Regression Methods

Stephen Jun Villejo

School of Statistics

Linear Regression

- Linear Regression is a simple supervised learning tool, and is useful for predicting a quantitative response.
- A *simple linear regression* assumes an approximately linear model between a quantitative response Y on the basis of a single predictor variable X.
- The model is given by:

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

- More precisely, we have the model

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

- The systematic part of the model is $\beta_0 + \beta_1 X.$
- The term ϵ is a mean-zero random error term.

Linear Regression

Example

- For example, to answer the question if TV advertising is linearly related with sales, we will fit the linear model given by:

$$\texttt{sales} \approx \beta_0 + \beta_1 \times \texttt{TV}.$$

- β_0 and β_1 are two unknown constants that represent the intercept and slope terms, respectively. Both are called the model *coefficients* or *parameters.*
- Once we have used our data to produce estimates $\hat{\beta}_0$and $\hat{\beta}_1$, we can predict sales on the basis of a particular value of TV advertising through

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

Linear Regression

Estimating the Coefficients

- Our goal is to find $\hat{\beta}_0$ and $\hat{\beta}_1$ such that the resulting line is as close as possible to the data points.
- There are a number of ways of measuring *closeness*.
- The most common approach involves minimizing the *least squares* criterion.
- Let $\hat{y}_i = \hat{\beta}_0 + \hat{\beta}_1 x_i$ be the predicted value of Y for *i*th observation.
- Define $e_i = y_i - \hat{y}_i$ as the residual of the *i*th observation.

Linear Regression

Estimating the Coefficients

- The **least squares approach** chooses $\hat{\beta}_0$and $\hat{\beta}_1$ that will minimize

$$\mathrm{RSS} = e_1^2 + e_2^2 + \cdots + e_n^2,$$

- The least squares estimators are:

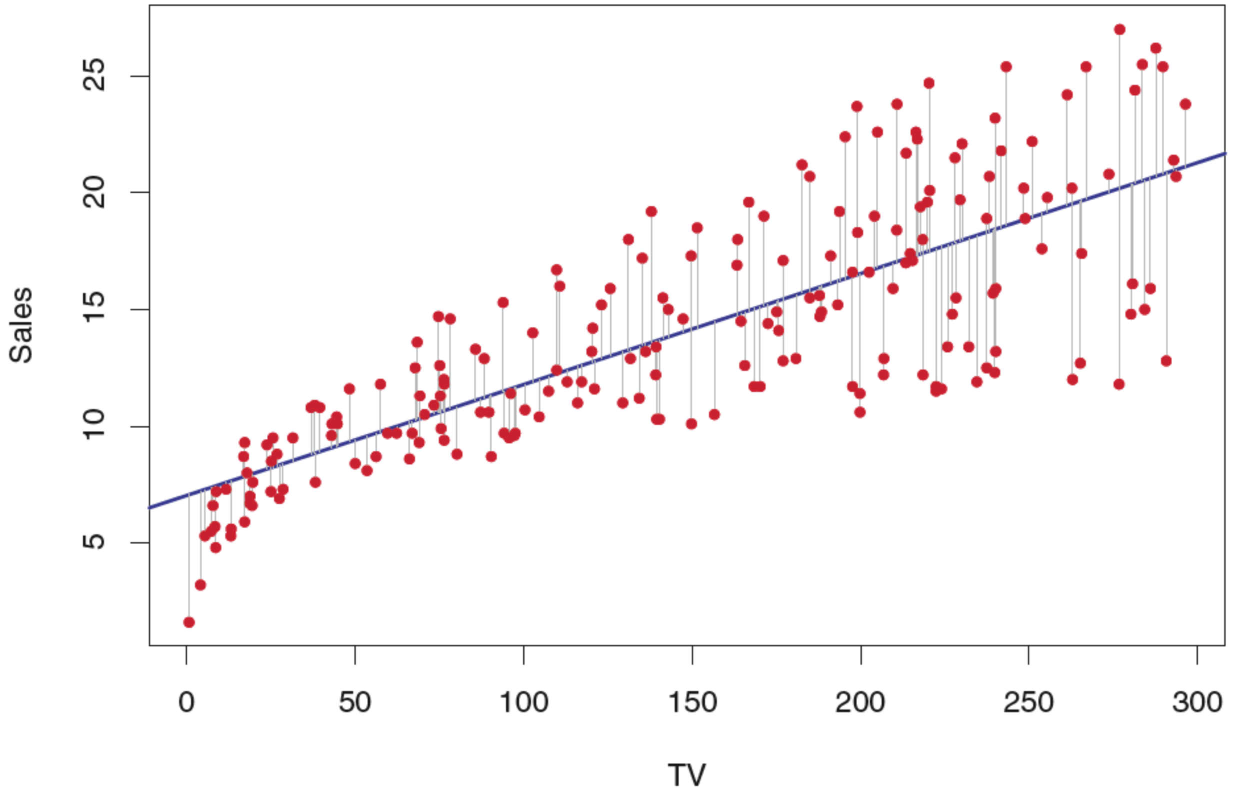
$$\hat{\beta}_1 = \frac{\sum_{i=1}^{n}(x_i - \bar{x})(y_i - \bar{y})}{\sum_{i=1}^{n}(x_i - \bar{x})^2},$$

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

Linear Regression

Estimating the Coefficients

- The figure below displays the simple linear regression fit where $\hat{\beta}_0 = 7.03$ and $\hat{\beta}_1 = 0.0475$.



Linear Regression

Standard Errors

- How accurate are $\hat{\beta}_0$ and $\hat{\beta}_1$ as estimates for β_0 and β_1?
- We answer this by computing the standard error of our estimates.
- Roughly speaking, the standard error tells us the average amount that the estimate differs from the actual value.

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

Linear Regression

Confidence Intervals

- Standard error can be used to compute **confidence intervals**.
- A 95% confidence interval is defined as a range of values such that with 95% probability, the range will contain the true unknown value of the parameter.
- 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.
- Similarly, for β_0 we have $\hat{\beta}_0 \pm 2 \cdot \mathrm{SE}(\hat{\beta}_0)$.

Linear Regression

Tests of Significance

- Standard error can also be used to perform **hypothesis tests** on the coefficients.
- The most common hypothesis is:

  $\mathrm{H_o}$: There is no linear relationship between X and Y.

  $\mathrm{H_1}$: There is a linear relationship between X and Y.
- Mathematically, this corresponds to testing:

  $\mathrm{H_o}: \beta_1 = 0$

  $\mathrm{H_1}: \beta_1 \neq 0$
- We look at the p-value of the test in making the decision whether to reject or not reject the null hypothesis.

Linear Regression

Tests of Significance

- Roughly speaking, we interpret the **p-value** as follows: a small p-value indicates that it is unlikely to observe such a substantial association between the predictor and the response due to chance.
- Thus, we *reject the null hypothesis* – that is, we declare a relationship to exist between X and Y – if the p-value is small enough.
- Typical cutoffs for rejecting the null hypothesis are 5% or 1%.

Linear Regression

Tests of Significance

- The computation of the p-value is based on the *t-statistic* given by

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

- In our Advertising example, we have:

	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

Linear Regression

Assessing the Accuracy of the Model

- The quality of a linear regression fit is typically assessed using two related quantities: **residual standard error** and $\mathbf{R^2}$ statistic.
- The residual standard error (RSE) is an estimate of the standard deviation, ϵ, of the linear regression model.
- It is computed using the formula:

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

- The RSE is considered a measure of the *lack of fit*.

Linear Regression

Assessing the Accuracy of the Model

- The $\mathbf{R^2}$ statistic takes the form of a proportion – the proportion of variance explained by the model – and so it always takes on a value between 0 and 1.
- To calculate $\mathbf{R^2}$, we have:

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

- TSS is the total sum of squares, defined as $\mathrm{TSS} = \sum (y_i - \bar{y})^2$
- The $\mathbf{R^2}$ statistic measures the amount of variability in Y that can be explained using X.

Linear Regression

Assessing the Accuracy of the Model

- The $\mathbf{R^2}$ statistic has an interpretational advantage over the RSE.
- However, it can still be challenging to determine what is a *good* R^2 value.
- Recall the correlation between X and Y defined as

$$\mathrm{Cor}(X, Y) = \frac{\sum_{i=1}^{n}(x_i - \overline{x})(y_i - \overline{y})}{\sqrt{\sum_{i=1}^{n}(x_i - \overline{x})^2}\sqrt{\sum_{i=1}^{n}(y_i - \overline{y})^2}},$$

- The R^2 is the square of $\mathrm{Cor}(\mathrm{X}, \mathrm{Y})$.

R Exercise

Multiple Linear Regression

- In practice we have more than one predictors. Instead of fitting a separate simple linear regression model for each predictor, we extend the simple linear regression model to

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

- Here, we interpret β_j as the average effect on Y of a one unit increase in X_j, holding all other predictors fixed.
- In our advertising example, we have

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

Multiple Linear Regression

Estimating the Regression Coefficients

- The parameters are also estimated using the same least squares approach.
- We choose $\beta_0, \beta_1, \ldots, \beta_p$ to minimize the sum of squared residuals

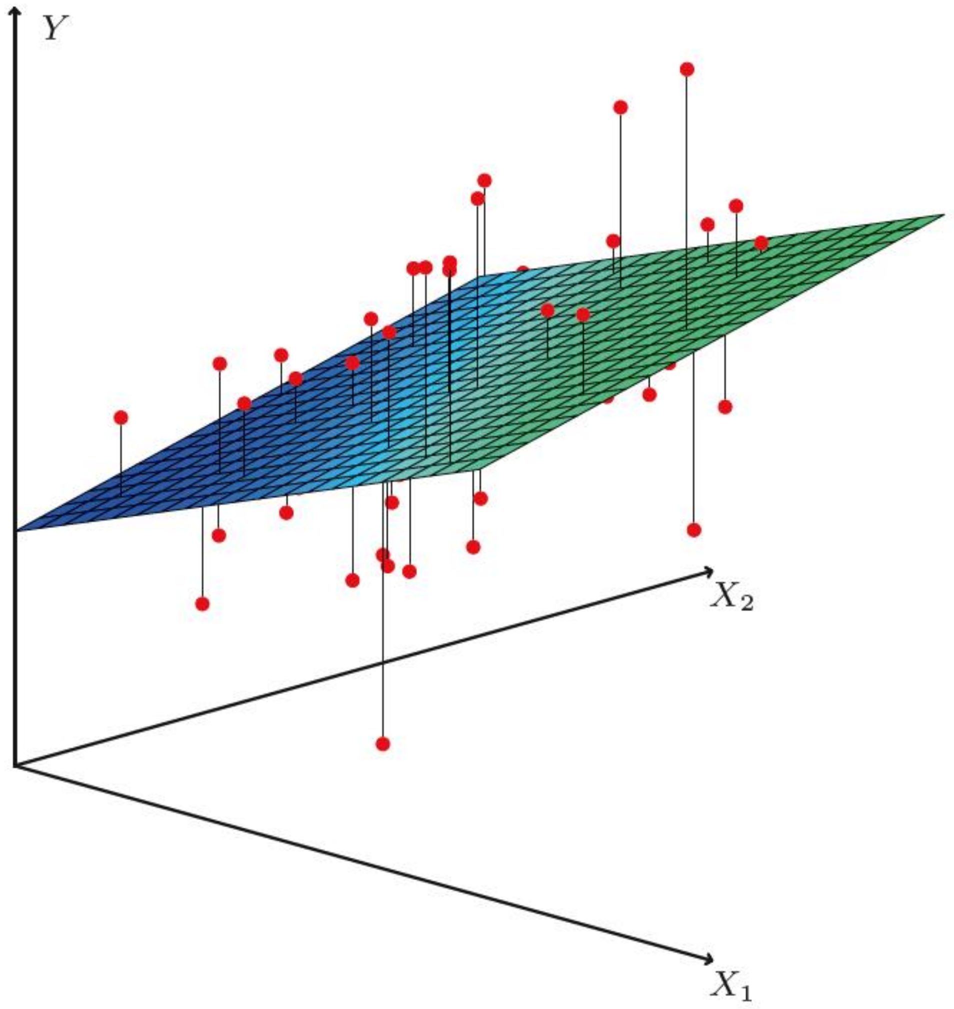
$$\begin{aligned}\mathrm{RSS} &= \sum_{i=1}^{n}(y_i - \hat{y}_i)^2 \\ &= \sum_{i=1}^{n}(y_i - \hat{\beta}_0 - \hat{\beta}_1 x_{i1} - \hat{\beta}_2 x_{i2} - \cdots - \hat{\beta}_p x_{ip})^2.\end{aligned}$$

- Unlike the simple linear regression coefficient estimates, the multiple linear regression coefficient estimates have somewhat complicated forms that are most easily represented using matrix algebra.

Multiple Linear Regression

Estimating the Regression Coefficients

- In a three-dimensional setting, with two predictors and one response, the least squares regression line becomes a plane.
- The plane is chosen to minimize the sum of the squared vertical distances between each observation and the plane.



Multiple Linear Regression

Example

- For the Advertising data, we have the following coefficient estimates:

	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

Multiple Linear Regression

Some Important Questions

- Is at least one of the predictors $X_1, X_2, \ldots, X_p$ useful in predicting the response?
- Do all the predictors help to explain Y, or is only a subset of the predictors useful?
- Given a set of predictor values, what response value should we predict, and how accurate is our prediction?

Multiple Linear Regression

Is There a Relationship Between the Response and Predictors?

- We use a hypothesis test to answer this question.
- We test the null hypothesis,

$$H_0 : \beta_1 = \beta_2 = \cdots = \beta_p = 0$$

versus the alternative

$$H_a : \text{ at least one } \beta_j \text{ is non-zero.}$$

- The hypothesis is performed by computing the *F-statistic*

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

Multiple Linear Regression

Is There a Relationship Between the Response and Predictors?

- When there is no relationship between the response and predictors, one would expect the F-statistics to take on a value close to 1.
- A large F-statistic suggests that at least one of the predictors is significantly related to the response.
- The p-value associated with the F-statistic is used to determine whether or not to reject H_0.

Multiple Linear Regression

Is There a Relationship Between the Response and Predictors?

- We also test the **partial effect** of each variable in the mode.
- These provide information about whether each individual predictor is related to the response, after adjusting for the other predictors.
- Test on the partial effect of the individual coefficients uses the t-statistic.
- In our Advertising example, we have:

	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
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Multiple Linear Regression

Remarks

- The approach of using an F-statistic to test for any association between the predictors and the response works when p is relatively small, and certainly small compared to n.
- If $p > n$, we cannot even fit the multiple linear regression model using least squars.
- When p is large, we use *high-dimensional* techniques.

Multiple Linear Regression

Deciding on Important Variables

- If we conclude that at least one of the predictors is related to the response, we want to know which are the *guilty* ones!
- Note that the RSS always decreases as more variables are added to the model.
- Determining which predictors (a subset) are associated with the response, in order to fit a single model, is referred to as ***variable selection***.
- For the many possible models, we determine the optimal model based on some criteria: Mallows's C_p, Akaike information criterion (AIC), Bayesian information criterion (BIC), and adjusted R^2.

Multiple Linear Regression

Deciding on Important Variables

Mallows's C_p

$$C_p = \frac{1}{n}\left(\mathrm{RSS} + 2d\hat{\sigma}^2\right),$$

- The C_p is an estimate of the MSE for a model with d predictors. The C_p adds a penalty to the RSS to adjust for the corresponding decrease in the RSS.
- We choose the model with the lowest C_p value.

Multiple Linear Regression

Deciding on Important Variables

AIC

$$\mathrm{AIC} = \frac{1}{n\hat{\sigma}^2}\left(\mathrm{RSS} + 2d\hat{\sigma}^2\right)$$

- AIC is proportional to the C_p value.

BIC

$$\mathrm{BIC} = \frac{1}{n}\left(\mathrm{RSS} + \log(n)d\hat{\sigma}^2\right)$$

- Like the C_p value and AIC, we select the model with the lowest BIC value.

Multiple Linear Regression

Deciding on Important Variables

Adjusted R^2

$$\text{Adjusted } R^2 = 1 - \frac{\text{RSS}/(n-d-1)}{\text{TSS}/(n-1)}.$$

- We select the model with the largest adjusted R^2.
- The intuition behind the adjusted R^2 is that once all of the correct variables have been included in the model, adding additional *noise* variables will lead to only a very small decrease in RSS.
- The adjusted R^2 statistic pays a price for the inclusion of unnecessary variables.

Multiple Linear Regression

Deciding on Important Variables

- Ideally, we try out all possible subset of the predictors. However, trying out every possible subset may be infeasible, even for moderate p.
- We have automated and efficient approaches to choose a smallest set of models to consider using: **Forward selection**, **Backward selection**, **Mixed** or **Stepwise selection**

Multiple Linear Regression

Deciding on Important Variables

Forward selection

- We begin with a null model.
- We then add to the model the variable that results in the lowest RSS.
- Then, we choose the next variable that will result in the lowest RSS for the new two-variable model.
- This is continued until some stopping rule is satisfied.

Multiple Linear Regression

Deciding on Important Variables

Backward selection

- We start with all variables in the model then remove the variable with the largest p-value, that is, the variable that is the least significant.
- The new (p-1)-variable model is fit, and the variable with the largest p-value is removed.
- This continues until all remaining variables have a p-value below some threshold.

Multiple Linear Regression

Deciding on Important Variables

Mixed selection

- This is a combination of forward and backward selection.

Multiple Linear Regression

Prediction

- The *least squares plane*

$$\hat{Y} = \hat{\beta}_0 + \hat{\beta}_1 X_1 + \cdots + \hat{\beta}_p X_p$$

  is only an estimate for the true population regression plane

$$f(X) = \beta_0 + \beta_1 X_1 + \cdots + \beta_p X_p.$$

- We can compute a confidence interval to determine how close $\hat{Y}$ will be to $f(x)$.
- Even if we know the true values β_0, $\beta_1, \ldots, \beta_p$, the response value cannot be predicted perfectly because of the random error.
- We use **prediction intervals** to quantify how much $\hat{Y}$ will vary from Y.
- **Prediction intervals** are wider than confidence intervals.

Other Considerations in the Regression Model

Qualitative Predictors

- To include qualitative predictors, we make use of dummy or indicator variables.

Predictors with Only Two Levels

- Here, we use only one indicator variable. For example, for *Gender:*

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

- This results to the model:

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

- β_1 is the average difference in Y between females and males.

Other Considerations in the Regression Model

Qualitative Predictors

Predictors with More Than Two Levels

- If a variable has d levels, we introduce (d-1) dummy variables.
- Example, for ethnicity = {Asian, Caucasian, African American} :

$$x_{i1} = \begin{cases} 1 & \text{if } i\text{th person is Asian} \\ 0 & \text{if } i\text{th person is not Asian,} \end{cases} \quad x_{i2} = \begin{cases} 1 & \text{if } i\text{th person is Caucasian} \\ 0 & \text{if } i\text{th person is not Caucasian.} \end{cases}$$

- Then we have the model:

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

Other Considerations in the Regression Model

Qualitative Predictors

Predictors with More Than Two Levels

- Then we have the model:

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

- β_1 can be interpreted as the difference in the average response between Asian and African American categories.
- β_2 is the average difference in the average response between Caucasian and African American.
- The level with no dummy variable is the **baseline** category.

Other Considerations in the Regression Model

Interaction Terms

- Previously, we concluded that both TV an radio seem to be associated with sales.
- We assumed that the effect of TV is independent of radio.
- 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?
- To account for this interaction, we include an **interaction term**.

Other Considerations in the Regression Model

Interaction Terms

- We have the model

$$Y = \beta_0 + \beta_1 X_1 + \beta_2 X_2 + \beta_3 X_1 X_2 + \epsilon.$$

- We can rewrite this as

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

- The effect of X_1 is no longer constant: adjusting X_2 will change the impact of X_1 on Y.

Other Considerations in the Regression Model

Interaction Terms

- **Example**
- Suppose we wish to predict credit balance using income and whether student or not.
- Without interaction term, the model is

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

Other Considerations in the Regression Model

Interaction Terms

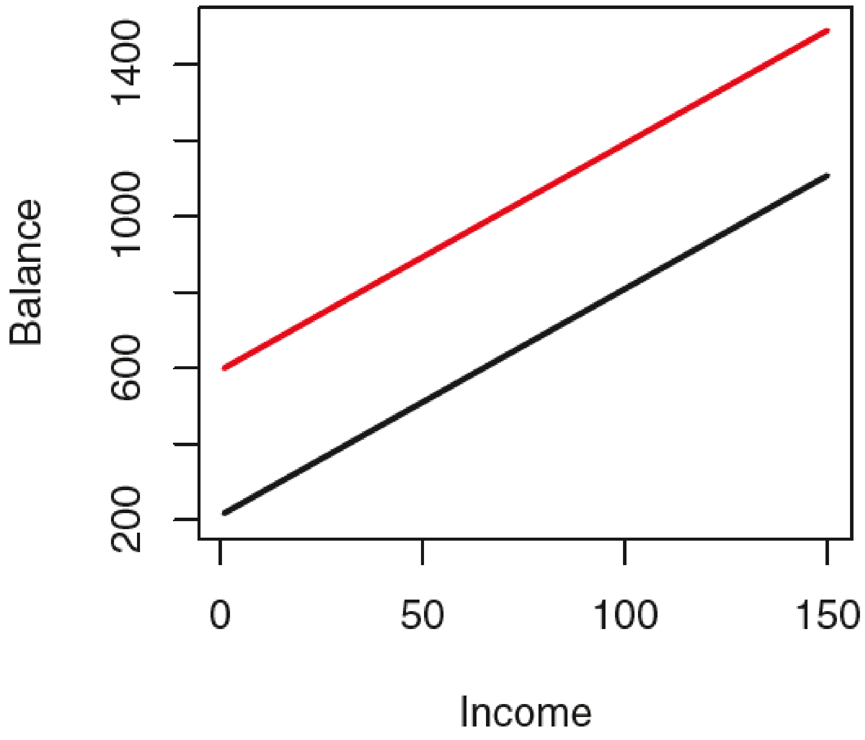
- **Example**
- Introducing the interaction term between student and income, we have:

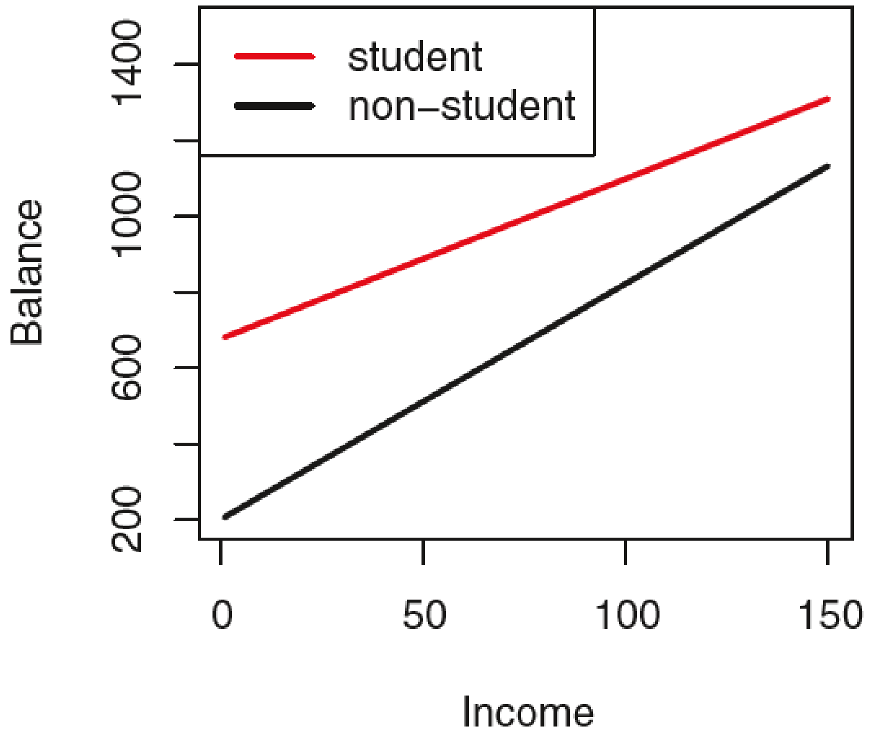
$$
\begin{aligned}
\texttt{balance}_i &\approx \beta_0 + \beta_1 \times \texttt{income}_i + \begin{cases} \beta_2 + \beta_3 \times \texttt{income}_i & \text{if student} \\ 0 & \text{if not student} \end{cases} \\
&= \begin{cases} (\beta_0 + \beta_2) + (\beta_1 + \beta_3) \times \texttt{income}_i & \text{if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

Other Considerations in the Regression Model

Interaction Terms

- **Example**





Potential Problems in the Model

The most common problems in a linear regression model are:

1. Non-linearity of the response-predictor relationships
2. Correlation of error terms
3. Non-constant variance of error terms
4. Outliers
5. High-leverage points
6. Collinearity

R Exercise