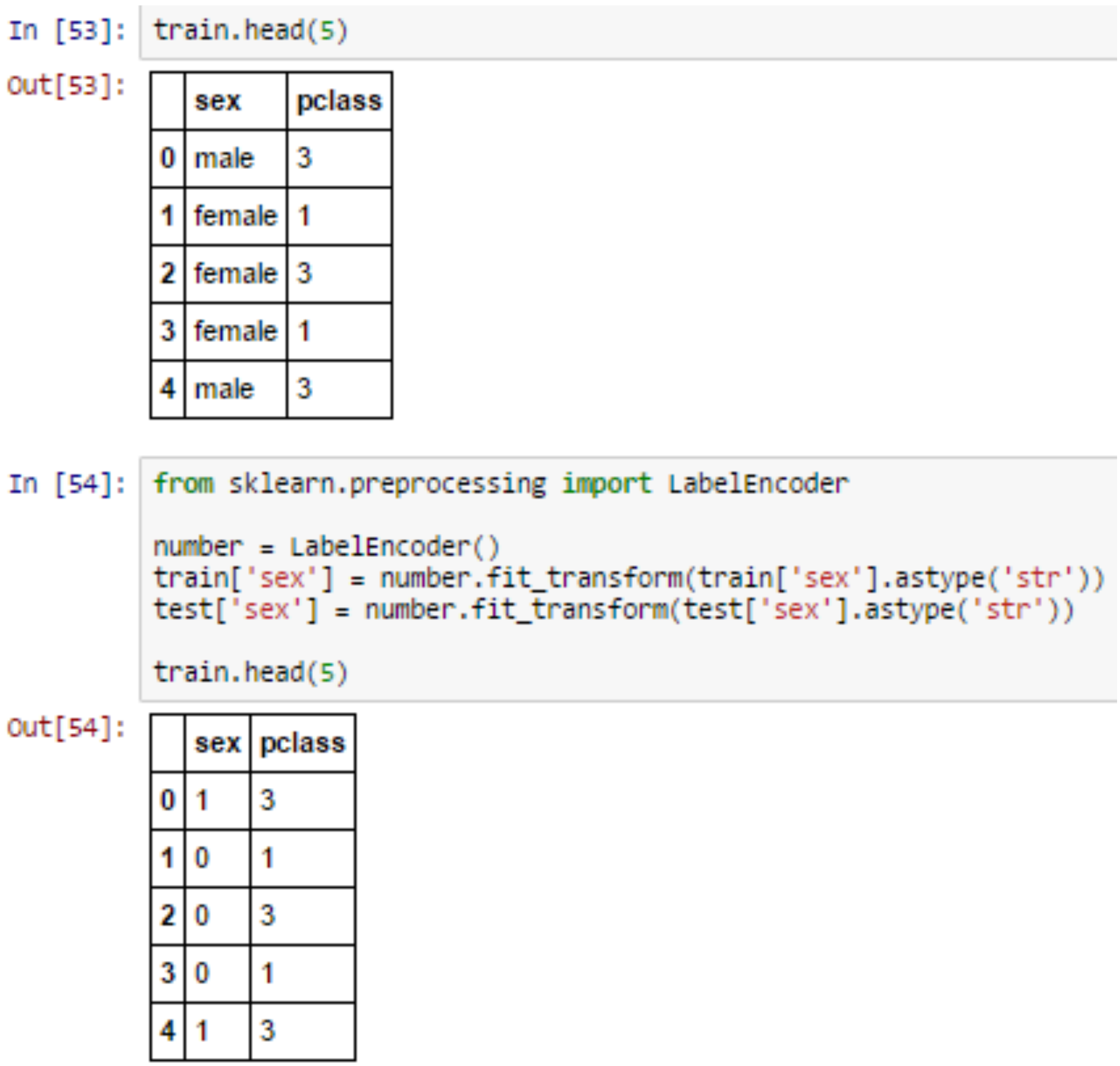
Methods to deal with Qualitative/ Categorical Variables

Convert to Number

Label Encoder: It is used to transform non-numerical labels to numerical labels (or nominal categorical variables). Numerical labels are always between 0 and n_classes-1.

Methods to deal with Qualitative/ Categorical Variables

Label Encoder:



```
In [53]: train.head(5)
```

Out[53]:

	sex	pclass
0	male	3
1	female	1
2	female	3
3	female	1
4	male	3

```
In [54]: from sklearn.preprocessing import LabelEncoder

         number = LabelEncoder()
         train['sex'] = number.fit_transform(train['sex'].astype('str'))
         test['sex'] = number.fit_transform(test['sex'].astype('str'))

         train.head(5)
```

Out[54]:

	sex	pclass
0	1	3
1	0	1
2	0	3
3	0	1
4	1	3

Methods to deal with Qualitative/ Categorical Variables

Label Encoder: A common challenge with nominal categorical variable is that, it may decrease performance of a model. For example: We have two features “age” (range: 0-80) and “city” (81 different levels).

Methods to deal with Qualitative/ Categorical Variables

Now, when we’ll apply label encoder to ‘city’ variable, it will represent ‘city’ with numeric values range from 0 to 80. The ‘city’ variable is now similar to ‘age’ variable since both will have similar data points, which is certainly not a right approach.

Methods to deal with Qualitative/ Categorical Variables

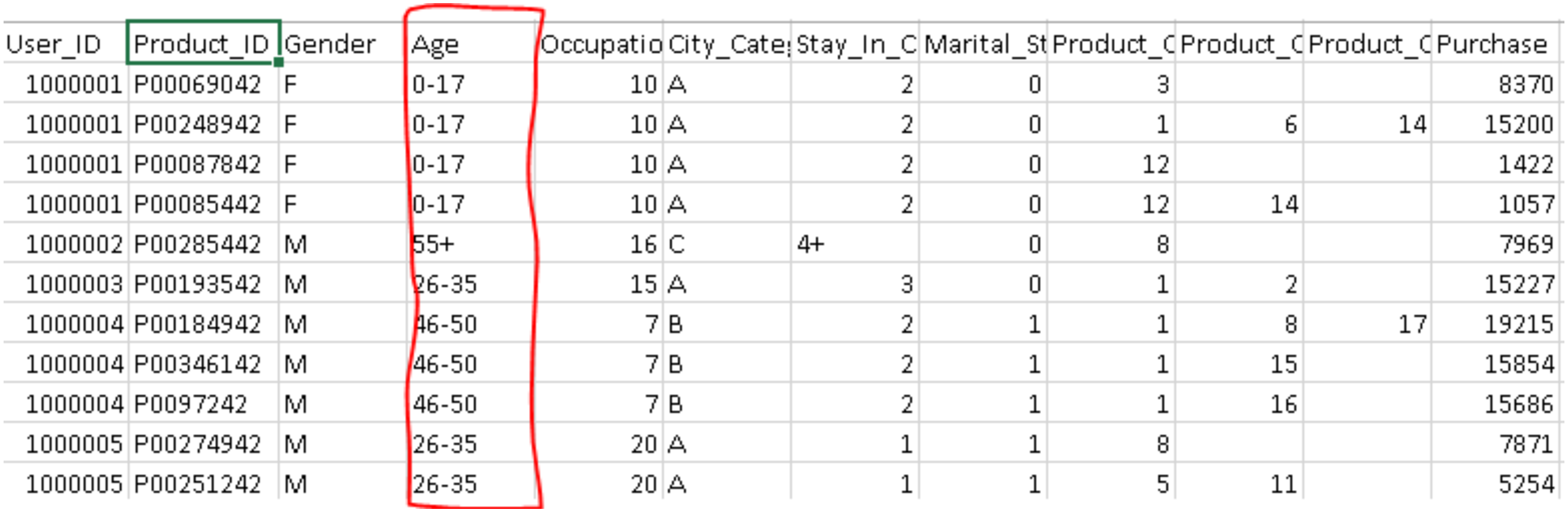
Convert to Number

Convert numeric bins to number: Let’s say, bins of a continuous variable are available in the data set (shown next).

Methods to deal with Qualitative/ Categorical Variables

Convert to Number

Convert numeric bins to number



User_ID	Product_ID	Gender	Age	Occupatio	City_Cate	Stay_In_C	Marital_St	Product_C	Product_C	Product_C	Purchase
1000001	P00069042	F	0-17	10	A	2	0	3			8370
1000001	P00248942	F	0-17	10	A	2	0	1	6	14	15200
1000001	P00087842	F	0-17	10	A	2	0	12			1422
1000001	P00085442	F	0-17	10	A	2	0	12	14		1057
1000002	P00285442	M	55+	16	C	4+	0	8			7969
1000003	P00193542	M	26-35	15	A	3	0	1	2		15227
1000004	P00184942	M	46-50	7	B	2	1	1	8	17	19215
1000004	P00346142	M	46-50	7	B	2	1	1	15		15854
1000004	P0097242	M	46-50	7	B	2	1	1	16		15686
1000005	P00274942	M	26-35	20	A	1	1	8			7871
1000005	P00251242	M	26-35	20	A	1	1	5	11		5254

Methods to deal with Qualitative/ Categorical Variables

Convert to Number

Convert numeric bins to number:

- Variable “Age” has bins (0-17, 17-25, 26-35 …). We can convert these bins into definite numbers using the following methods:
  - Using label encoder for conversion. But, these numerical bins will be treated same as multiple levels of non-numeric feature. Hence, wouldn’t provide any additional information

Methods to deal with Qualitative/ Categorical Variables

Convert to Number

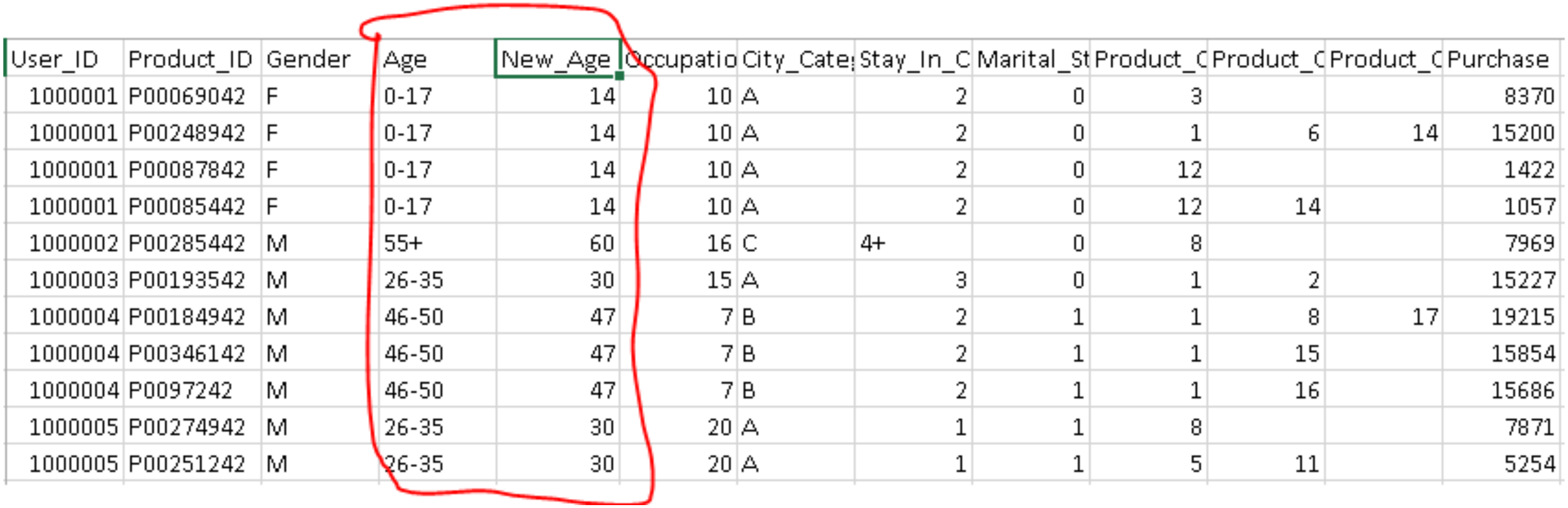
Convert numeric bins to number:

- Variable “Age” has bins (0-17, 17-25, 26-35 …). We can convert these bins into definite numbers using the following methods:
  - Create a new feature using mean or mode (most relevant value) of each age bucket. It would comprise of additional weight for levels.

Methods to deal with Qualitative/ Categorical Variables

Convert to Number

Convert numeric bins to number:



User_ID	Product_ID	Gender	Age	New_Age	Occupatio	City_Cate	Stay_In_C	Marital_St	Product_C	Product_C	Product_C	Purchase
1000001	P00069042	F	0-17	14	10	A	2	0	3			8370
1000001	P00248942	F	0-17	14	10	A	2	0	1	6	14	15200
1000001	P00087842	F	0-17	14	10	A	2	0	12			1422
1000001	P00085442	F	0-17	14	10	A	2	0	12	14		1057
1000002	P00285442	M	55+	60	16	C	4+	0	8			7969
1000003	P00193542	M	26-35	30	15	A	3	0	1	2		15227
1000004	P00184942	M	46-50	47	7	B	2	1	1	8	17	19215
1000004	P00346142	M	46-50	47	7	B	2	1	1	15		15854
1000004	P0097242	M	46-50	47	7	B	2	1	1	16		15686
1000005	P00274942	M	26-35	30	20	A	1	1	8			7871
1000005	P00251242	M	26-35	30	20	A	1	1	5	11		5254

Methods to deal with Qualitative/ Categorical Variables

Convert to Number

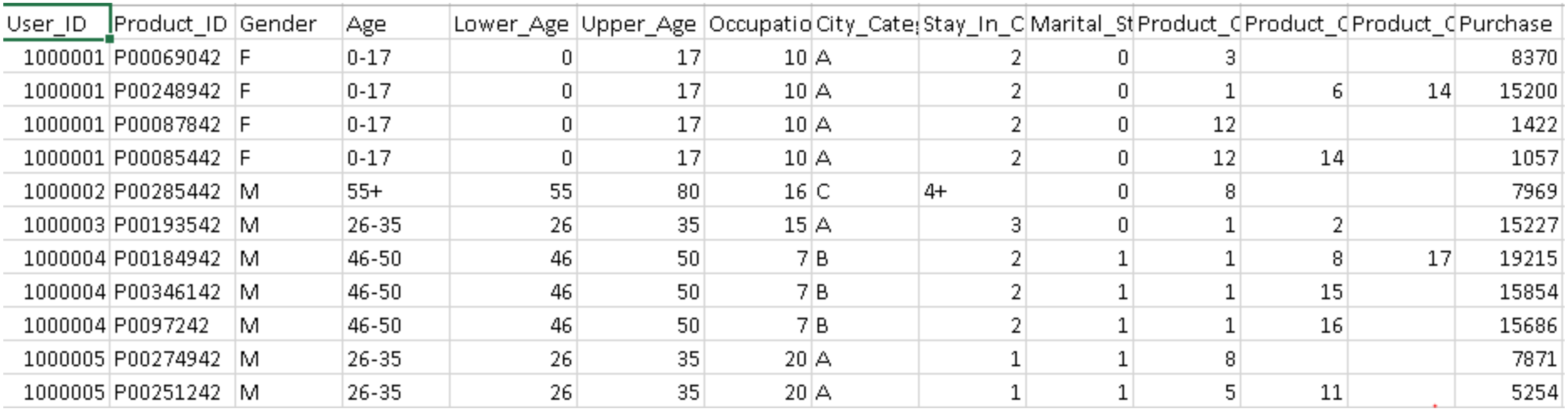
Convert numeric bins to number:

- Variable “Age” has bins (0-17, 17-25, 26-35 …). We can convert these bins into definite numbers using the following methods:
  - Create two new features, one for lower bound of age and another for upper bound. In this method, we’ll obtain more information about these numerical bins compare to earlier two methods.

Methods to deal with Qualitative/ Categorical Variables

Convert to Number

Convert numeric bins to number:



User_ID	Product_ID	Gender	Age	Lower_Age	Upper_Age	Occupatio	City_Cate;	Stay_In_C	Marital_St	Product_C	Product_C	Product_C	Purchase
1000001	P00069042	F	0-17	0	17	10	A	2	0	3			8370
1000001	P00248942	F	0-17	0	17	10	A	2	0	1	6	14	15200
1000001	P00087842	F	0-17	0	17	10	A	2	0	12			1422
1000001	P00085442	F	0-17	0	17	10	A	2	0	12	14		1057
1000002	P00285442	M	55+	55	80	16	C	4+	0	8			7969
1000003	P00193542	M	26-35	26	35	15	A	3	0	1	2		15227
1000004	P00184942	M	46-50	46	50	7	B	2	1	1	8	17	19215
1000004	P00346142	M	46-50	46	50	7	B	2	1	1	15		15854
1000004	P0097242	M	46-50	46	50	7	B	2	1	1	16		15686
1000005	P00274942	M	26-35	26	35	20	A	1	1	8			7871
1000005	P00251242	M	26-35	26	35	20	A	1	1	5	11		5254

Methods to deal with Qualitative/ Categorical Variables

Combine Levels: one can sometimes simply combine the different levels. There are various methods of combining levels. Here are commonly used ones:

Using Business Logic

Methods to deal with Qualitative/ Categorical Variables

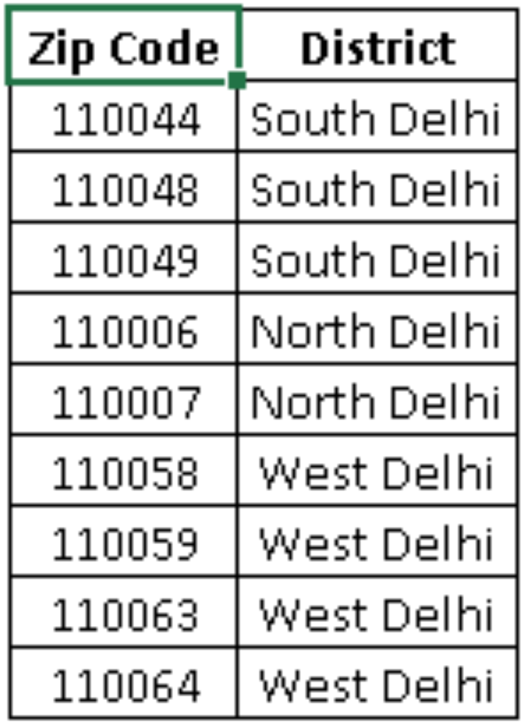
Combine Levels:

Using Business Logic

For example, we can combine levels of a variable “zip code” at state or district level. This will reduce the number of levels and improve the model performance also.

Methods to deal with Qualitative/ Categorical Variables

Combine Levels: Using Business Logic



Zip Code	District
110044	South Delhi
110048	South Delhi
110049	South Delhi
110006	North Delhi
110007	North Delhi
110058	West Delhi
110059	West Delhi
110063	West Delhi
110064	West Delhi

Methods to deal with Qualitative/ Categorical Variables

Combine Levels:

Using frequency or response rate:

When we don’t have domain knowledge about the levels, we combine levels by considering the frequency distribution or response rate.

Methods to deal with Qualitative/ Categorical Variables

Combine Levels:

Using frequency or response rate:

Consider the frequency distribution of of each level and combine levels having frequency less than 5% of total observation (5% is standard but you can change it based on distribution). This is an effective method to deal with rare levels.

Methods to deal with Qualitative/ Categorical Variables

Combine Levels:

Using frequency or response rate:

We can also combine levels by considering the response rate of each level. We can simply combine levels having similar response rate into same group.

Methods to deal with Qualitative/ Categorical Variables

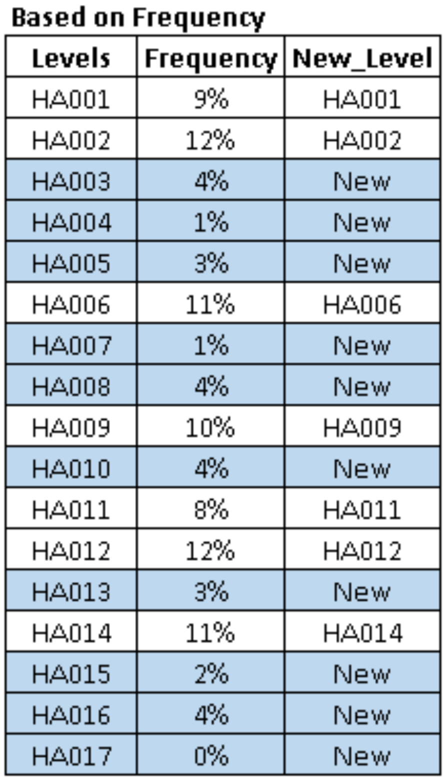
Combine Levels:

Using frequency or response rate:

Finally, you can also look at both frequency and response rate to combine levels. You first combine levels based on response rate then combine rare levels to relevant group.

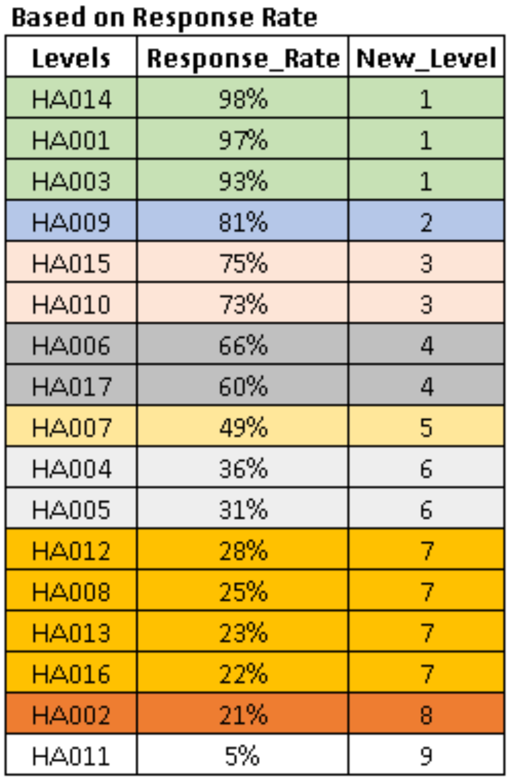
Methods to deal with Qualitative/ Categorical Variables

Combine Levels:



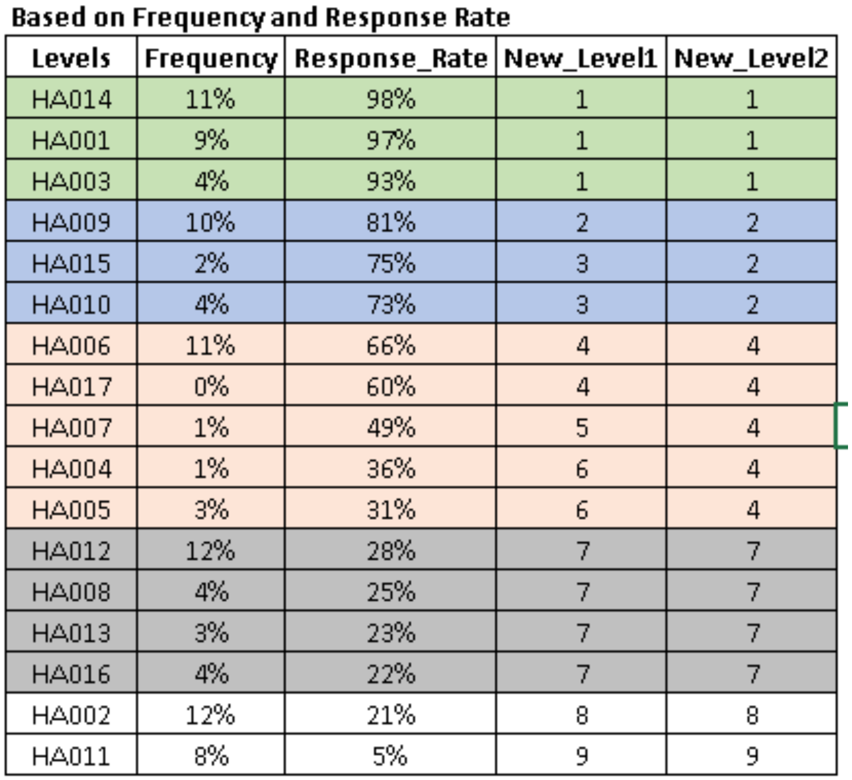
Based on Frequency

Levels	Frequency	New_Level
HA001	9%	HA001
HA002	12%	HA002
HA003	4%	New
HA004	1%	New
HA005	3%	New
HA006	11%	HA006
HA007	1%	New
HA008	4%	New
HA009	10%	HA009
HA010	4%	New
HA011	8%	HA011
HA012	12%	HA012
HA013	3%	New
HA014	11%	HA014
HA015	2%	New
HA016	4%	New
HA017	0%	New



Based on Response Rate

Levels	Response_Rate	New_Level
HA014	98%	1
HA001	97%	1
HA003	93%	1
HA009	81%	2
HA015	75%	3
HA010	73%	3
HA006	66%	4
HA017	60%	4
HA007	49%	5
HA004	36%	6
HA005	31%	6
HA012	28%	7
HA008	25%	7
HA013	23%	7
HA016	22%	7
HA002	21%	8
HA011	5%	9



Based on Frequency and Response Rate

Levels	Frequency	Response_Rate	New_Level1	New_Level2
HA014	11%	98%	1	1
HA001	9%	97%	1	1
HA003	4%	93%	1	1
HA009	10%	81%	2	2
HA015	2%	75%	3	2
HA010	4%	73%	3	2
HA006	11%	66%	4	4
HA017	0%	60%	4	4
HA007	1%	49%	5	4
HA004	1%	36%	6	4
HA005	3%	31%	6	4
HA012	12%	28%	7	7
HA008	4%	25%	7	7
HA013	3%	23%	7	7
HA016	4%	22%	7	7
HA002	12%	21%	8	8
HA011	8%	5%	9	9

Methods to deal with Qualitative/ Categorical Variables

Dummy Coding

Dummy coding is a commonly used method for converting a categorical input variable into continuous variable. ‘Dummy’, as the name suggests is a duplicate variable which represents one level of a categorical variable.

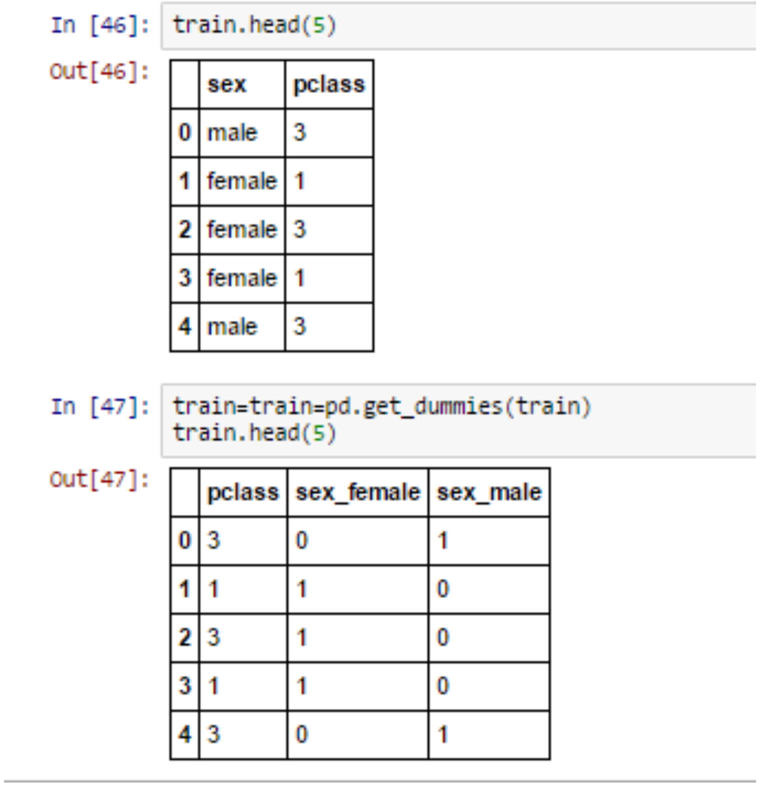
Methods to deal with Qualitative/ Categorical Variables

Dummy Coding

Presence of a level is represent by 1 and absence is represented by 0. For every level present, one dummy variable will be created. Look at the representation below to convert a categorical variable using dummy variable.

Methods to deal with Qualitative/ Categorical Variables

Dummy Coding



In [46]:
```
train.head(5)
```

Out[46]:

	sex	pclass
0	male	3
1	female	1
2	female	3
3	female	1
4	male	3

In [47]:
```
train=train=pd.get_dummies(train)
train.head(5)
```

Out[47]:

	pclass	sex_female	sex_male
0	3	0	1
1	1	1	0
2	3	1	0
3	1	1	0
4	3	0	1

Methods to deal with Qualitative/ Categorical Variables

Dummy Coding

Note: Assume, we have 500 levels in categorical variables. Then, should we create 500 dummy variables? If you can automate it, very well. Or else, I'd suggest you to first, reduce the levels by using combining methods and then use dummy coding. This would save your time. This method is also known as "One_Hot Encoding".

Methods to deal with Qualitative/ Categorical Variables

Feature Hashing

Read:

https://blog.myyellowroad.com/using-categorical-data-in-machine-learning-with-python-from-dummy-variables-to-deep-category-66041f734512