CS 397: Topics in Computer Science–Probability & Statistics

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Regression & Correlation

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Although it has been around for a very long time, it is still one of the most widely used statistical learning methods

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Several questions we can answer with linear regression are:

- Is there a relationship between two or more variables?
- How strong is the relationship?
- What are the effects of the different variables?
- Can we make accurate predictions?
- Is the relationship linear?
- Is there synergy among the variables?

Simple Linear Regression In the simple linear regression (SLR) model there is one independent variable and has the form

$$Y \approx \beta_0 + \beta_1 X$$

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β_0, β_1 are coefficients, or model parameters

Model training results in the estimates $\hat{\beta}_0$ and $\hat{\beta}_1$

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We can use these estimates to predict the response value for a given input

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

where $\hat{y} = \mathbb{E}[Y|X = x]$

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- SLR is based on the idea of least squares – find the coefficients $\hat{\beta}_0$ and $\hat{\beta}_1$ that describe the line that minimizes the squared errors

$\hat{y}_i$ is the predicted value for the i-th observation

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$$RSS = e_1^2 + e_2^2 + e_3^2 + \cdots + e_n^2 = \sum_{i=1}^{n} e_i^2 = \sum_{i=1}^{n} (y_i - \hat{y}_i)^2$$

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Least squares minimizes RSS

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Using calculus we can find the values of $\hat{\beta}_0$ and $\hat{\beta}_1$ that minimize RSS are

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

and

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

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- ϵ is the error term

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$\hat{\beta}_0$ and $\hat{\beta}_1$ are *unbiased* estimates – if we estimate $\hat{\beta}_0$ and $\hat{\beta}_1$ repeatedly over many data sets drawn from the same population then $\hat{\beta}_0 \to \beta_0$ and $\hat{\beta}_1 \to \beta_1$

If we estimate the population mean as $\hat{\mu}$ then

$$\mathrm{Var}\left(\hat{\mu}\right) = \frac{\sigma^2}{n} = SE(\hat{\mu}) \tag{14.1}$$

where $\sigma^2 = \mathrm{Var}\left(\epsilon\right)$

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where $\sigma^2 = \operatorname{Var}(\epsilon)$

The standard error $SE(\hat{\mu})$ gives the average amount by which $\hat{\mu}$ differs from μ

Additionally,

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

and

$$SE(\hat{\beta}_1)^2 = \frac{\sigma^2}{\sum_{i=1}^{n}(x_i - \overline{x})^2}$$

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What does this mean?

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What does this mean? There's a 95% chance that the interval contains the true β_i

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- Does the estimate $\hat{\beta}_1$ differ significantly from zero?

- This depends on the value of $\hat{\beta}_1$ and $SE(\hat{\beta}_1)$

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- This statistic has a t-distribution with $n - 2$ degrees of freedom
- The p-value associated with this t-statistic helps us make a decision about H_0

Definition

p-value is the probability of observing a value of $|t|$ or greater (absolute value) when H_0 is true

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- A small p-value suggests there is enough evidence to reject H_0 and conclude $\beta_1 \neq 0$
- In other words, with a small p-value it is unlikely that H_0 is true

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Table 14.1: Least squares coefficients for Regressing Sales on TV ads from the **`Advertising`** data.

	Coefficient	Std. Error	t-statistic	p-value
`Intercept`	7.0325	0.4578	15.36	< 0.0001
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The results show that there is a statistically significant relationship between money spent of **TV** ads and **Sales**

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Recall $RSE = \sqrt{\frac{1}{n-2}RSS}$, and we define the **Total Sum of Squares**

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

and

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

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- $R^2 \in [0, 1]$ so R^2 from different models are comparable

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- For SLR $R^2 = r^2$, however this does not hold for Multiple Linear Regression – thus R^2 is the measure we'll use

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- Above we looked at the sample correlation r which is an estimate of the population correlation, ρ

Exercise

Compute and interpret the correlation coefficient for the following grades of 6 students selected at random:

Math Grade	70	92	80	74	65	83
English Grade	74	84	63	87	78	90

Multiple Linear Regression

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Instead we fit a MLR model using all the variables

$$Y = \beta_0 + \beta_1 X_1 + \beta_2 X_2 + \cdots + \beta_p X_p \tag{14.19}$$

Estimating the Coefficients

Given $\hat{\beta}_0, \hat{\beta}_1, \ldots, \hat{\beta}_p$ we can make predictions via

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Like SLR we find the $\hat{\beta}$'s that minimize the RSS

$$\begin{aligned} RSS &= \sum_{i=1}^{n} (y_i - \hat{y})^2 \\ &= \sum_{i=1}^{n} (y_i - \hat{\beta}_0 - \hat{\beta}_1 x_1 - \cdots - \hat{\beta}_p x_p)^2 \end{aligned}$$

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In matrix notation the coefficients are

$$\hat{\beta} = \left(\mathbf{X}^{\mathrm{T}}\mathbf{X}\right)^{-1} \mathbf{X}^{\mathrm{T}}\mathbf{y}$$

Let's compare ...

Table 14.3: Simple regression of **sales** on **radio** (top) and **sales** on **newspaper** (bottom)

	Coefficient	Std. error	t-statistic	p-value
Intercept	9.312	0.563	16.54	< 0.0001
radio	0.203	0.020	9.92	< 0.0001

	Coefficient	Std. error	t-statistic	p-value
Intercept	12.351	0.621	19.88	< 0.0001
newspaper	0.055	0.017	3.30	< 0.0001

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Both **radio** and **newspaper** are statistically significant

Table 14.4: Multiple regression of **sales** on **TV, radio, newspaper**

	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

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When all three predictors are in the model, **`newspaper`** is no longer significant *given* **`TV`** and **`radio`** are already included

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The F-statistic in the MLR case is

$$F = \frac{(TSS - RSS)/p}{RSS/(n-p-1)} \tag{14.23}$$

Linear Regression

If the linear model assumptions are correct and H_0 is true then

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If H_a is true then

$$\mathbb{E}[(TSS - RSS)/p] > \sigma^2$$

so we expect $F > 1$

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We find the p-value associated with the F-statistic and make a decision

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We then fit a models using all the variables except the last q and find RSS_0, the RSS for the reduced model

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We don't have this problem with F because the statistic adjusts for p

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If $p > n$ we cannot fit a model

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- Bayesian Information Criterion (BIC)
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We will discuss these more in Chapter 6

Given some value for p there are 2^p possible models and as p grows it becomes infeasible to try them all

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Three approaches to model building

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Forward Selection: Start with a null model using β_0. Fit p individual (SLR) models and add the variable with the lowest RSS to the null model. Keep going until you cannot add more.

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Backward Selection: Start with all the variables and remove the one with the highest p-value. Continue until there are no variables with a p-value $> \alpha$.

Mixed Selection: Start with the null model and add variables like forward selection. If the p-value of a variable already in the model goes above α take it out. Continue until all the variables in the model have p-values less than α and adding more would have p-value $> \alpha$

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- Mixed selection always works and doesn't have these issues

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RSE in MLR is

$$RSE = \sqrt{\frac{1}{n-p-1}RSS}$$

which reduces to the equation we for SLR when $p = 1$

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Visualization

Visualization

Graphs are essential and can highlight problems not detectable with numerical statistics

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The residuals in the following graph suggest a non-linear relationship which is probably due to an interaction between variables (more later)

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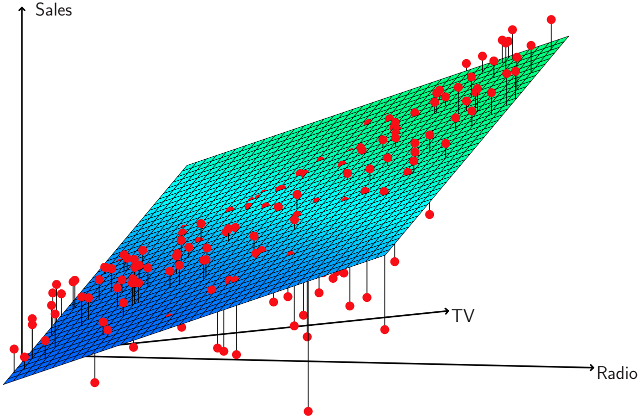

Figure 14.5: Response surface **Advertising** data **sales**∼**TV**+**radio**

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We can use our model to predict the reponse Y given a set of predictors $X_1, X_2, \ldots, X_p$

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(a) $\hat{\beta}$'s are estimates for the true β's

$$\hat{Y} = \hat{\beta}_0 + \hat{\beta}_1 X_1 + \cdots + \hat{\beta}_p X_p \text{ vs. the true}$$
$$f(X) = \beta_0 + \beta_1 X_1 + \cdots + \beta_p X_p$$
$$f(X) - \hat{Y} : \text{Reducible error}$$

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Prediction intervals quantify the uncertainty around a specific predicted value given X

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- The **`Credit`** data set has a number of quantitative variables and four qualitative ones: **`gender`**, **`student`**, (marital) **`status`**, and **`ethnicity`**

Qualitative variables are also known as categorical variables, or factors `gender` has two levels so we use a "dummy" variable

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

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In a regression model this becomes

$$y_i = \beta_0 + \beta_1 x_i + \epsilon_i = \begin{cases} \beta_0 + \beta_1 + \epsilon & \text{if female} \\ \beta_0 + \epsilon & \text{if male} \end{cases}$$

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For the **Credit** data, β_0 is the average card balance for males, and $\beta_0 + \beta_1$ is the average card balance for females

Here we list the regression model output and notice that there is no statistically significant evidence that card balance varies by gender (p-value $= 0.6690$)

Table 14.7: Least squares estimates for `balance` on `gender`

	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

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$$x_i = \begin{cases} 1 & \text{if female} \\ -1 & \text{if male} \end{cases}$$

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The **`ethnicity`** variable in the **`Credit`** data set has three levels African-American, Asian and Caucasian

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The `ethnicity` variable in the `Credit` data set has three levels African-American, Asian and Caucasian

$$x_{i1} = \begin{cases} 1 & \text{if Asian} \\ 0 & \text{if not Asian} \end{cases}$$

and

$$x_{i1} = \begin{cases} 1 & \text{if Caucasian} \\ 0 & \text{if not Caucasian} \end{cases}$$

$$y_i = \beta_0 + \beta_1 x_{i1} + \beta_2 x_{i2} + \epsilon_i = \begin{cases} \beta_0 + \beta_1 + \epsilon_i & \text{if Asian} \\ \beta_0 + \beta_2 + \epsilon_i & \text{if Caucasian} \\ \beta_0 + \epsilon_i & \text{if African-American} \end{cases}$$

African-American in this example is the *baseline*

Table 3.8 shows the R output for this model, but the **ethnicity** variable is not statistically significant

Table 14.8: Least squares estimates for **balance** on **ethnicity**

	Coefficient	Std. Error	t-statistic	p-value
Intercept	531.00	46.32	11.646	< 0.0001
ethnicity[Asian]	-18.69	65.02	-0.287	0.7740
ethnicity[Caucasian]	-12.50	56.68	-0.221	0.8260

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Of course we can use quantitative and qualitative variables in the same MLR model

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Sometimes the effects of the predictors are not independent as assumed

When the change in one variable affects another we say there is an *interaction* effect (marketing people call this *synergy*)

Suppose we have a linear model with two variables

$$Y = \beta_0 + \beta_1 X_1 + \beta_2 X_2 + \epsilon$$

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We can extend this model to include an *interaction term* $X_1 X_2$

$$Y = \beta_0 + \beta_1 X_1 + \beta_2 X_2 + \beta_3 X_1 X_2 + \epsilon \qquad (14.31)$$

We can re-write (14.24) as

$$
\begin{aligned}
Y &= \beta_0 + (\beta_1 + \beta_3 X_2)X_1 + \beta_2 X_2 + \epsilon \\
&= \beta_0 + \tilde{\beta}_1 X_1 + \beta_2 X_2 + \epsilon
\end{aligned} \tag{14.32}
$$

where $\tilde{\beta}_1 = \beta_1 + \beta_3 X_2$

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where $\tilde{\beta}_1 = \beta_1 + \beta_3 X_2$

From (14.32) it's apparent that as X_2 changes so does $\tilde{\beta}_1$ which changes the effect of X_1 on Y, thus the interaction

Example

Suppose that we are interested in studying the productivity of a factory. We wish to predict the number of **`units`** *produced on the basis of the number of production* **`lines`** *and the total number of* **`workers`***. It seems likely that the effect of increasing the number of production* **`lines`** *will depend on the number of* **`workers`***, since if no* **`workers`** *are available to operate the* **`lines`***, then increasing the number of* **`lines`** *will not increase* **`production`***. This suggests that it would be appropriate to include an interaction term between* **`lines`** *and* **`workers`** *in a linear model to predict* **`units`***.*

Example

Say we get the following results after fitting the model

$$\begin{aligned}\texttt{units} &\approx 1.2 + 3.4 \times \texttt{lines} + 0.22 \times \texttt{workers} \\ &\qquad + 1.4 \times \texttt{lines} \times \texttt{workers} \\ &= 1.2 + (3.4 + 1.4 \times \texttt{workers}) \times \texttt{lines} + 0.22 \times \texttt{workers}\end{aligned}$$

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For additional `line` added the number of `units` goes up by $3.4 + 1.4 \times \texttt{workers}$

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Using the `Advertising` data from earlier, we regress `sales` on `radio`, `TV`, and the interaction between the two

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$$\begin{aligned}\texttt{sales} &= \beta_0 + \beta_1 \times \texttt{TV} + \beta_2 \times \texttt{radio} + \beta_3 \times (\texttt{radio} \times \texttt{TV}) + \epsilon \\ &= \beta_0 + (\beta_1 + \beta_3 \times \texttt{radio}) \times \texttt{TV} + \beta_2 \times \texttt{radio} + \epsilon\end{aligned} \tag{14.33}$$

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Hereto we see that the effect of one variable (**TV**) is a function of another variable (**radio**)

The fitted model from (14.33) gives the following results

Table 14.9: Least squares estimates for **`sales`** on **`radio`**, **`TV`**, and their interaction.

	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` $\times$ **`radio`**	0.0011	0.000	20.73	< 0.0001

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From the table we note that the main effects and interaction term are all statistically significant

From Table 14.9 we see all the variables, main effects and interaction, are significant

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The *hierarchical principle* tells us if the interaction term is significant we should include the main effects even if one or both are not

Interactions also work with qualitative variables

Interactions also work with qualitative variables
From the **Credit** data we regress **balance** on **income** and the qualitative variable **student**

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

$$= \beta_1 \times \texttt{income}_i + \begin{cases} \beta_0 + \beta_2 & \text{if student} \\ 0 & \text{if not} \end{cases}$$

It's possible that income has a different effect on students and non-students so we test this by including an interaction term

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

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- Polynomial Regression a linear model with polynomial functions as predictors
- Using the **Auto** data we regress **mpg** on **horsepower** and plot the results for a linear model a second-degree polynomial and a fifth-degree polynomial on the next slide

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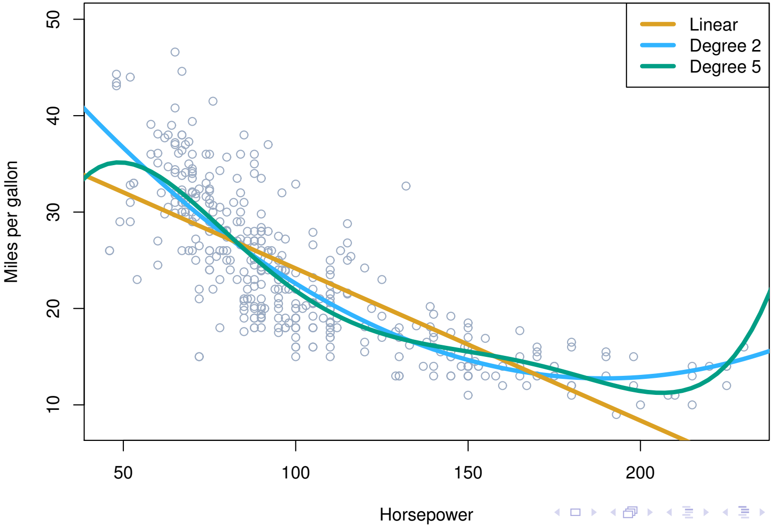
Comparing a linear fit with a second-degree and fifth-degree polynomial



- The quadratic polynomial fits the data the best suggesting the model

$$\texttt{mpg} = \beta_0 + \beta_1 \times \texttt{horsepower} + \beta_2 \times \texttt{horsepower}^2 + \epsilon$$

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- Although we use a non-linear function of horsepower this is still alinear model because it is linear in its parameters

$$Y = \beta_0 + \beta_1 X_1 + \beta_2 X_2 + \epsilon$$

where $X_1 = \texttt{horsepower}$ and $X_2 = \texttt{horsepower}^2$

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Exercise

Fit the quadratic model using the `Auto` data

It seems too good to be true!

- We may encounter problems after we fit a linear regression model

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    1. Non-linearity of the X, Y relationship
    2. Correlation of the error terms
    3. Non-constant variance of the error terms
    4. Outliers

It seems too good to be true!

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- Many of these challenge the underlying assumptions of our model
    1. Non-linearity of the X, Y relationship
    2. Correlation of the error terms
    3. Non-constant variance of the error terms
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- Plot the residuals against $\hat{y}_i$ for MLR

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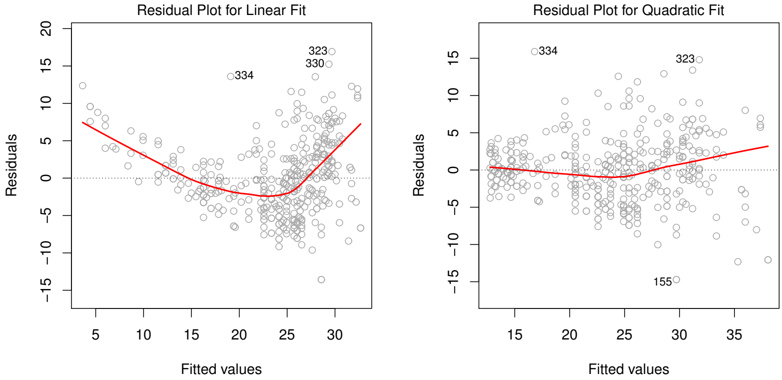
Resdiual Plots left: linear fit; right: quadratic fit



To remove the non-linearity we can transform the predictors with non-linear transformations such as $\log X, \sqrt{X}, X^2$

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- *If* the errors *are* correlated the standard error will be underestimated
- Correlated error terms occur frequently in time series data
- Often observations in adjacent time periods will be correlated

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- Sometimes the variance of the error terms is not constant known as *heteroscedasticity*
- If the error terms have non-constant variance the residual plot will show a funnel shape

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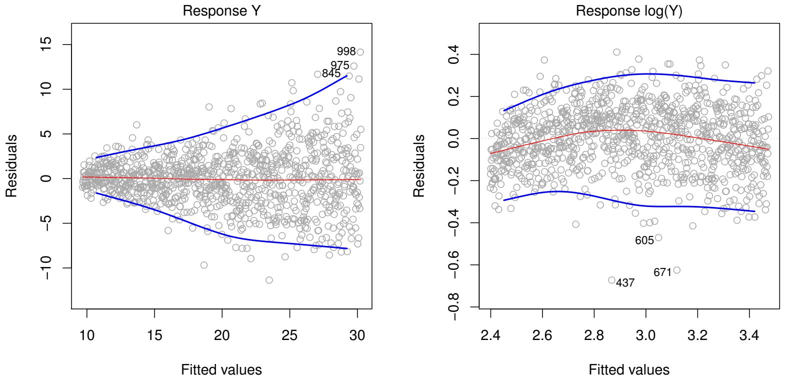
Residual plots for the original data showing heteroscedasticity (left) and for the transformed data (right)



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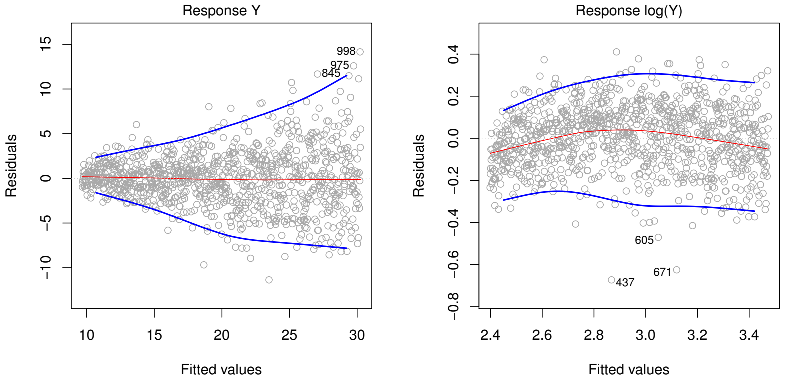

Transforming Y using $\log Y$ (as in the left plot) or $\sqrt{Y}$ generally reduces heteroscedasticity

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- Residual plots help identify outliers, we plot Studentized residuals, $e_i/SE(e_i)$, against fitted values
- Any data point for which $\left|\frac{e_i}{SE(e_i)}\right| > 3$ is a possible outlier

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- Removing a high-leverage point has a bigger impact on the model than removing an outlier
- The leverage statistic for SLR is

$$h_i = \frac{1}{n} + \frac{(x_i - \overline{x})^2}{\sum_{i'=1}^{n} (x_{i'} - \overline{x})^2}$$

which extends to MLR but for thr latter we'll let R calculate it

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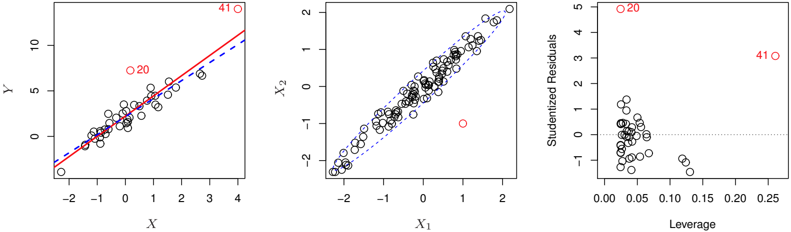

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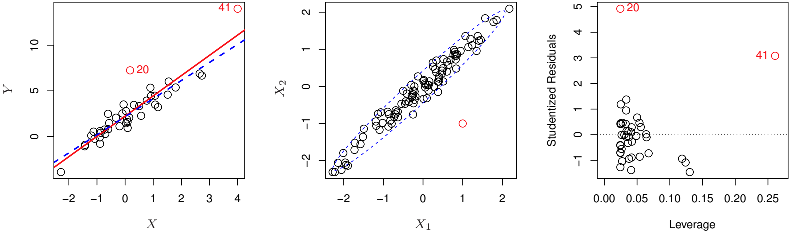

- Point 41 is an outlier *and* a high leverage point that can greatly influence our regression

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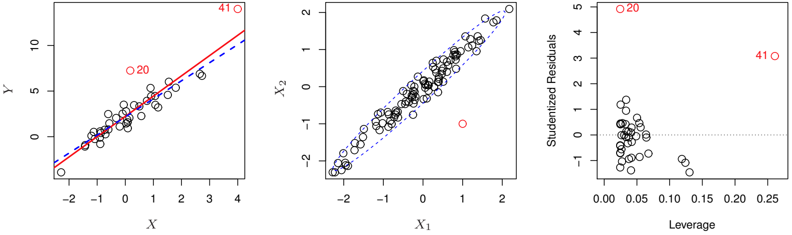

- Point 41 is an outlier *and* a high leverage point that can greatly influence our regression
- Point 20 is an outlier but has very low leverage thus has little effect on the regression

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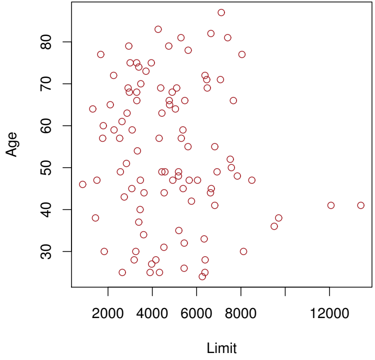
- Using the `Credit` data Figure 3.14 (next slide) illustrates collinearity
- In the left panel `age` and `limit` have no relationship but on the right it's clear that `rating` and `limit` are highly correlated
- Since they are so strongly correlated it's difficult to determine how each relates to the response

The variables on the left are uncorrelated but those on the right are highly correlated



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- Collinearity causes one variable to be insignificant when another, correlated variable is in the model

Variance Inflation Factor

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The closer $R^2_{X_j|X_{-j}}$ is to one, the larger VIF gets, indicating the presence of multicollinearity

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R output for a multiple linear regression model

```
Call:
lm(formula = mpg ~ . - name, data = Auto)

Residuals:
    Min      1Q  Median      3Q     Max
-9.5903 -2.1565 -0.1169  1.8690 13.0604

Coefficients:
               Estimate Std. Error t value Pr(>|t|)
(Intercept)  -17.218435   4.644294  -3.707  0.00024 ***
cylinders     -0.493376   0.323282  -1.526  0.12780
displacement   0.019896   0.007515   2.647  0.00844 **
horsepower    -0.016951   0.013787  -1.230  0.21963
weight        -0.006474   0.000652  -9.929  < 2e-16 ***
acceleration   0.080576   0.098845   0.815  0.41548
year           0.750773   0.050973  14.729  < 2e-16 ***
origin         1.426141   0.278136   5.127 4.67e-07 ***
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

Residual standard error: 3.328 on 384 degrees of freedom
Multiple R-squared:  0.8215, Adjusted R-squared:  0.8182
F-statistic: 252.4 on 7 and 384 DF,  p-value: < 2.2e-16
```

References

Miller, I. and Miller, M. (2014).
John E. Freund's Mathematical Statistics with Applications.
Pearson, 8th edition.